INTERNATIONAL RESEARCH AND PRACTICE CONFERENCE “NANOTECHNOLOGY AND NANOMATERIALS”

The NANO-2023 Conference is dedicated
to the brave men and women serving in the Armed Forces
of Ukraine, who safeguard freedom and peace in Ukraine

16-19 of August 2023

Bukovel, UKRAINE

Abstract book

УДК 536:669

The International research and practice conference "Nanotechnology and nanomaterials" (NANO-2023). Abstract Book of participants of the International research and practice conference, 16–19 August 2023, Bukovel. Edited by Dr. Olena Fesenko. – Kyiv: LLC APF POLYGRAPH SERVICE, 2023. – P. 640.

This book contains the abstracts of contributions presented at the International research and practice conference "Nanotechnology and Nanomaterials" (NANO-2023).

The NANO-2023 Conference was organized by the Institute of Physics of NAS of Ukraine with the participation of the University of Tartu (Estonia), the Lviv Polytechnic National University, University of Turin (Italy) and Pierre and Marie Curie University – Paris 6 (France).

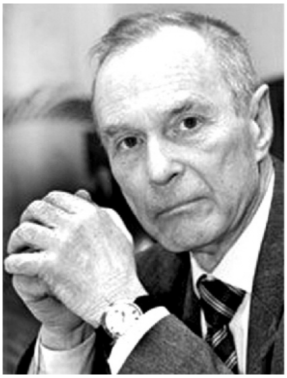
NANO-2023 was the 11th conference in the series of NANO-conferences initiated by the Institute of Physics of NAS of Ukraine in 2012 in the framework of FP7 Nanotwining project. From year to year, they attract more attention and participants. In 2012, the first meeting was held in the format of International Summer School for young scientists «Nanotechnology: from fundamental research to innovations». The 2013 and 2014 conferences were organized in conjunction with the International Summer Schools for young scientists under the same title. In 2013, this event was attended by more than 300 scientists, in 2014-2017, 450 scientists took part and in 2018 it gathered above 650 participants. In 2021 conference was attended by more than 700 scientists from Ukraine, Poland, Italy, Estonia, France, Austria, Germany, Greece, Turkey, USA, Romania, Moldova, Czech Republic, Taiwan, Lithuania, Egypt, Iran, India, Algeria, Indonesia and other countries. In 2021 and 2022 the Organizer Committee has received more than 500 application forms from about 25 countries of the world each years.

The NANO-2023 conference brought together leading scientists and young researchers from many countries of the world. This year its topics were as follows: Nanobiotechnology for health-care; Nanochemistry and biotechnology; Nanocomposites and nanomaterials; Nanoobjects microscopy; Nanooptics and photonics; Nanoplasmonics and surface enhanced spectroscopy; Nanoscale physics; Nanostructured surfaces; Physico-chemical nanomaterials science.

Website of the NANO-2023 conference: http://nano-conference.iop.kiev.ua

ISBN: 978-617-8092-32-0

Welcome to International Conference «NANOTECHNOLOGY AND NANOMATERIALS»!



It gives me a great pleasure to welcome you all at the International Conference "Nanotechnology and nanomaterials" (NANO-2023) that will be held in Lviv from August 16 to 19, 2023. Its aim is to promote scientific contacts and discussions between researchers representing various fields.

Previous NANO Conferences, held in Ukraine in 2013-2022, allowed the participants, including young scientists, to familiarize with current research and application problems in this area and thus forward implementation of nanotechnologies into innovations meeting public needs. The events also gave the opportunity to young and early-career researchers to attend lectures of internationally recognized experts and roundtable discussions on the emerging fields in nanosciences and nanotechnologies.

Our previous International Conferences and Summer Schools received positive feedback from international experts and from the media. Now we are holding the 11th such meeting, for which we are deeply grateful to its indefatigable initiator and organizer, Dr. Olena Fesenko and all her assistants, as well as to the universities and institutes that hospitably welcome the participants.

This year above 600 registration forms have been received from scientists representing more than 30 countries. We especially appreciate the participation in the conference of our foreign colleagues, both those who attend here and those who communicate their works remotely.

The fruitful cooperation of scientists is highly important not only to science itself. It helps us to overcome political and war conflicts and misunderstandings and to find our just peaceful future, which is now vitally important not only to Ukraine but also to other countries.

I wish the participants of the Conference to successfully share and broaden their knowledge in nanoscience and nanotechnologies, to advance the networking and launch new contacts between academia and research players in this area and thus to create a good basis for further practical contributions.

May good health serve us and promote creative success in our research!

Academician of NAS of Ukraine,
Professor **Anton G. Naumovets**

Group photo of participants of the 1st International Summer School for young scientists "NANOTECHNOLOGY: from fundamental research to innovations" (Bukovel 2012)

Interview with Prof. Dr. Thomas A. Klar, Director of the Institute of Applied Physics, Johannes Kepler University of Linz, Austria

At the lecture during the 1st International Summer School

Summer school participants on the background of the monument, which is a symbol of the geographical center of Europe (Rakhiv district)

Closing ceremony of the 1st International Summer School for young scientists "NANOTECHNOLOGY: from fundamental research to innovations"

Group photo of the 2nd International Summer School participants
(Bukovel 2013)

Summer School participant
PhD. Vorokhta M. (Czech Republic)
tries to play trembita

Plenary Session

The organizing committee
working hard

PhD. Lyashchova A.G.
(Ukraine)

Group photo of 1st International NANO–2013 Conference participants
(Bukovel 2013)

Opening speech by Dr. habil.
Emmanuelle Lacaze (France)

Online presentation of the Springer book
with selected proceedings of the 1st
International Summer School

Head of the Local organizing
committee Dr. O.Fesenko

Excursion to the city of Lviv

Group photo of 3rd International Summer School participants (Yaremche 2014)

Discussion with speaker

Hiking the path of Dovbush, Carpathians

Director of Institute of Physics of NAS of Ukraine Prof. Leonid Yatsenko awards prizes to the winners of competition

Interview with Prof. Leonid Chernozatonskiy from Prokhorov Institute of general physics (Russia)

Group photo of the 3rd International NANO-2014 Conference participants (Lviv, 2014)

Choir of Lviv National Ivan Franko University performsthe national anthem of Ukraine

Opening speech of Rector of Ivan Franko National University of Lviv, Prof. Volodymyr Melnyk

Report of Prof. Francesco Bonaccorso, leading specialist in graphene investigations

Scientific discussion with the audience

Group photo of the 3rd International NANO-2015 Conference participants (Lviv 2015)

Scientific discussion with the audience

Report of Prof. Dr. Thomas A. Klar, Director of the Institute of Applied Physics, Johannes Kepler University of Linz, Austria

Ivan Franko National University of Lviv violin ensemble performans

"Cheremosh" folk song and dance ensemble during the Conference opening ceremony

Group photo of the 4th International NANO-2016
Conference participants (Lviv 2016)

Scientific discussion with the audience

Report of Prof.Dr S. S. Choi (South Korea)

Registration of participants

Excursion to the Museum of Folk Culture and Rural Life in Lviv

Group photo of 5th International Summer School participants
(Bukovel 2017)

Scientific reporting

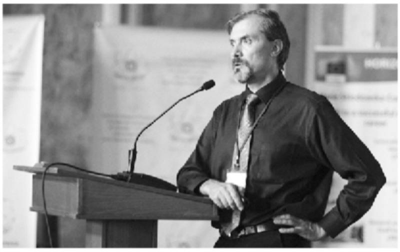
Report of Prof. Dr Stefano Bellucci

Tourist complex Mygovo

Don’t forget for dinner barbeque

Group photo of the 5th International NANO-2017 Conference participants (Chernivtsi 2017)

Report of heads of conference



Report of Prof. Dr. Vadym Mochalin (USA)

Registration of participants

Symphonic orchestra of Chernivtsi

Group photo of the 6th International NANO-2018
Conference participants (Kyiv 2018)

Registration of participants

Report of Dr. Hanna Morozovska
(Ukraine)

Discussion during the poster session

Organizing committee
of NANO-2018

Presentation of Philippe Mariani, CEO of Sophia Antipolis Foundation

Interview for a media

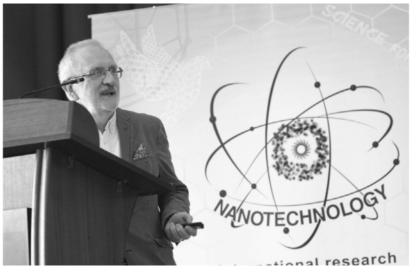
Experts in innovative ecosystem

Discussion with the audience

Expexerpt commmittemitet chee choooseosses the best startups

Presentation of Philippe Mariani, CEO of Sophia Antipolis Foundation

Registration of the participants

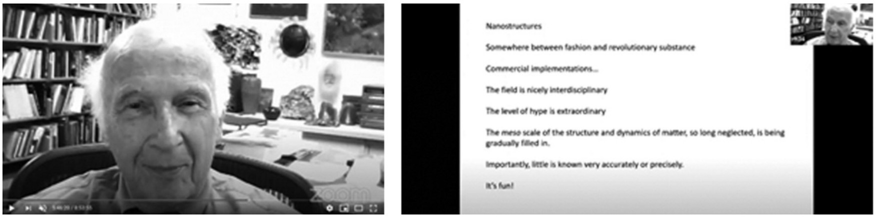


Report of Prof. Andzey Suchocki (Austria)

Mr. Jastin Taruska, member of the Innovation start-ups competition jury

Awarding the winners of the Innovation start-up competition

A collective photo of the participants of the NANO-2020 conference
on the stairs of the Lviv House of Scientists



Nanostructures

Somewhere between fashion and revolutionary substance

Commercial implementations...

The field is nicely interdisciplinary

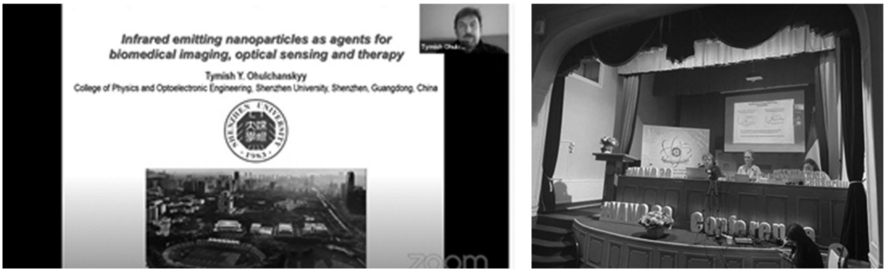
The level of hype is extraordinary

The meso scale of the structure and dynamics of matter, so long neglected, is being gradually filled in.

Importantly, little is known very accurately or precisely.

It's fun!

Online speech by Nobel laureate Roald Goffman

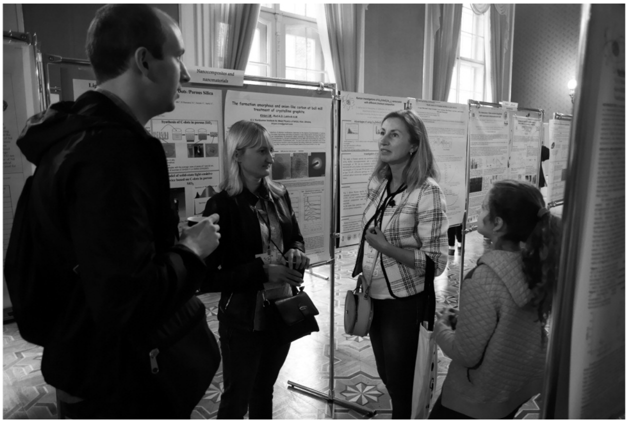


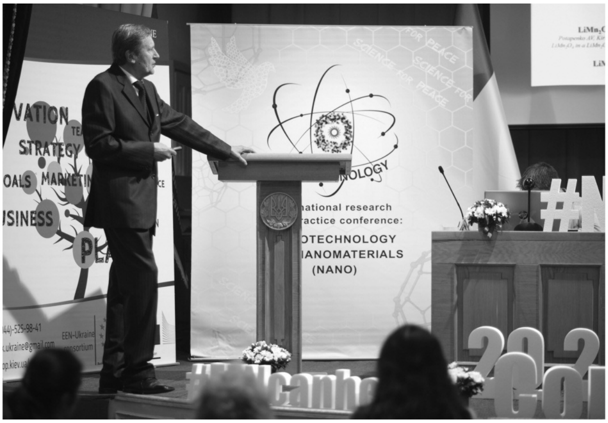
Infrared emitting nanoparticles as agents for biomedical imaging, optical sensing and therapy

Tymish Y. Ohulchanskyy

College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, Guangdong, China

Online and offline speech by Prof. Tymish Y. Ohulchanskyy
and Dr. Sergey Kolotilov respectively


A participant of the NANO-2021 conference presents his poster to colleagues


Participant of the NANO-2021 conference presents his oral report


General photo of NANO-2021 conference participants after all official events

General photo of NANO-2022 conference participants after all official events

A participant of the NANO-2022 conference presents her poster

Organizing committee of NANO-2022

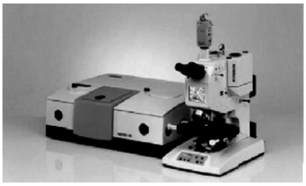
Participant of the NANO-2022 conference presents his oral report

INTERNATIONAL LABORATORY “SURFACE ENHANCED SPECTROSCOPY”

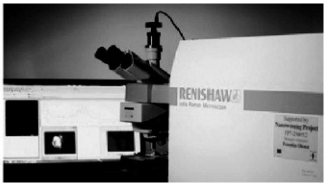
The International “Surface enhanced spectroscopy (SES)” laboratory was created at the International Research and Innovation Cooperation, Technology Transfer Department of the Institute of Physics NAS of Ukraine in the framework of implementation of Nanotwinning Project. This laboratory has a close cooperation with its Partners: Institute of Physics of the University of Tartu (Estonia), Pierre and Marie Curie University (France) and University of Turin (Italy).

Main activity: Study of mechanisms and effects of the enhancement of optical signals from bioorganic molecules near metal and non-metal (carbon, graphene) surfaces using IR and Raman spectroscopy, creation of a new type of substrates for spectroscopy, applications of Surface enhanced Infrared absorption (SEIRA) and Surface enhanced Raman scattering (SERS) spectroscopy.

Equipments: FTIR Spectrometer VERTEX 70 equipped with FTIR microscope HYPERION 1000 (Bruker, Germany), inVia micro-Raman spectrometer (Renishaw, England), UV-260 spectrophotometer (Shimadzu, Japan) with diffuse reflectance attachment and all needed equipment for sample preparation.



FTIR Spectrometer VERTEX 70 (Bruker, Germany)



InVia micro-Raman spectrometer with lasers λ = 786 and 633 nm (Renishaw, England)

The International Laboratory Team has many years' experience in preparation, implementation and management of International Projects.

Laboratory's Projects:

– STCU Project “Rose”;
– FP7-PEOPLE-2013-IRSES, Marie Curie actions;
– FP7 Nanotwinning project No 294952;
– NATO “Science for Peace” Project NUKR.SFPP 984702;
– Horizon2020_COS-EEN Project for 2016–2020 years.

We are interested in cooperation in the field of development of scientific and infrastructural International projects in the frame of Horizon2020 and others Programs.

Head of Laboratory
Dr. Olena Fesenko

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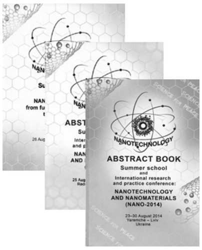
Our publications



Abstracts Book of the 1st International Summer School (2012)

Abstracts Book of the 1st International Summer School and International Conference NANO 2013

Abstracts Book of the 2nd International Summer School and International Conference NANO 2014

Abstracts Book of the 3nd International Conference NANO-2015

Abstracts Book of the 4nd International Conference NANO-2016

Abstracts Book of the 5nd International Conference NANO-2017

Abstracts Book of the 6nd International Conference NANO-2018

O. Fesenko, L.Yatsenko and M. Brodin et al. (eds.), Nanomaterials, Imaging techniques, Surface Studies, and Applications, Springer Proceedings in Physics 146, DOI: 10.1007/978-1-4614-7675-7, ©Springer Science+Business, Media, New York 2013

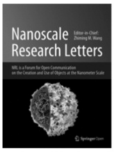
O. Fesenko, L. Yatsenko (eds.), Nanocomposites, Nanophotonics, Nanobiotechnology, and Applications, Springer Proceedings in Physics 156, DOI: 10.1007/978-3-319-0661-0, ©Springer International Publishing, Switzerland 2014

O. Fesenko, L. Yatsenko, Nanoplasmonics, Nano-Optics, Nanocomposites, and Surface Studies 167, DOI: 10.1007/978-3-319-18543-9, ©Springer International Publishing, Switzerland 2015

O. Fesenko, L. Yatsenko, Nanophysics, Nanophotonics, Surface Studies, and Applications 183, DOI: 10.1007/978-3-319-30737-4, ©Springer International Publishing, Switzerland 2016

O. Fesenko, L. Yatsenko, Nanocomposites, Nanostructures, and Their Applications 221, DOI: 10.1007/978-3-030-17759-1, ©Springer International Publishing, Switzerland 2019

O. Fesenko, L. Yatsenko, Nanophotonics, Nanooptics, Nanobiotechnology, and Their Applications 222, DOI: 10.1007/978-3-030-17755-3, ©Springer International Publishing, Switzerland 2019



Participants of International Summer Schools and International NANO Conferences - published their articles in Special Issue of Springer Open Journal “Nanoscale Research Letters” (in 2013, 2014 and 2015) dedicated to NANO Conferences. Impact Factor of Journal - 2.779.

In 2016-2018 it was also possible to publish an articles for participants of the NANO conference in Applied Nanoscience Journal, The European Physical Journal Plus (EPJ Plus) and Applied Sciences Journal (SN).

www.springer.com/materials/nanotechnology/journal/11671

Also, since 2017 year it was possible to publish the articles for participants of NANO Conference in the Molecular Crystals and Liquid Crystals Journal

https://www.tandfonline.com

Our Partners:

The Enterprise Europe Network helps businesses innovate and grow on an international scale. EEN-Ukraine Consortium can help you to find investors, international partner and promote your innovation products. Our contacts:

Website of Consortium: http://www.iop.kiev.ua/~een/

E-mail: een.network.ukraine@gmail.com

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The Enterprise Europe Network (EEN) is a service that provides support for Small and Medium-sized Enterprises (SMEs) with international ambitions. Co-funded by the European Union's COSME and Horizon 2020 programmes, the Network's aim is to help businesses innovate and grow internationally.

The Enterprise Europe Network was launched on 7 February 2008 by former EU Commissioner Günter Verheugen. The Enterprise Europe Network combines the previous Euro Info Centres and the Innovation Relay Centres. From 2008 to 2014, the Network was co-financed by the EU's Competitiveness and Innovation Framework Programme (CIP), in cooperation with institutions at national and regional levels. From 2015-2020, the Network is co-financed under the European Union's programme for the competitiveness of SMEs (COSME) and Horizon 2020.

Under the responsibility of the European Commission's Directorate-General for Internal Market, Industry, Entrepreneurship and SMEs, the Enterprise Europe Network is managed by the Executive Agency for Small and Medium-sized Enterprises (EASME).

The Network is active in more than 70 countries worldwide. It brings together 6,000 experts from more than 600 member organisations, including:

- chambers of commerce and industry
- technology poles
- innovation support organisations
- universities and research institutes
- regional development organisations

Enterprise Europe Network innovation support services are available based on an assessment of the needs and development phase of the business.

At an entry level, Network services include:

- information on innovation-related policies, legislation and support programmes
- links with local innovation stakeholders
- information about access to local sources of funding/support

Network experts can provide one-to-one services to support innovation capacity building. Services include innovation audits, advice on intellectual property, marketing and access to finance.

Finally, the Network provides key account management services to businesses benefitting from the Horizon 2020 SME instrument programme, part of the European Innovation Council (EIC) pilot.

In 2017, Ukraine joined the European Enterprise Network (EEN) within the framework of the COSME program, which promotes the competitiveness and innovative development of SMEs, innovation organizations and institutes/universities. For this purpose in Ukraine was created a Consortium EEN-Ukraine, which included representatives of business and government agencies, as well as scientific organizations. The Partner of the EEN-Ukraine Consortium is Institute of Physics of NAS of Ukraine.

To contact EEN-Ukraine please follow the website

http://eenukraine.com/uk/

E-mail: een.network.ukraine@gmail.com

Телефон: +380 44 525 9841

Session 1

Nanocomposites and Nanomaterials

Synthesis of tungsten carbides submicron powder with high-frequency electroerosion method

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A high-frequency electroerosion method for the synthesis of submicron tungsten carbide powder from tungsten granules in a carbon-containing organic liquid has been developed. The developed pulsed power supply provides the specified characteristics of discharge current in the range from 10 to 100 A and voltage in the range from 100 to 600 V. The specified performance of up to 3 g/hour is achieved by the high frequency up to 10 kHz of discharge pulses passage. The specific energy consumption of the synthesis of tungsten carbides reaches 20 g/kW*hour.

X-ray structural analysis of the obtained powder, which was carried out on DRON-4-07 diffractometer with the copper tube, showed fractions of tungsten and tungsten carbides. The image of the surface morphology of the particles of the obtained powder obtained with JSM-6700F scanning electron microscope confirms that the particles have the linear size from 40 to 200 nm.

Complex Method of Ni-Co-P Chemical Deposition and Chemical-Thermal Treatment

Stetsko A.E.

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Diffusion saturation is carried out on parts made of steel. The complex method consists of several stages [1], [2]. The main stages are the chemical deposition and diffusion saturation of the surfaces of the machine parts.

The machining of the surfaces of the parts is carried out to a size that takes into account the surface build-up during chemical deposition and diffusion saturation. Mechanical cleaning, degreasing and then decapitation are required, which significantly activates the surface prior to deposition. The decapitation is carried out in acids, followed by washing. During chemical deposition, care should be taken to ensure that suspended specimens do not come into contact with each other and that the medium is maintained at a pH of 9–10.

Chemical-thermal treatment was carried out in saturated powder mixtures. Retorts with the parts placed in them in powder mixtures have fusible closures (fusible caps) to seal saturated media. Such retorts provide quality diffusion coatings on the surfaces.

The chemical deposition applied to the surface of the reinforcing part before chemical-thermal treatment significantly changes the morphology of the diffusion layers.

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1. Stetsko A.E., Stetsko Y.T. (2020) Formation of Composite Reinforced Coating by Chemical Deposition and Chemical-Thermal Treatment of Boron and Carbon. In: Pogrebnjak A., Bondar O. (eds) Microstructure and Properties of Micro- and Nanoscale Materials, Films, and Coatings (NAP 2019). Springer Proceedings in Physics, vol 240. Springer, Singapore, P.261–270.

2. Stetsko A.E., Stetsko Y.T. (2021) The Influence of Carbon, Carbon, and Boron on the Formation of Diffusion Nanocomposite Hardened Layers on the Surfaces of Steel Parts. In: Fesenko O., Yatsenko L. (eds) Nanomaterials and Nanocomposites, Nanostructure Surfaces, and Their Applications. Springer Proceedings in Physics, vol 246. Springer, Cham. P. 699-708.

The effect of pressure on the anisotropy of the properties of a nanocomposite with Fe^{3+} iron

***Shapovalov V.A.*[1], *Shapovalov V.V.*[2]**

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The use of mineral nanocrystals of kaolinite $Al_2Si_2O_5(OH)_4$ has become widespread [1]. However, it is not taken into account that the location of kaolinite crystals in the composite changes during mechanical action when working with the material. This is due to the fact that kaolinite crystals are thin plates. High pressures transform an isotropic composite with a chaotic distribution into an anisotropic composite with a specific distribution of nanocomplexes with iron. The orientation of kaolinite nanocrystals in the composite depending on the pressure gradient is shown. The electron paramagnetic resonance spectra of Fe^{3+} iron ions in a polymer with kaolinite nanocrystals have been studied at high pressures in the temperature range T=4.2K-300K. The spectrum consists of two lines belonging to the Fe^{3+} iron ion. The value of the g-factor of line 1 $g_1 = 4.13 \pm 0.16$. The value of the g-factor of line 2 $g_2 = 2.15 \pm 0.1$. The dynamic characteristic is determined - the height of the barrier of the crystal field potential at the location of Fe^{3+} iron ions [2].

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1. Shapovalov V.V., Shapovalov V.A., Sluzhbin Yu.A., Drokina T.V., Vorotynov A.M., Valkov V.I. Characteristics of Nanocomplexes with iron Fe^{3+} in Glass Ionomer Cement Powder by ESR method // FTT-2023.-65, -P. 302-304.

2. V.A. Shapovalov, V.V. Shapovalov, M. Rafailovich, S. Piechota, A. Dmitruk, E. Aksimentyeva, A. Mazur. Dynamic Characteristic of Molecular Structure of Poly(orthomethoxyaniline) with Magnetic Probes // J. Phys. Chem.- 2013.-C 117, -P. 7830-7834.

Electrospinning of nonwoven materials based on biocompatible polymers

***Ohrimenko I.V.**, Ishchenko O.V., Plavan V.P., Koliada M.K., Liashok I.O.*

Chemical Technology and Resource Saving Department, Kyiv National University of Technologies and Design, Nemyrovycha-Danchenka Street, 2 Kyiv 01011, Ukraine. E-mail: e.ishchenko5@gmail.com

Nanofibrous nonwoven materials successfully obtained by the method of electrospinning. First, this is due to the possibility of sourcing nano- and microstructures from several biodegradable, biocompatible and bioinert polymers. In addition, this technology allows adding various active pharmaceutical ingredients, even at the stage of development of the formulation solution [1].

Presenter study aimed creating nonwoven nanofibrous materials with antiseptic properties based on PVA, PVAc with the addition of gelatin and chlorhexidine.

The parameters of obtaining fibers by the electrospinning method were determined by the optimal voltage of 30 kV and the distance between the electrodes – 14 cm, using a capillary with a diameter of 1.1 mm.

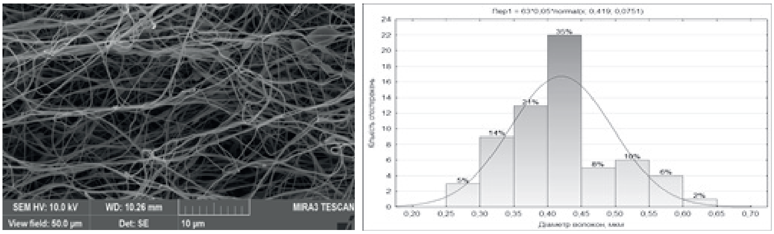

***Fig. 1** – Photomicrograph and histogram of fiber diameter distribution based on the composition of PVA/Gelatin (8:2 ratios)*

The obtained nonwoven materials from PVA/Gelatin and PVAc/Gelatin compositions have a fiber diameter in the range of 0.10-0.65 microns (Fig.1). Materials based on PVA/Gelatin have most fibers with a diameter of 0.12-0.32 µm, and in materials based on PVA only 19% of such fibers.

Thus, the addition of gelatin makes it possible to obtain fibers with a uniform diameter distribution. The use of gelatin allows to expand the scope of applications of the obtained nonwoven polymer materials due to the reactive groups of collagen and the possibility of their combination with other active pharmaceutical ingredients.

---

1. Koliada M., Ishchenko O., Plavan V., Bessarabov V. Characterisation of electrospun fibers made of PVA or PVAc and collagen derivative / // Vlakna a textile. – 2018. –25 (2). – P. 48–52.

Probing the multilevel structure of nanodiamond aggregates in thin layers of a nematic liquid crystal

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The last ten years have been marked by a sharp increase in the research of colloidal systems based on liquid crystals (LCs) and nanoparticles (NPs). The great attention to such researches is related to the possibility of radical changes of physicochemical properties of the LC matrix, as a major component of modern liquid crystal devices. One of the most interesting classes of the fillers is formed by carbonaceous materials including such unique objects as carbon nanotubes (CNTs). In the previously studies we detailed investigated structure of LC-CNTs composites [1, 2]. In the present work, we investigate LCs filled by diamond nanoparticles (DNPs), which is a different allotropic form of carbon matter.

We revealed the structural features of LCs filled with nanodiamond particles in a size range from a few nanometers to hundreds of micrometers combining small-angle neutron scattering and polarizing optical microscopy (Fig. 1).

It was shown that the primary assembling of DNPs leads to the developed structures with the fractal dimension $D = 2$, which means the lower averaged density of these formations in comparison with similar objects in polar isotropic

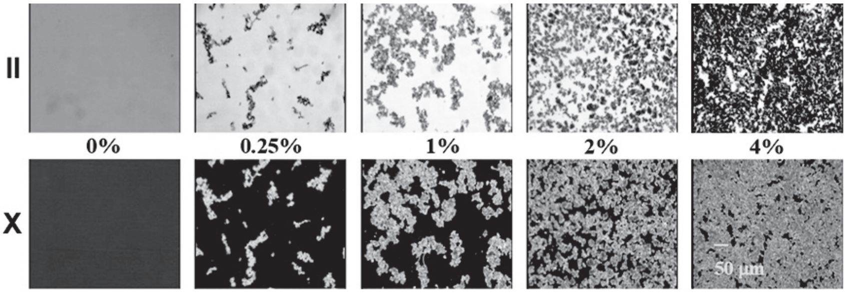

Fig. 1. *Microscopic images of planar-oriented LC-DNPs samples in the configurations with crossed polarizers (X) and with the analyzer removed (II). DNP concentration is given in wt. %. The thickness of the LC layer in all cases is 25 μm.*

solvents [3]. Further, these clusters assemble into elongated aggregates, which can be observed with the help of polarizing optical microscopy at low concentrations. An increase in DNPs content in the system leads to the formation of a continuous network, which naturally increases the viscosity of the system and, in fact, making it impossible to prepare samples with $\varphi \geq 5$ wt.% according to the described procedure. It was also shown that the spatial limitation in the direction perpendicular to the nematic director does not affect the aggregation processes. Neutron scattering is a proper technique to investigate such systems, provided there is sufficient concentration. The use of quartz as the container material can somewhat improve the scattering data quality while maintaining the possibility of using optical microscopy. As the next stage, the studies using ultra-small-angle neutron scattering (USANS) are foreseen to test the proposed structural model in the size scale interval of 0.1–5 μm.

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Thermodynamic Analysis of features of Phase Formation processes in Amorphous Alloys of the Fe-B system

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Amorphous metal alloys of the Fe-B system are characterized by a wide range of unique physical properties and are widely used as the latest functional materials, so the study of their properties and conditions of formation has both fundamental and practical significance. Thermodynamic analysis of the features of phase formation processes in amorphous alloys of the Fe-B system has been carried out. A new expression is proposed to describe the concentration dependence of the relative Gibbs free energy for the initial amorphous phase, which takes into account the dependence of entropy on the volume change during alloy formation. The constructed concentration dependences of the relative integrated Gibbs free energy for the original amorphous phase do not have a specific S-shaped shape, which indicates the impossibility of phase separation within the amorphous state for these binary alloys. It is shown that the obtained equations qualitatively correctly describe the processes of phase formation in amorphous alloys of the Fe-B system, and the agreement of the results of theoretical calculations with the experiment is observed. Theoretical calculations of the kinetics of the process of crystallization of binary amorphous alloys of the Fe-B system under continuous slow heating and pulsed laser processing have been carried out. The possibility of explosive crystallization during pulsed laser annealing in binary amorphous alloys of the Fe-B system has been theoretically confirmed. It is shown that the phenomenon of explosive crystallization occurs at temperatures significantly lower than the temperature of the beginning of intensive crystallization under slow heating. The temperature at which explosive crystallization due to a laser pulse is possible was found to be (50-80) K lower than the temperature of the intensive crystallization beginning under slow heating. This fact should be taken into account when choosing technological modes of processing amorphous materials in their practical application.

Electrical conductivity of polymer nanocomposites with a novel type of carbon filler

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Polymer composites filled with well-known carbon fillers, especially carbon nanotubes (CNT), nanofibers (NF), graphene nanoplatelets (GNP), reduced GNP, thermally expanded graphite (TEG) are characterized by good electrical, thermal, and mechanical properties. But their number of applications in industry is not so large because these fillers are quite expensive. One of the solutions to this problem is the creation of new types of fillers based on coal and their further modification.

Novel types of carbon filler with a graphene-like layer structure were obtained from coal coke (CP) and crude oil pitch (PET). The composites studied were based on ultrahigh molecular weight polyethylene (UHMWPE) filled with new carbon fillers CP and PET, also as well-known fillers such as anthracite, graphene, carbon black (CB) multi-walled carbon nanotubes (MWCNT).

All composites shown in Fig.1 were filled with 10 vol.% of different types of carbon fillers. It can be seen that the electrical conductivity of both composites with a novel type of fillers CP and PET is higher than the composite filled with anthracite for 1.5 orders. Composite with CP filler has the value log σ = -2.49 S/cm which is close to the composite filled with graphene, and slightly smaller than the composite filled with CB log σ = -2.06 S/cm or MWCNT log σ = -2.11 S/cm.

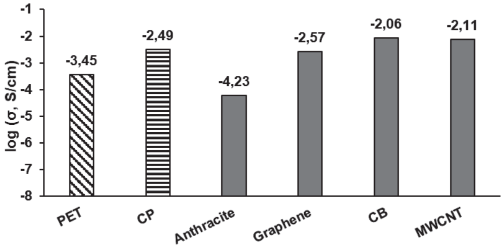

Fig.1. Electrical conductivity of composites filled with 10 vol.% of carbon fillers.

This research demonstrates that polymer composites filled with novel types of fillers CP and PET have similar values of electrical conductivity compared to well-known carbon fillers, and they are perspective for further study of their mechanical characteristics and EMI shielding properties.

Adsorption of dyes by ferromagnetic carbon nanocomposites synthesised from organic raw materials

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The industrial production of food, pharmaceuticals and textiles uses thousands of different dyes, the manufacture and use of which generates significant volumes of contaminated wastewater. Among the methods of purification of such waters, adsorption processes are widely used. In this work, the structure, magnetic and adsorption properties of ferromagnetic carbon composites (FCC) in relation to methylene blue (MB) and congo red (CR) dyes were studied.

For the synthesis of FCC dried beet pulp was used, the activator was a mixture of $FeCl_3$ and $ZnCl_2$ salts. In the first method of synthesis, the pulp impregnated with salts was subjected to pyrolysis in an inert atmosphere (argon) at 800 °C for ~90 min (sample FC1). In the second synthesis method, first, beet pulp was pre-pyrolysed at a temperature of ~400 °C for ~90 min, then this carbonizate was impregnated with an aqueous solution of $FeCl_3$+$ZnCl_2$. The resulting mixture was subjected to pyrolysis in an inert atmosphere at 800 °C for ~90 min (sample FC_2). Industrial activated carbon was used to compare the adsorption of dyes.

X-ray studies of both synthesized FCC samples revealed an amorphous structure of the carbon phase, which clearly shows peaks identified as Fe_3O_4 magnetite. The coercive force, residual specific magnetization and relative residual magnetization of the synthesized FCC were determined by hysteresis loops.

The adsorption isotherms of both dyes by all types of the studied FCC belong to type II. This indicates a weak bonding of the dye molecules with the surface mainly due to electrostatic interaction and allows the Langmuir model to be used to analyse all isotherms. The adsorption value decreases significantly when moving from MB to CR. The synthesized nanocomposite FC_2 has the highest adsorption capacity among the studied carbon materials, and compared to industrial carbon it adsorbs MB by 10% more and CR by 30% more.

Magnetisation switching of a synthetic antiferromagnet by a magnetic field pulse

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Functional systems consisting of uniformly magnetised thin magnetic discs have been intensively investigated for decades in both quasi-static and dynamic modes for their potential use, for example, in magnetic recording [1]. In turn, uniformly magnetised soft synthetic antiferromagnets (SAFs) are of great interest for possible applications in magnetoresistive random-access memory (MRAM).

SAFs, in contrast to conventional AFMs, have the ferromagnetic layers coupled relatively weakly. This makes possible low-field, essentially barrier-free switching of small elliptical SAF elements, the mechanism of which is described in detail and is based on using perpendicular-to-the-plane field pulses of specific duration and amplitude, tuned to be in sync with the intrinsic dynamics of the SAF trilayer. Such field pulses can be generated, for example, by circularly polarised laser pulses via the inverse Faraday effect, concentrated into the individual SAF using an optical antenna.

The regime of barrier-free switching in nanoscale SAF elements using low-amplitude field pulses is investigated theoretically. It has been proven that under a coherent rotation of the two ferromagnetic moments in the AP state with zero total magnetization allow us to neglect the shape-induced magnetostatic barrier and makes switching fast and with low energy consumption, which is desirable in various technological applications such as MRAM. It is shown that in combination with the barrier-free regime of SAF switching, laser-induced normal-to-the-plane field pulsing can form the base of an efficient method of information writing on to SAF-type media.

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Electrochemical synthesis of functional nanocomposite metal-oxide coatings on titanium alloys

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The use of electrolytic thin-film coatings with photocatalytic properties is promising for the destruction of toxic organic compounds and gases, for the disinfection of water, air and surfaces from viruses and bacteria. Valve metals are used as platforms for photocatalytic materials, and the plasma-electrolytic oxidation (PEO) method is used to form the coatings.

Heterooxidic coatings based on titanium (IV) oxide were synthesized on substrates made of alloy VT1-0 from aqueous solutions, to which dopant compounds were injected either as soluble salts (Co, Cu, Mn, Sn, Mo, W) or phase oxides (ZnO, ZrO_2) [1]. The morphology of the surface was investigated using an atomic force microscopy and the visualization of the results was carried out using 2D and 3D topographic maps. The results of our authentic research into the development, studying the morphology, and testing the photocatalytic materials clearly indicate in favor of the use of the PEO to create heterooxidic composites based on titanium. Synthesized coatings are distinguished by a specific morphology. Thus, in comparison with the original structure of TiO_2, heterooxidic coatings of $TiO_2 \cdot ZnO$ have a more developed surface. Over time, the surface grows and during heat treatment acquires a uniform distribution of globular nanostructures and micropores. One of the characteristic features of PEO technology was the ability to form heterooxidic coatings, which include compounds of alloying elements. It’s content and surface morphology can be varied by changing the composition of electrolytes and electrolysis modes. Testing of photocatalytic activity of heterooxidic systems showed the expected fact of increasing the functional properties due to the doping of *d*-elements.

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Photo-domain effect in ferroelectric nanoparticles

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The photo-domain effect in nanosized photo-ferroelectric-semiconductors is of high fundamental interest as the interaction of light quanta with an electron-phonon subsystem under nanoscale confinement conditions. To the best of our knowledge, the photo-domain effect in photo-ferroelectric nanoparticles **(NPs)** has not been studied theoretically, so we devoted our work to research of light-induced phase transitions, accompanied by transformations of polar state and domain morphology in the NPs. The calculations are performed in the framework of Landau-Ginzburg-Devonshire approach for the $Sn_2P_2S_6$ NPs under continuous light exposure [1]. Since the free carrier density in the photovoltaic NPs essentially depends on the light intensity, the latter strongly influences the screening length of ferroelectric. Due to this dependence the intensity increase induces phase transitions from the nonpolar paraelectric phase to the polar ferroelectric state, causes the changes of domain morphology in the state, and controls phase diagrams of free and stressed NPs. The analysis showed that the light exposure can control the appearance and vanishing of domains and induce strong changes of polarization switching scenario and hysteresis loop shape in NPs. When exposed to light, polar, dielectric and piezoelectric responses of an ensemble of weakly interacting stressed photo-ferroelectric NPs can reveal superparaelectric-like features in the point, such as strongly frequency-dependent giant piezoelectric and dielectric responses, which can be important for advanced piezoelectric applications. Acknowledgements: The work is supported by the NATO SPS Programme Grant G5980 “FRAPCOM”.

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The anti-corrosion pigments based on zeolite nanocontainer for paints coatings

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One of the most common methods of protecting metal products is the use of paint coatings, in particular "smart" coatings, the action of which consists of the generation of an inhibitor at the moment of the onset of underfilm corrosion. Such coatings contain multifunctional nanocontainers, which are added to the polymer for active anti-corrosion protection. Environmentally friendly nanoporous zeolites with intercalated corrosion inhibitors can be perspective anticorrosion components of "smart" paint coatings.

The corrosion resistance of an aluminium alloy in the presence of Na-A zeolite, modified with divalent metal cations by the liquid phase ion exchange method was investigated, whose inhibitory effect is due to the formation of oxide-hydroxide layers and increases in the range Ca-zeolite <Mn-zeolite <Zn-zeolite [1]. It was established that the pigment based on zeolite and monocalcium phosphate obtained by the mechanochemical method exhibits an inhibitory effect on low-carbon steel due to the formation of a protective film of calcium and iron phosphates [2]. The obtained pigments are used in the coating only at the moment of the onset of underfilm corrosion of the metal due to the dissolution of their active nanosized phosphate phase and ion exchange with the corrosive medium. The main advantage of the created inhibitory pigments is environmental safety in coatings, industrial production without environmental pollution and high anti-corrosion efficiency.

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Bimetallic nanoparticles Ni_xAg_{100-x} as fillers with a low percolation threshold for electroconductive polymer composites

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Taking into account the relevance of the wide practical application of nanosystems in various fields, there is currently a need for a new ecological and cheap technologies for the synthesis of metal nanoparticles, to expand the fields of their application in industry, in particular, in the production of electrically conductive composite materials.

We have synthesized and studied bimetallic nanopowders based on nickel and silver of different composition by the method of co-precipitation of Ag^+ and Ni^{2+} ions with nickel hydroxide in ethylene glycol solutions with subsequent reduction of the formed suspension with hydrazine. As the result the Ni_xAg_{100-x} nanoparticles were obtained with the size of 30–50 nm. The phase composition of the obtained Ni_xAg_{100-x} bimetallic nanopowders was investigated using the XRD method. It was established that there are no unidentified peaks within the range of 2ϴ angles from 200 to 1000, which indicates the absence of non-target products, namely, metal oxides or hydroxides in the obtained Ni_xAg_{100-x} bimetallic nanopowders.

The obtained Ni_xAg_{100-x} bimetallic nanopowders were studied as conductive fillers for conductive polymer composites. It was found that the electrical conductivity of thin films of nanocomposites based on Ni_xAg_{100-x} is quite significant at an extremely low content of metal filler, only 10 % by volume (50 % by weight) and reaches the values of more than 3500 S/m. It was shown that the reason for the high electrical conductivity of nanocomposite films is the self-organization of the filler particles and the formation of an electrically conductive 3D network in the polymer matrix due to the high coercive force of the synthesized nickel-based nanopowders. Taking into account the low values of the percolation threshold for the obtained bimetallic nanosystems, the synthesized Ni_xAg_{100-x} can be considered a promising material for the development of electrically conductive polymer nanocomposites.

FORC signatures versus phase composition in W/SmCo/W films

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High remnant magnetizations and storage of high magnetic energy are the main features attracting great interest to SmCo structures for application in Micro Electromechanical System. The mixed-phase SmCo samples is often encountered in practice. The investigation of the interaction between different phases could give rise to predict magnetic properties. Thick SmCo films of 500 nm thickness were deposited by RF sputtering on Si substrate (Fig. 1a). We used annealing at 650 °C and 750 °C for tuning the magnetic properties of the films (Fig. 1b).

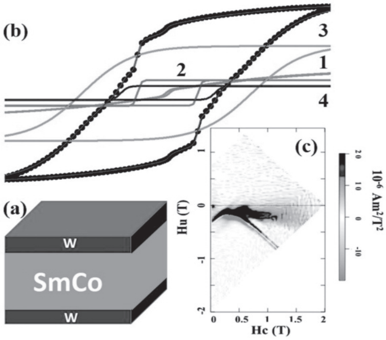

Fig.1. *(a) Sketch of the W/SmCo/W structure; (b) Decomposition of hysteresis loop of the film annealed at 650 °C using the following components: 1 is amorphous intergrain phase, 2 is 1-5 grain phase, 3 is intergrain 1-5 phase, and 4 is 2-17 phase; (c) FORC plots presented in Hu and Hc coordinates, where Hu is shift of the center of symmetry due to the intergrain coupling and field Hc is grain switching field.*

After annealing at 650 - 750 ºC as grown amorphous and/or nanocrystalline structure was transformed to a mixture of Sm_2Co_{17} magnetic phase with 12 kOe coercive field and SmCo5 magnetic phase. Increase of annealing temperature results in dispersion of the magnetic phases and corresponding increase of the interphase coupling, decreasing the switching field of the hard phase. Decrease of switching field of 2-17 phase under intergrain interaction revealed by FORC agrees well with the decrease of the effective average anisotropies.

High-speed heating of oxidized graphite particles for their thermoexpanding in reactors of different types of feedstock loading. CFD simulation

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The article studied in detail the process of thermally expanded graphite generation (TEG) [1] due to high-speed heating of oxidized graphite (OG) particles [2] in methane-fuelled vertical reactors.

Three types actually operating reactors served as initial data for the calculations (Fig.), which differ in the method of heat supply to the initial product [3]. The methane combustion process, the supplying of GO particles into the hot zone and their heating during thermal expanded are simulated.

As a result, the particle heating rates for these reactors types were obtained and their technological features were analyzed.

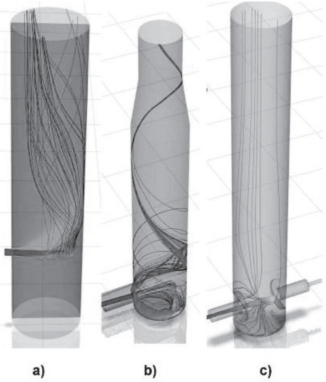

Fig. *Studied reactors are: a) co-flow, b) cyclone type, c) opposed type.*

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Formation of nanoscaled $Zr_{1-x}Ti_xC$ solid solution at mechanical alloying of 80ZrC-20TiC blend

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Refractory TiC and ZrC carbides, as is known, have unique complex of available properties ensures there as hardening additives for materials and protective coatings using for cutting tools. In addition to pure ZrC and TiC carbides, their $Zr_{1-x}Ti_xC$ solid solution has certain prospects for practical application, too. Since the *Ab initio* phase diagram of the ZrC-TiC system, calculated in Ref [1], is asymmetric with greater solubility on the ZrC side, mechanical alloying (MA) synthesis was carried out here by treatment in a high-energy planetary mill (HEPM) of ZrC rich blend (mol. %): 80ZrC–20TiC. The test MA treated samples were studied comprehensively using X-ray method [2].

It`s shown that the crystal structures of ZrC and TiC carbides, existing in test samples, are described well within the framework of the NaCl-type but with some vacancies of metal atoms in 4*a* set. That is, the impact loading, applied on the blend during MA, causes metal atoms knocked out of carbides with their gradual accumulation in the reaction zone of the HEPM in a form of individual clusters. As result of this process, at the first stage of MA the lattice parameter of ZrC carbide decreases substantially, while the TiC carbide begins to collapse fully. The next stage of the MA process there is a diffusion penetration of smaller titanium atoms into the ZrC lattice, which leads to a stepwise increase in its lattice parameter. It`s shown that after 5 hour of MA treatment in HEPM, the ZrC carbide dissolves about 12 at. % Ti while after its HPHT sintering these solubility increases well.

It`s first shown that sequential MA and HPHT treatments of the 80ZrC–20TiC blend lead to the formation of the nanoscaled (up to 30 nm) $Zr_{1-x}Ti_xC$ solid solution, containing up to 20 at. % Ti. The compact material obtained here will be tested for its further application.

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Structure, optical properties and photocatalytic activity of undoped, La_2O_3-doped ZnO nanocomposites

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Zinc oxide is an important material due to its optical, photocatalytic, and magnetic properties. ZnO can be an effective photocatalytic nanomaterial due to the high generation rate and distribution of photoinduced electrons e and holes h^+. Doping ZnO with rare earth elements has a great influence on the photocatalytic efficiency of ZnO [1].

The undoped and La_2O_3-doped ZnO nanoparticles were synthesized using a chemical method from Zn^{2+} and La^{3+} nitrates solutions. Investigate the X-ray diffraction patterns of undoped and La_2O_3-doped ZnO nanoparticles on a "Dron-3M" X-ray diffractometer. The undoped ZnO nanoparticles are identified as a wurtzite structure ZnO. The XRD patterns of the La_2O_3-doped ZnO do not show any other peaks corresponding to La, La_2O_3 or any other additional phases associated with impurities. These indicate the ideal solubility and homogeneity of La^{3+} ions in the ZnO lattice.

Micro-Raman scattering measurements were carried out to study the influence of La^{3+} doping on the structural and vibrational properties of ZnO samples.

This work supported by the research project of the NAS of Ukraine "Creation of promising materials based on ZnO doped REE for use in catalysis".

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Composite sorbent based on fibrous anion exchange polymer containing nanoparticles of hydrated Sn (IV) oxide: water purification from U(VI) compounds

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Both the nanoparticles of hydrated tin(IV) oxide (HTO) and their aggregates were embedded into fibers of a Fiban A-6 polymer anion-exchanger. In order to control the particle size, a thermodynamical approach based on Ostwald-Freudlich equation has been developed. The approach considers not only the solubility of compounds being deposited, but also sorption capacity of polymer matrix, concentration of reagents, their volume etc. According to the literature data, HTO is characterized by the lowest solubility among other hydrated oxides of multivalent metals. It means, HTO is able to form non-aggregated nanoparticles inside polymer phase. As found using TEM and SEM, some aggregates were also formed, but their content is inconsiderable. Specific surface area and porous characteristics were determined using a method of nitrogen adsorption-desorption. The composites were applied to the removal of U(VI) carbonate compounds from aqueous solutions, main regularities of adsorption have been established.

The composites show higher sorption rate comparing with pristine fibers: the half-time of the equilibrium is achieved after 6 min, the total removal is after 25 min. In the case pristine fibers these values are 10 and 40 min, respectively. The models of Weber-Morris and Yelovich as well as the models of pseudo-first and pseudo-second order were applied. The isotherms were fitted with Henry, Langmuir, Freundlich, Dubinin-Radushkevich, Frumkin models. The constants of these formulas were determined, sorption thermodynamical parameters were estimated. U(VI) sorption is a spontaneous endothermic process, since entropy increases. The composite was used for the removal of U(VI) from the model technological solution. It should be stressed that a growth of U(VI) ions concentration from 1 to 4 mg dm^{-3} improves their recovery from 58 to 95 % (pristine polymer) and from 68 to 100 % (composite).

Micro- and nanocomposites of barium zirconate incorporated in polymer matrix

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Inorganic/organic nanosystems based on semiconductor nanocrystals and conducting or thermoplastic polymers are actively investigated nowadays [1,2]. These polymers are useful for optical applications due to complete transparency in the visible range of the spectrum and relatively high stability. Recently $BaZrO_3$ (BZO) perovskite has attracted attention as a substrate for superconductor synthesis, a high-temperature microwave dielectric, and a fluorescent material. The luminescence characteristics of BZO significantly depend on the fabrication technology of micro- and nanocrystals. In this report, the irradiative properties and structure of hybrid composites based on polystyrene (PS) and micro- (d < 10 μm) and nanocrystals (d < 50 nm) of BZO have been studied using luminescent spectroscopy and X-ray analysis. A strong cathodoluminescence (CL) was found for BZO-nanocrystals. Results demonstrate high-temperature stability CL intensity and spectral composition after 2 hours of annealing at 400, 500, 700, and 800ºC. This behavior is also attributed to micro-BZO (d< 10 μm) powders. For the BZO-PS composites, a significant reduction of the CL intensity is observed. At the same time, the low-energy and high-energy bands (near 4 eV) appeared. The coexistence of an amorphous halo with the diffraction peaks of BZO is clear evidence of the nanocomposite formation. According to XRD analysis, BZO presents a cubic perovskite-type structure in crystalline form with space group Pm_3m, and the average size of domains is 23 nm. The lattice parameter a for BZO decreases from 4.19083(6) Å to 4.1879(2) Å in the BZO–PS composite. All this suggests that polystyrene considerably alters the subsurface structure of BZO.

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Thermodynamic of interactions and relaxation properties of the POSS-containing nanocomposites based on polyurethane matrix

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The nanocomposites based on crosslinked polyurethane (PU), synthesized from adduct of trimethylolpropane with toluene diisocyanate (TMP-TDI adduct) and polyester poly(diethylene glycol) adipinate with mol. mass 2000 (PDEGA 2000), contained 1,2-propandiolisobutyl-POSS were created and the impact of different amount of POSS on the thermodynamic of interactions and dynamic-mechanical behavior of the nanocomposites were investigated.

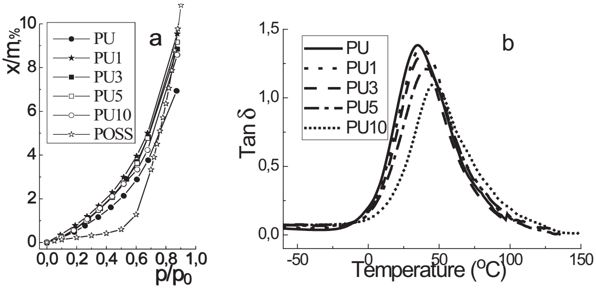

Fig. 1.The isotherms of methylene chloride vapors sorption (a) and Tan delta of mechanical loss (b) by nanocomposites with POSS content 1 (2), 3 (3), 5 (4), 10 % (5).

From Fig.1(a), the sorption isotherms of solvent vapors by POSS-containing PU nanocomposites are higher than of the native PU. With an increase in the amount of POSS, the vapor sorption values increase, thereby demonstrating a decrease in the density of the obtained nanocomposites. The free energy of polyurethane and POSS mixing was calculated and was shown that it is positive for all systems with different amount of POSS. That means the thermodynamic incompatibility between this PU and hydroxy-POSS takes place.

From Fig.1(b), the temperature dependences of tan δ for the native PU and nanocomposites, obtained by DMA method, could be seen. The introduction of POSS led to a shift of tan δ maximum towards higher temperatures. This means that the segmental motion in polyurethane decreases with an increase of POSS content, while the glass transition temperature of nanocomposites increases. This indicates the restriction of the segmental motion of PU chains, which causes by the introduction of POSS nanoparticles into the system.

Effect of Neutral-to-Acceptor substituents replacement on self-action nonlinear response under picosecond laser excitation

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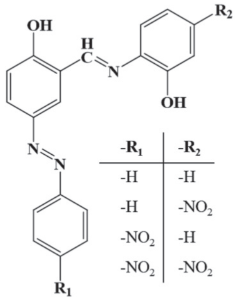
Polymers with π-conjugated electron system, like azobenzene or azomethine, represent a promising class of nonlinear optical (NLO) polymers, being widely recognized as candidates for many practical applications such as data storage, photoswitchable sensors, holographic recording, optoelectronic devices, etc. [1]. Impact of two several photoactive groups' joint contribution on NLO properties of polymers was not properly investigated yet.



$-R_1$	$-R_2$
-H	-H
-H	$-NO_2$
$-NO_2$	-H
$-NO_2$	$-NO_2$

In the presented study we have investigated self-action effects manifestation and neutral/acceptor substituents influences in PMMA thin films doped with 1% (wt.) of azo-azomethines within picosecond range pulsed laser excitation at 1064 nm [2]. Aforementioned azo-azomethines were synthesized through standard azo-coupling procedure with further condensation between aldehyde containing azobenzenes and hydroxy-aniline.

Refractive NLO response efficiency magnitude $|\mathrm{Re}(\chi^{(3)})| \sim 10^{-7}$ esu rises two times both for unsubstituted $(R_2=–H)$ imine moiety and nitro-analogue $(R_2=–NO_2)$ one due to replacing a neutral $(R_1=–H)$ group with an electron-acceptor $(R_1=–NO_2)$ substituent. Enhancement of $|\mathrm{Re}(\chi^{(3)})|$ for the dyes with $R_1=-H$ is accompanied with switching sign of the NLO refractive response from self-focusing to self-defocusing mode.

The obtained results are promising for design of efficient NLO nanocomposite materials with wide possibility to control both sign and magnitude of photoinduced refractive index variations in near IR range.

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Effect of $–CH_3$/-H/-NO_2 substitution on the self-action in azo- and azo-azomethines derivatives in polymeric thin films under picosecond laser excitation at 1064 nm

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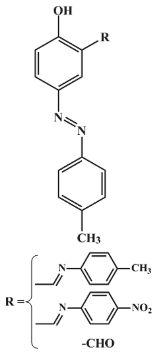
Advanced light-responsive polymeric materials containing -A=B- chromophore groups undergo reversible *trans-cis-trans* photo-isomerization cycle, like –N=N- or –CH=N-, are used in a number of modern electronic photoswitchable systems like sensors, liquid crystal displays [1], elements of optical information storage devices, etc.



In the present work we have prepared composite “host-guest” films, containing host PMMA and azo- ***(Azo)*** or azo-azomethine ***(Azo-CH_3/Azo-NO_2)*** “guest” (1% wt.) subsystem. The laser beam self-action effects in thin films were studied within fundamental wavelength of mode-locked Nd:YAG laser pulses at 1064 nm [2].

Analysis of photoinduced refractive/absorptive nonlinear optical (NLO) response manifestation has shown that the dyes demonstrated slight < 4% photobleaching phenomenon, being saturated at laser intensity of about I ~ 25 MW/cm². Self-defocusing effect with efficiency $|Re(\chi^{(3)})| \sim 10^{-8}$ esu was observed in the same range. Azomethine group incorporation provides twice enhancement of the cubic NLO susceptibility $|Re(\chi^{(3)})|$ in the following order -NO_2>-CH_3>Azo without significant donor/acceptor substituents’ origin impact.

The obtained data is important for design of novel photoswitchable media.

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Lithium ion diffusivity in nanoporous carbon material

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The process of electrostimulated diffusion of lithium ions in a power source based on nanoporous carbon material (NCM) obtained by hydrothermal carbonization of plant raw materials at a temperature of 750°C was considered in the work using the method of galvanostatic intermittent titration technique. The method is based on the chronopotentiometry procedure [1], during which lithium ions are intercalated (deintercalated) in the electrode material when a small direct current is applied for a limited period of time τ. At the end of this time, the material is characterized by the lithium content (or intercalation degree) x ± Δx depending on the current direction.

The diffusion coefficient of lithium ions in the case of a straight-line dependence $E = \mathrm{f}(\tau^{-1/2})$ (E is the voltage of the electrochemical cell) was calculated by the formula $D = \frac{4}{\pi\tau}\left(\frac{mV}{MA}\right)\cdot\left(\frac{\Delta E_s}{\Delta E_\tau}\right)^2$, where M, m are the molar mass and mass of NCM, respectively, V is the molar volume of the formed intercalation compound, A is the area of the electrode, dE_τ is the change in the voltage of the electrochemical element under the applied current during time τ, dE_s is the relaxation voltage during this time.

Calculations of the diffusion coefficient of lithium ions in NCM using the galvanostatic intermittent titration technique according to the above formula indicate a significant decrease in the D value (Fig. 1) when the intercalation degree x increases from 0 to 0.435 due to the formation of solid electrolyte interphase enriched with introduced lithium ions, the electrostatic interaction of which complicates the process of further intercalation.

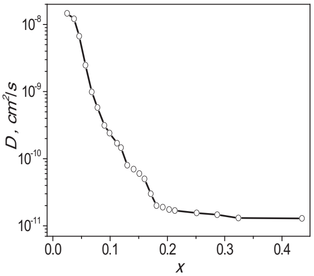

Fig. 1. Dependence D versus x for NCM.

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Inorganic membranes modified with nanoparticles of Li-selective composite

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The development of deposits and the extraction of lithium from primary and secondary resources are associated with environmental risks: the alienation of fertile lands, the salinization of fresh water sources, high costs of fresh water, and its contamination with soluble lithium compounds (the maximal allowable concentration for Li^+ ions is 0.03 mg dm^{-3}) and other toxic impurities. It is known that membrane methods are promising for extracting valuable components from the the solutions of technological and natural origin. There is currently no information about selective membranes specifically for continuous lithium extraction. Moreover, such membranes should be characterized by mechanical strength, because this property determines their suitability for separation technologies.

The purpose of the work is to develop ion-selective membranes for the selective removal of Li^+ ions from salt solutions. The tasks are to study the diffusion permeability of membranes to these ions, as well as to establish the possibility of their extraction from solutions by a combined membrane-sorption method.

A method of modifying ceramic membranes with lithium-titanium spinel ($Li_4Ti_5O_{12}$) has been developed. The modifier was embedded to the pores of the membranes. This sorbent is selective for lithium ions. The amphoteric properties of the modifier ensure a constant rate of salt diffusion.

The modifier was investigated with X-ray analysis and TEM, the last method was also applied to the composite membrane, the modifier particles were shaded with organic acid. A size of embedded particles is 15-20 nm. Potentiometric method was also used to estimate charge selectivity of the membranes. This property is provided by aggregation of nanoparticles, which screen the macropores of ceramic matrix.

Due to the formation of a concentration gradient in the volume of the membrane, a diffusion flow arises, which is determined by the diffusion coefficient of Li^+ ions in the membrane, its thickness and the concentrations of ions in the surface layers of the solution on both sides of the membrane.

Organic- inorganic membranes were obtained by impregnating ultrafiltration membranes with a composite modifier - hydrated zirconium (IV) dioxide (HZD) containing oxidized graphene (GO, 0.5 wt.%). The modifier was precipitated in the active layer of the membrane forming a "secondary active layer". The layer thickness calculated according to the Kozeny-Carman equation is 0.66-1.38 μm. A thinner layer is formed in the membrane with smaller pore size, which is identified according to the rejection of calibrant (polyvinylpyrrolidone, molexular mass of which is 40 kDa). The diffusion coefficients of Li^+ and Na^+ ions were determined, the effect of HZD and HZD-GO composite on the ion transport was discussed. The influence of the modifier on the retention ability relatively to hardness ions (10-14%) and to protein compounds (95-98%) was established. The mathematical modeling of the dependence of the permeate flux versus time showed that the ion exchanger particles in the polymer active layer prevents the accumulation of organic substances in pores. Therefore, only the outer surface of the membrane is contaminated, and the precipitate can be easily removed mechanically. It was shown that the insertion of GO into pores of the membranes is advisable only in the case of a finely porous active layer. In particular, the performance of the initial polymer membrane (20 $dm^3\ m^{-3}\ h^{-1}$) and the selectivity to the calibrant of 40 kDa (99%) is the criteria of the choice of polymer matrix. In comparison with a membrane modified only with inorganic ion-exchanger, the membrane containing GO shows high filtration rate of protein solutions and considerable resistance against contamination. The results are discussed from the point of view of hydrophilic-hydrophobic properties of composite membranes.

Influence of vacuum annealing on the dispersion of chromium nanofilms deposited onto non-metallic materials

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In order to join ceramics and other non-metallic materials to metals by brazing, non-metallic surfaces often have to be coated with various metals, in particular chromium, in the form of thin films. This metal in the form of coatings is widely used in such industries as semiconductor technology, magneto-optics, touch sensors, and magnetic devices for storing information, etc. Adhesion of a metal film to non-metal surface, especially in the process of its annealing which occurs anyway during brazing or welding, plays an important role in these materials joints formation. For this reason, it is important to study the behavior and properties (in particular, the morphology) of metal nanofilms during their heating.

In this work, we study the dispersion kinetics of chromium nanofilms 100 nm thick deposited both onto oxide (alumina ceramics, sapphire, quartz glass) and non-oxide (silicon nitride ceramics and glassy carbon) materials and annealed in vacuum at temperatures of 1000-1200 °C with exposure at each temperature during from 2 up to 20 min.

The initial chromium films on all substrates were continuous and practically retained their continuity at annealing temperatures up to 1000 °C. After a long exposure (20 min) at 1000 °C, the films on all substrates begin to decompose. This process is intensified at 1100 °C; as a result of annealing at 1200 °C, chromium films disintegrate completely into separate fragments and drops.

As a result of long exposure at 1100 °C, chromium films on silicon nitride ceramics interact with the substrate material, and this interaction is significantly enhanced with an increase of the annealing temperature up to 1200 °C.

Using the obtained results, it is possible to recommend the use of chromium coatings on all the studied materials for subsequent brazing with appropriate solders at temperatures not exceeding 1100 °C, given that at these temperatures these films do not completely disintegrate, and the non-metallic substrates surface area coated by the metal films is 60-70 % of the original substrates area. At the same time, the units brazing time at 1100 °C should not exceed 10 min.

Stability and regularities of changes in transport properties of polymer composites with nanocarbon filler under thermal load

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In the work the questions of stability and regularities of transport properties of polymer composites with nanocarbon filler under thermal load are considered. The analysis has been carried out on the basis of the results of the temperature dependence of the electrical resistance studies for polymer composites based on epoxy resin with different types of nanocarbon filler with a filler concentration of up to 10% by mass.

The temperature dependence of the electrical resistance of the composite material is determined, in the first approximation, by the change with temperature of three parameters: 1) the electrical resistance of the nanocarbon filler particles R_f; 2) contact electrical resistance between nanocarbon filler particles R_c; 3) the number of continuous conductive chains (current paths) through the specimen N_{ch}.

For all nanocarbon materials used as fillers, the main mechanism of charge carrier scattering is temperature-independent charge carrier scattering at crystallite boundaries. Thus, for all nanocarbon fillers, electrical resistance R_f decreases with temperature due to an increase in the concentration of charge carriers. The temperature dependence of the contact electrical resistance R_c is determined by the temperature dependence of the nanocarbon filler itself and the change with temperature of the contact spot radius. Thus, the temperature dependence of the contact resistance is quite complex. Moreover, if the temperature coefficients of linear expansion (TCLE) for the particles of the nanocarbon filler and the polymer matrix are different, then the increase in the size of the polymer layers between the nanocarbon particles or their chains with increasing temperature results in the exclusion of these chains from the current transfer process.

It is shown in the work that there is a clear correlation between the structural and morphological state of the surface of nanocarbon filler particles, their shape and *aspect ratio*, and the character of the temperature dependence of the electrical resistance of the composite material. The factors that lead to such a correlation are analyzed in detail in the work.

Synthesis and structure peculiarities of proton conducting solid electrolytes of enhanced thermal stability

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A method for modifying polymer proton-conducting cation-exchange materials with a two-component modifier has been developed. The modifier involves tin (IV) hydrophosphate and carbon quantum dots. It was taken into consideration that Sn(IV) is in a form of anionic complexes in aqueous solutions, the surface of carbon constituent is charged negatively. In order to overcome this barrier, the modifier was deposited from the solution of non-equivalent sorbed electrolyte. Its content in polymers was controlled to prevent the formation of aggregated nanoparticles. Cation exchange resin was a model object for investigations. Porous structure of these materials in a swollen state is similar to that of ion exchange membranes. The composite based on this resin contains only non-aggregated nanoparticles, a size of which is 4-20 nm. These particles are in hydrophilic pores. Additions of carbon nanodots results in a partial aggregation of inorganic nanoparticles, the size of aggregates is up to 50 nm. They can be located only in hydrophobic pores. The effect of carbon constituent on electrical conductivity of the Nafion membrane under elevated temperatures has been found. The maximal value (0.32 $Ohm^{-1}m^{-1}$) is reached, when the content of carbon constituent in the modifier is 4 %. This is larger in 2 times than the conductivity of membrane containing only tin hydrophosphate and more than in 1000 times higher comparing with the conductivity of pristine membrane. The growth of conductivity is due to participation of protons of carboxyl groups, which are located on the surface of nanodots, in charge transfer. Further increasing the content of carbon nanodots causes a decrease of conductivity due to localization of aggregates in hydrophobic pores. The advantages of the composite modifier over other inorganic substances is a possibility to obtain it from relatively cheap and available reagents. Moreover, the synthesis method is eco-friendly: it provides no usage of chemical reagents.

Silver-containing polymer nanocomposites

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Using the methods of green chemistry, three types of silver-containing biomaterials (powders, films, solutions) with effective antimicrobial and antiviral action were developed.

Powdered silver-containing materials based on polyelectrolyte complexes with the participation of polysaccharides (pectin – chitosan, pectin – cationic starch, carboxymethylcellulose (CMC)–cationic β-cyclodextrin, anionic starch – cationic starch) were developed.

Silver-containing film materials based on polylactide biopolymer were created in various ways: *(i)* thermochemical reduction of Ag^+ ions in PLA-AgPalm-chitosan polymer systems to metal nanoparticles; *(ii)* by using green tea extract Ag^+ ions were reduced in the polymer matrix of PLA-AgPalm (*in situ* method); *(iii)* cathodic sputtering of silver nanoparticles on the surface of the PLA.

Silver-containing solutions (sprays) were synthesized by reducing silver ions with green tea extract, mint, propolis, and pectin.

The obtained materials were characterized by physico-chemical methods, and their antimicrobial, antiviral and cytotoxic properties were studied. The relationship between the structure, morphology, antimicrobial and antiviral properties of the obtained materials was studied.

The obtained materials can be promising for the treatment of wounds of various infectious origins; for the formation of antimicrobial coatings in medical, pharmacological, and biological laboratories to ensure sterile conditions; for creating packaging materials for long-term, high-quality and safe storage of food; for creating antimicrobial air filters in ventilation systems in hospitals and microbiological laboratories; for creating medical masks, etc.

On the miscibility gap in tungsten-based alloys

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In this work we establish an approach to model miscibility gaps of alloys using statistical physics, lattice dynamics from first-principles calculations. We carefully calculate the entropy to include all processes introducing disorder to the system, i.e., combining the electronic, phononic, and configuration entropies. Furthermore we present our algorithm for generating Special Quasirandom Structures (SQS). We model the miscibility gap in tungsten - chromium and tungsten - molybdenum systems, obtaining the agreement with the experimental data. Furthermore, we propose an enhancement for the tungsten-chromium $W_{70}Cr_{30}$ alloy with tantalum and hafnium, leading to the modified stabilization temperatures TS, where the solid solution is miscible.

We acknowledged the financial support by the Czech Science Foundation through grant No. 20-18392S as well as the Czech MŠMT via project e-INFRA CZ (ID:90140).

Keywords:

tungsten-chromium system, alloy, ab-initio, miscibility gap, solid solution, special quasirandom structures

Silica Based Lithium Ion Battery Anode Nanomaterial

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Lithium-ion battery (LIB) anodes are usually composed of graphite or other carbon materials. The graphite anode has a stable structure, good electrical conductivity, and can embed up to 1 lithium atom for every 6 carbon atoms in its crystal lattice. However, graphite has a low capacity (372 mA·h/g), which limits the performance of LIB and cannot meet the ever-increasing need for batteries.

This paper briefly discusses the trends, current problems and prospects for the use of silicon Si and its oxides SiO, SiO_2, which have a high theoretical capacity (4200, 2600 and 1965 mA·h/g, respectively). This means they can store more energy per unit mass compared to traditional graphite. However, anode materials based on Si and its oxides are associated with a large volume of expansion during charging and discharging of the battery, which can lead to damage to the anode structure, as well as low electrical conductivity. SiO_2 is considered as a potential replacement for the Si anode in LIB as it has moderate volume expansion (100 %) and low cost. However, SiO_2 has a weak electrochemical kinetics.

The results of the synthesis of the composite nanomaterial for LIB anodes based on highly dispersed SiO_2 and carbon C are presented. SiO_2 powder was synthesized from the metallurgical industry wastes with particle sizes in the range of 100–200 nm. The SiO_2/C nanocomposite was obtained by annealing in an argon atmosphere at the temperature of 500°C, which results in the formation of a layer on the surface of SiO_2 spherical particles, which ensures the electrical conductivity of the entire anode material.

It is shown that the carbon content in the SiO_2/C composite can have a significant effect on the electrical conductivity of the anode. The anode based on the obtained nanocomposite demonstrates good electrochemical characteristics. After 500 cycles at a current density of 1.0 A/g, the LIB capacity remains at 786 mA·h/g, and at 0.2 A/g, the specific discharge capacity is 900 mA·h/g.

Thus, the SiO_2/C nanocomposite material synthesized using metallurgical waste is a promising anode material for LIB.

Evaluation of the influence of physical and chemical factors on the properties of Alginate-Gelatin-Chitosan hydrogel for tissue engineering application

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In recent years, researchers have attracted the attention of hydrogels based on natural polymers, which are used in tissue engineering for bone treatment, as heart or nerve implants [1]. Alginate (Alg), chitosan (CS), gelatin (Gel) are often used to create materials that aim to mimic the natural extracellular matrix of native tissue. These polymers are biocompatible and biodegradable, at the same time their concentration, ratio and technological conditions of use have a huge impact on the physicochemical properties of the created hydrogel systems [1]. The combination of these biopolymers and the selection of technological conditions for their creation provides an optimal composition that meets the requirements for materials of the specified direction. To solve the task, a number of samples were synthesized with a ratio of Alg:Gel equal 3:1; 1:1; 1:3. The results of the study proved that an increase in the proportion of gelatin leads to a decrease in the degree of swelling (SW) from 550% (for Alg:Gel 3:1) to 400% (for Alg:Gel 1:3) in samples cross-linked simultaneously with chitosan and calcium ions.

In samples cross-linked exclusively by calcium ions, a sinusoidal curve of swelling in physiological solution is observed, which is obviously related to the participation of Ca^{2+} in ion exchange processes and the reverse diffusion of calcium ions due to the concentration gradient. SWs of these samples are generally smaller than that of samples cross-linked with CS, and are 260-360%. However, the degradation degree (DD) is significantly higher than for samples cross-linked with CS. Degradation of samples synthesized at pH 7 begins after 24 hours, and samples synthesized at pH 4.10 - after 96 hours. Increasing the crosslinking time with calcium ions from 20 minutes to 24 hours significantly increases the time before the degradation of the samples begins. The Alg : Gel 1:3 and Alg : Gel 1:3 samples are especially noteworthy, which show shape stability after 432 hA of testing.

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Effect of phase transitions on the electrical conductivity of graphite intercalation compound with bromine

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In presented work the peculiarities of phase transitions in the bromine layers and their effect on the electrical conductivity of intercalation compounds based on fine crystalline pyrolytic graphite are considered.

As recently conducted studies of the structure of GICs with bromine in the temperature interval of (150-300) K by the methods of X-ray diffraction and Raman spectroscopy [1, 2] have shown, that three phase transitions occur in the layers of the intercalate in this temperature range. These are transition of bromine in from "quasiliquid" state to the incommensurate with the graphite layer lattice at the temperature > 290 K (1); the transition of bromine from incommensurate with the graphite layer to commensurate lattice at the temperature ~ 250 K (2) and the transition of bromine from one commensurate with the graphite layer lattice to another commensurate lattice at temperature ~ 150 K (3).

Figure presents the dependence $\rho_a(T)$ for second stage GIC with bromine. As can be seen from the Figure, in the indicated temperature intervals, there are indeed peculiarities in the dependence $\rho_a(T)$. Moreover, at temperature ~ 150 K, the value of resistivity changes 100 times. In work factors causing peculiarities in the temperature dependence of resistivity in the intervals of phase transitions are analyzed in detail.

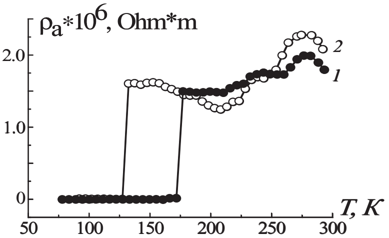

Fig. Dependence ρa(T) for second stage GIC with bromine: 1 – cooling, 2 - heating

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The Influence of Co^{2+} Substitution on the Structural, Mössbauer, and Dielectric Properties of Spinel-type Copper Ferrites

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This research studies the effects of replacing the d-block element Cu^{2+} with Co^{2+} ions in the copper ferrite-spinel composition [$Cu_{1-x}Co_xFe_2O4$ (x=0.0; 0.2; 0.4; 0.6; 0.8; 1.0)] and its influence on the material's structural, vibrational, and dielectric properties. The samples are prepared using the sol-gel autocombustion technique. The tetragonal phase of copper ferrite diminishes progressively upon introducing cobalt ions, and at x=0.6, the spinel phase Fd3m becomes predominant. The spinel-type cubic structure at room temperature for $Cu_{1-x}CoxFe_2O_4$ ($0.6 \leq x \leq 1.0$) was verified by analyzing X-ray diffraction patterns using the Rietveld method. Raman spectroscopy investigations identified 2(5) optically active modes in $CuFe_2O_4$ ($CoFe_2O_4$) at ambient conditions. Mössbauer spectroscopy of $Cu_{1-x}Co_xFe_2O_4$ (x=0.0; 0.2; 0.6) samples revealed two sextets for each specimen, signifying the presence of Fe in both A and B positions. Position identification was conducted based on the distribution of superexchange interactions and isomer shift data. The dielectric constant and the dielectric loss tangent were evaluated within a frequency range of 0.01 Hz to 105 Hz at room temperature, revealing a decrease in these values as the frequency increased.

The synthesized nano-sized ferrite particles were evaluated as photocatalysts for removing dyes from aqueous media using photo-Fenton. The $Co_{0.4}Cu_{0.6}Fe_2O_4$ composition demonstrated 97% elimination of Methylene Blue dye, and complete removal of Congo Red and Malachite Green dyes within 200, 80, and 100 minutes, respectively, under exposure to visible light from a 150 W halogen lamp. In addition, the study demonstrates that incorporating a transition metal ion (Co^{2+}) into $CuFe_2O_4$ establishes the foundation for diverse applications of the resulting material. Previous conclusions are supported by the material's structural properties, including crystallinity, lattice constant, magnetic characteristics, and dielectric properties.

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Structural modification of poly(DL-lactic acid) material by equal-channel multi angular extrusion

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A promising method for realizing plastic deformation by simple shear under high-pressure conditions is the equal-channel angular extrusion (ECAE) process and its modified version, the equal-channel multi-angle extrusion (ECMAE) process, which allows changing the spatial orientation of the shear planes, the intensity and the extent of accumulated deformation in one cycle of the process, which is not possible in the case of the ECAE process. Studies [1-3] have shown that such a process is suitable for the structural modification of synthetic polymers. At the same time, the possibilities of ECAE and ECMAE in the case of biodegradable polymers have been little studied. The key parameters of processes based on deformation by simple shear are the intensity of deformation (the value of the cutting angle of the channels), the degree of accumulated deformation, temperature, speed and pressure of extrusion. The direction of shear deformation, i.e., the deformation pathway, also has a significant effect on the type of microstructure formed and the properties of the polymers.

In this work, the effect of the key parameters of the ECMAE process on the efficiency of the structural rearrangements and the physical and mechanical properties of the processed polymers was studied using polylactides with a different content of D and L forms of lactide as an example.

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Nanocomposites based on polyurethane and modified montmorillonite: thermodynamic approach to reinforcement

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Nanocomposites based on thermoplastic polyurethane and montmorillonite (Mt) modified with oligourethaneammonium chloride (OUACH) were synthesized. The Mt of the Askan deposit (Georgia) was used. The method of Mt modifying is described in a previous work [1]. The nanocomposites were obtained by the method of exfoliation in a solution. The influence of the filler content on the thermodynamics of interactions, physical and mechanical properties, and morphology of the created nanocomposites was investigated.

For the thermodynamic compatibility investigation of polyurethane and Mt modified with oligourethaneammonium chloride, the sorption of acetone vapors by samples was studied using a vacuum installation with McBain balances. The thermodynamic parameters calculations have shown that the free energy of mixing the filler and the matrix during the formation of the nanocomposites decisively determines the physical and mechanical properties of the created nanocomposites. In case of thermodynamic compatibility between the matrix and the filler, dense surface layers of the matrix on the filler, high-quality polymer-filler contacts in the system are formed, which leads to the creation of nanocomposites with increased parameters of physical and mechanical properties. Mt modified with urethane-containing compounds, can form strong hydrogen bonds with the polar polymer matrix such as polyurethanes, polyamides, polyamidoimides, thus this method allow to create high performance polymer systems.

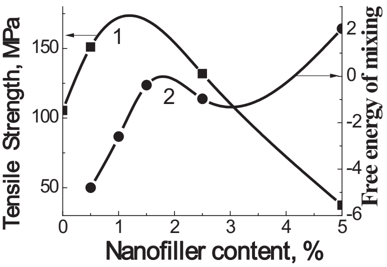

Fig. 1. *Concentration dependence of the tensile strength of the nanocomposites (1) and the free energy of polymer-filler mixing during the nanocomposites formation (2)*

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Specific electrochemical characteristics of $LiMn_2O_4$/graphene composite electrodes for lithium-ion batteries

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Lithium-manganese spinel $LiMn_2O_4$ is one of the most intensively researched cathode materials for lithium-ion batteries. The morphology and particles size of $LiMn_2O_4$ significantly affect its specific capacity and stability at high discharge current densities. There are a number of methods in the literature that allow to increase the specific characteristics of $LiMn_2O_4$ and ensure their stability under long-term cycling conditions [1].

Composite electrodes with a conductive matrix based on graphene are able to maintain a high specific capacity even under high discharge current densities [2]. This is due to the ability of graphene to create structures with improved electronic and ionic charge transfer properties. However, the surface and morphological properties of $LiMn_2O_4$ in composite electrodes may have additional influence depending on the properties of the graphenes used.

In the work discusses the results of capacitive and resource testing of composite electrodes depending on the physicochemical characteristics of $LiMn_2O_4$ and industrial graphenes of XG Sciences Inc. It is shown that the size of spinel particles, their geometric configuration and the size and shape of agglomerates as well as similar properties of graphenes significantly affect the rate characteristics of composite electrodes improving them compared to electrodes containing traditional conductive components.

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Effect of Post-Synthesis Annealing Temperature and Chelating Agent on Photocatalytic Properties of Nanosized Copper Ferrite.

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anoferrites possessing a spinel crystal structure have demonstrated good performance as photocatalysts in the visible light range. This is due to the fact that some spinel ferrites keep an optical band gap of approximately 1.5-2 eV, which enables the excitation of valence band electrons by visible light photon energy. The synthesis of these materials using the sol-gel self-combustion technique requires a specific chelating agent, which serves as an oxidizing agent in the initial precursor. The use of different chelating agents during the sol-gel self-combustion synthesis of ferrites significantly influences the resulting product's morphology and physicochemical characteristics.

The produced specimen underwent annealing in air at temperatures of 500°C and 800°C for three hours. The decrease in the degradation efficiency, as the annealing temperature increased, can be attributed to two factors. Firstly, an increase in particle size led to a reduction in specific surface area. Secondly, the combustion of the remaining carbon scaffold, which functioned as an additional sorbent for the dye.

A modified sol-gel autocombustion method was utilized to synthesize a nanosized, single-phase $CuFe_2O_4$ ferrite with an average crystallite size of 27 nm. This product was used to photodegrade Methylene Blue dye in an aqueous medium. Due to the small optical band gap of 1.55 eV, photodegradation was possible under visible light exposure. Results indicate that the degradation capability decreases with an increase in the post-synthesis annealing temperature. Moreover, the synthesized product's photocatalytic characteristics rely on the type of chelating agent utilized during synthesis. When glycine was used as the oxidizing agent, there was a 12% increase in degradation capacity.

Formulation of physically based constitutive models to reproduce the mixing process of immiscible polymers in the solid state under conditions of severe plastic deformation

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Homogeneous mixing of chemical substances is crucial in chemistry, materials and technology. Commercial attention has been devoted to compatibilization of macromolecules in efforts to produce new materials with tailored properties. However, different from low-molecular-weight compounds, the entropy of mixing for macromolecules is inherently very low; therefore, in most cases, the mixing of two or more polymers results in phase separation on the macroscopic scale. This fatal problem poses a significant barrier to producing many scientifically and technologically relevant homogeneous blends. To overcome the limitations of the existing approaches, several new strategies have appeared to prepare polymer blends using supramolecular complexation, porous coordination polymers, polymer nanoparticles, fluid interfaces. However, it remains difficult to improve versatility, mass-productivity and/or compatibility. Hence, the search for an easy and efficient strategy to achieve the perfect mixing of polymers at the molecular level continues.

In this work, we have attempted to mathematically model the mixing of immiscible polymers under conditions of ultrahigh plastic deformation, taking into account the peculiarities of the mechanics and physics of polymers. For this purpose, various viscoelastic-plastic models were created taking into account the peculiarities of polymer mechanics using professional software packages based on the finite element method. In addition, the well-known VPSC code, which is well suited for modeling the plastic deformation of metals, was extended to polymeric materials.

Formation of polymers in the presence of dispersed mineral phase

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The polymerization of vinyl monomers in the presence of dispersed mineral fillers allows obtaining materials with interesting properties. This paper presents the results of a study of the polymerization of various vinyl monomers in the presence of aerosols. The monomers used were styrene (ST), methyl methacrylate (MMA), methyl acrylate (MA), butyl methacrylate (BMA), and butyl acrylate (BA). In all experiments, industrial samples of aerosols were used, namely: A-175, alumina aerosil (AlA), titanium aerosil (TiA), and methyl aerosil (MeA). The specific surface area of the studied samples determined by low-temperature nitrogen adsorption was 190 m^2/g for A-175, 170 m^2/g for AIA, 120 m^2/g for TIA, and 190 m^2/g for MeA. The particle size of the fillers was in the range of 10-40 nm and the bulk density was 40-60 g/l. The content of aluminum oxide in AlA was 3.5 %. The content of titanium oxide in TIA samples was 4.0 %. Methyl ester contained 4.0 % methoxyl groups. Benzoyl peroxide (BP), oligomeric sebacic acid peroxide (OPSA), and diperoxide (DP) were used as initiators of radical polymerization. The introduction of aerosil into the polymerization system leads to a slowdown in the polymerization rate of ST, while in the case of MA, MMA, BMA, the polymer formation rate increases. The polymerization rate of monomers was studied by the dilatometric method up to 10 % conversion. The polymerization mixture was intensively stirred during the polymerization study, with the aerosil being evenly distributed throughout the system.

Was study of the adsorption of OPSA and DP on aerosil in styrene solution. The adsorption of OPSA on aerosil occurs due to the formation of hydrogen bonds between peroxide groups and OH-groups of aerosil. The thermodynamic parameters of the adsorption process and the area occupied by the OPSA link in the adsorption layer were determined. In the case of MA, MMA, and BMA, competitive adsorption of peroxide and vinyl monomer takes place. The increase in the polymerization rate of MA, MMA, BA, and BMA is associated with an increase in the viscosity of the polymerization mixture, which reduces the rate constant of polymer chain breakage. In some cases, a slight increase in the order of the initiator in the filled systems was found, indicating that part of the growing polymer chains breaks linearly. The molecular weights of the polymers formed in homogeneous and filled systems were determined.

Electrical conductivity and thermal stability of polyaniline and water-soluble polymer nanocomposites

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Polymer-polymer composites (PPCs) based on a conductive polymer – polyaniline (PANI) and water-soluble polymers such as: polyvinyl alcohol (PVA) and polymethacrylic acid (PMAA), have unique properties. Such PPCs have good electrical conductivity and can form strong films on various surfaces. Composites with such properties can be successfully used for the construction of chemic sensors, protection of metals from corrosion, etc. In our work, PPCs were obtained mechanic chemically by mixing the calculated amounts of PVA or PMAA with PANI in a small amount of water and treating the resulting mixture with ultrasound for 15 minutes. After drying, the obtained composites were investigated for their physical and chemical properties. The study of the X-ray spectra of the original polymers and composites based on them showed that intermolecular hydrogen bonds are formed between the components of PPC. Quantum chemical calculations confirmed the formation of hydrogen bonds between the components of the composite. Different conformational states of PANI and PMAA macromolecules lead to the formation of several types of hydrogen bonds, which are characterized by different energies and lengths.

The electrical conductivity of the obtained composites was studied. Electrical conductivity depends on the ratio of PANI and PMAA or PVA and is characterized by a maximum. The study of the dependence of electrical conductivity on temperature made it possible to determine the activation energy of charge transfer, which varies within fairly wide limits.

The study of thermal destruction of PANI, PMAA and PPCs was carried out by the method of thermogravimetry. The destruction of PMAA takes place in stages at temperatures higher than 100 °C, the macromolecule splits off water molecules, with further heating, and deep decomposition takes place. The destruction of PVA is also characterized by a complex nature and has several stages. Thermal decomposition of PANI also takes place in several stages. The decomposition of composites occurs in stages, and the temperature of destruction depends on the ratio between the components. This fact confirms the conclusion about the intermolecular interaction between the macromolecules that form the composite.

Patterns of the *in situ* formation of nanocomposites from polymer-inorganic hybrids and nickel nanoparticles: the role of the matrix structure and the concentration of components

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Polymer/inorganic hybrids consisting of a silica sol and polyacrylamide (SiO_2-g-PAAm) with different numbers and lengths of grafted chains have been synthesized and characterized. Their main molecular and structural parameters were determined using elemental analysis, DTGA, static light scattering, viscometry, potentiometric titration, and TEM. The functional properties of hybrids as hydrophilic matrices in the *in situ* synthesis of nickel nanoparticles (NiNPs) were controlled by UV-Vis spectroscopy and the original approach developed. The kinetic features and efficiency of the formation of NiNPs in hybrid solutions have been established depending on the structure and concentration of the hybrid matrices and the concentration of Ni-salt.

The accumulation rate and yield of NiNPs in hybrid solutions increased with an increase in the concentration of Ni-salt from 0.010 to 0.078 $kg \cdot m^{-3}$, and the reaction rate mainly decreased with an increase in the concentration of hybrid matrices from 0.5 to 2.0 $kg \cdot m^{-3}$. The structure of the hybrid matrices, determined by the number and length of grafted chains and the permeability of the polymer layer, was one of the key factors affecting the formation rate and yield of NiNPs. This provided greater or lesser accessibility of the active groups of the polymer "corona" and the inorganic "core" for metal ions and reducing agent molecules. A number of morphological studies of purified reduction products using TEM showed that the main structural elements of NiNPs/SiO_2-g-PAAm nanocomposites are swollen "hairy" particles of hybrids with small amorphous NiNPs (1.7±0.8 nm) embedded in the polymer "corona".

Natural heteropolysaccharide xanthan with nanogel particles as the basis for synthesis of new polymer hybrids

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Xanthan gum of microbial origin is currently considered one of the most interesting, studied and widely used natural polysaccharides due to its remarkable biocompatibility, biodegradability and non-toxicity. Having a regularly branched chemical structure and a negative charge in the side chains, its macromolecules can take both an elongated (helical) and a coiled conformation in solutions, depending on the balance of intra- and intermolecular electrostatic interactions and hydrogen bonds. Xanthan coils in aqueous solutions are physical nanogels with a micelle-like structure (Fig. 1), which can be used to create new hybrid materials of the type: nanogel "core" – polymer "corona". This work presents the implementation of this idea to obtain new xanthan/poly-N-isopropylacrylamide (K-*g*-PIPAAm) hybrids.

The chemical structure, molecular parameters, morphology, solution behavior, and coil size of a xanthan sample produced by the bacteria *Xanthomonas campestris* were characterized using FTIR, viscometry, potentiometric titration, DTGA, and TEM. Synthesis of hybrids was carried out by radical graft polymerization IPAAm from the surface of the xanthan coils. As a result, a number of hybrids were obtained with predicted the same length, but a different number of PIPAAm grafts. Their properties were studied by FTIR, DTGA and TEM.

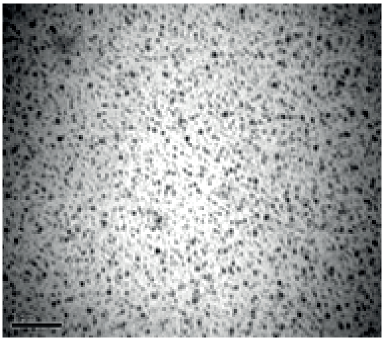

Fig. 1. *TEM image of xanthan coils.*

Silica phosphate nanomaterials containing multivalent metals: synthesis, functional properties and practical applications

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In this review, nanomaterials based on $SiO_2 \cdot P_2O_5 \cdot Me_xO_y$ (where Me is multivalent metal) are considered. Main approach to their synthesis is sol-gel technique. Multicomponent reactions, where three or more reactants takes part in a single reaction, are often used to prepare composites. A size of the primary particles of 20-100 nm is reported. As a result, a new material is formed, it includes two of more components. The composites can be also obtained with sol-gel synthesis, In this case, both support matrix an active components are formed simultaneously. The properties of glass-ceramics depends on the main crystalline phases and microstructures, which is determined on the composition of the parent glass. Nucleating agents also plays a key role, P_2O_5 promotes the separation of glass phase, increases the size of spherical droplets, and reduces the temperature of crystallization. Other approaches to the composite synthesis are reinforcement of preliminarily formed active component with a matrix, and embedding active component into the preliminarily formed matrix. It is stressed that the promising technique to obtain silica phosphates is ore processing.

Functional properties of the nanomaterials are sorption and catalytic ability, as well as proton conductivity and bioactivity. Their exceptional chemical stability and mechanical durability allow us to consider them as promising materials for technological processes. TiO_2 was found to promote crystallization and to enhance mechanical strength of $MgO–Al_2O_3–SiO_2–P_2O_5$ glass. This glass is used as dental material. Dual role of ZtO_2 on the crystallization temperature of Li-containing glass is suggested. The ion exchange capacity towards ammonia for the composite based on zirconium-containing silica phosphate, reaches about 3 mmol g^{-1} under ambient conditions. The composite was used as an adsorbent of ammonia The materials retain high capacity value up to 1300 K, where ZrP_2O_7 is formed. At lower temperatures, the composites are characterized by amorphous structure.

Transparent glass-like ceramics consisting of nanocrystals are recommended for electronic devices of different applications, Silica phosphate Zr-containing gels are also in a focus of attention as promising materials for the fabrication of hybrid organic-inorganic proton exchange membrane for low temperature fuel cells. The material is able to retain water up to 573 K.

Effect of physiological solution for different time on morphology of biogenic hydroxyapatite/magnetite/chitosan biocomposites

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Hydroxyapatite (HA) composites are the most promising for bone tissue engineering, especially like magnetosensitive materials that could promote regeneration processes during the treatment of bone injuries.

In our previous work [1] it was shown that not only the content but also the type of used magnetite significantly influence on the resorption rate of biogenic HA/magnetite/chitosan (BHA/M/Ch) composites in physiological saline for 2 days. Moreover, no cytotoxic effect was detected for all composite materials, regardless of the ratio of components and the method of magnetite synthesis.

The aim of the present work was study effect of physiological solution for different time on morphology of BHA/M/Ch composites.

BHA/M/Ch composites (1, 5, 25 and 50 wt.% of magnetite) were obtained by technology described in our previous work [2]. Composites were maintained in physiological solution (saline, 0.9% NaCl) for 2, 10, 16 and 31 days (solid: liquid =1:50) at 36.5±0.5ºC followed by control of phase composition, specific surface area (BET), density (helium pycnometry), and microstructure (SEM).

It was established that increasing maintaining in saline leads to increasing specific surface area and decreasing particle size. The higher amount of magnetite, the higher dissolution rate. At the same time, for long maintaining in saline the higher influence of BHA takes place. No clear correlation between density and composition has been shown. It was found no change in the phase composition.

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Plasmon Properties of Non-Spherical Copper Monosulphide Nanoparticles

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Plasmon phenomena in noble metal nanoparticles are well studied and widely used in contrast to semiconductor crystals, where this is a relatively new field of research [1]. One of the promising semiconductor materials capable of localized surface plasmon resonance is copper monosulfide (CuS). Moreover, the peak of its plasmon absorption falls on the NIR region, which attracts the special attention of researchers to this material and opens up interesting application possibilities. As in noble metals, in CuS the oscillator strength and the position of the plasmon resonance peak can vary depending on the size and shape of the particles, as well as the dielectric properties of the environment.

In this work, the dependence of the extinction cross section of CuS nanoparticles on their geometrical parameters was modeled. In particular, the extinction cross section of CuS nanoparticles was calculated from the incident radiation wavelength at different values of the ellipsoid semi-axis length (10, 30, 50, 70 and 90 nm) with constant values of the semi-axes b and c = 10 nm. It was established that the deviation from the spherical shape of the particle leads not only to the shift of the extinction maximum to the long-wavelength spectral region, but also to an increase in the maximum value of the extinction cross section. For instance, changing the length of the ellipsoid semi-axis a from 10 to 90 nm at constant values of the semi-axes b and c led to a shift in the position of the extinction peak by 1.48 μm (from 0.92 to 2.4 μm), and its value increased from 1.7×10^{-4} to 3×10^{-3} cm^{-2}. Thus, changing the ratio between the ellipsoid semi-axes makes it possible to adjust the optical response of CuS nanoparticles in the NIR region without loss in the intensity of plasmon absorption. It can be successfully used when solving problems in electronics or medicine, as well as when developing dual-purpose systems.

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Determination by striping voltammetry of cerium ions using nanomaterial-based electrodes

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Among the rare Earth elements cerium is the most widely distributed in the Earth's crust. This element is widely used in pharmaceuticals and photographic industries, metallurgy, microelectronic, organic synthesis starting materials, scintillation counters, catalysts, glass additives, fuel additives, as one of the active components of catalytic converts in vehicles. Cerium is also used in agriculture, forestry and animal husbandry, and as such, more and more attention is now being paid to the study of cerium in the environment. Cerium, like other rare Earth metals, has low to moderate toxicity. However, there are also other reports on the toxicity of cerium. The animals were given large amounts of cerium, they died of cardiovascular collapse. This element has also been found to cause pneumoconiosis due to inhalation of dust containing cerium. The growing industrial use of cerium and reports on its toxicity make it essential to have analytical procedures suitable for monitoring cerium in the environment [1,2]. Electrochemical methods, such as stripping voltammetry, are used to directly measure trace concentrations of metal ions in environmental samples. Voltammetry techniques are relatively easy, fast and inexpensive. In recent times, there has been an increasing use of nanomaterials for the manufacture of electrodes used in voltammetry. For the construction of electrodes, nanomaterials are sought that are chemically passive, widely available, have high mechanical strength and good conductivity [3]. The research presented here proposes the development of a new voltammetric procedure for the determination of trace amounts of Ce(III) using carbon nanotubes as the working electrode preparation material. The electrode prepared on the basis of nanotubes ensured low detection limits for cerium determination and very good selectivity towards other ions.

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Manifestation of Molecular Vibrations of Polymers in Thermoluminescence of Nanocomposites

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An experimental and theoretical study of the thermoluminescence (TSL) of a PDHS/MCM-41 nanocomposite (NC) with the introduction of a silicon organic polymer poly(di-n-hexylsilane) (PDHS) into MCM-41 nanopores with a pore diameter of 2.8 nm has been carried out. It is shown that the NC TSL curve is shifted toward low temperatures by 32 K relative to the polymer film, while its half-width is reduced by a factor of 6 and its shape is changed. The TSL curve consists of two bands: a very narrow intense band at 17 K with a half-width of 8 K, as well as a weaker and broader band with a maximum at 29 K and a half-width of 23 K. The energy spectrum of charge carrier traps is quasi-continuum. The positions of shelves in fractional TL method for a determination of energy spectra are discrete, they coincide with the energies of optical vibrations quanta.

The model [1, 2] was used to explain the experiment. In the model, the contributions from optical vibrations to the TSL curve and from other states are considered separately. The observed position of the peak of the TSL curve and the value of the activation energy in TSL allow to make a suggestion that the narrow peak of the TSL curve is a result of charge transfer to the conductive region of the polymer in the pore due to the absorption of an optical vibration quantum with an energy of 0.042 eV. The less intense broad band on the TSL curve arises due to the broadening of the distribution of the polymer segments. This broadening for a polymer in a pore is much smaller than in a film due to decrease of intermolecular interactions.

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Comparison of the piezoresistive response of Polystyrene/3D graphene and Polystyrene/Nanotubes composite films for sensors of deformation

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The growing scientific interest in the research of piezoresistive sensors in recent years is due to their wide application in such areas as the construction, automotive, aviation industries, as well as in robotics, biology and biomedicine, rehabilitation and personal health monitoring. The objective of this research was to develop high performance conductive polymer composite (CPC) materials for flexible piezoresistive sensors using hollow three-dimensional (3D) graphitic shells (GS) as a highly conductive particulate component. Polystyrene (PS), a cost-effective and robust polymer widely used in various applications such as household appliances, electronics, automotive parts, and packaging, was chosen as the polymer matrix. Hollow spherical three-dimensional graphene shells (GS) synthesized by chemical vapor deposition (CVD) using magnesium oxide (MgO) nanoparticles as a substrate, which were removed after synthesis, were used as conductive fillers. Commercial multi-walled carbon nanotubes (CNTs) were applied as a reference graphene material.

The main focus of this study was to investigate the impact of the GS on the piezoresistive response of graphene/polymer composite thin films. The performed studies allow to confirm that PS/GS composites can be characterized by a different type of piezoresistive response than composites with CNTs. So, it is shown that if the electrical conductivity of polymer films filled with CNTs decreases linearly with deformation, then for composites filled with GS this dependence has a complex character. The use of empty carbon shells greatly affects the sensors response during bending of composite, due to GS deformation, which leads to the absence of a response under elastic deformation. The sensitivity of PS/GS composites becomes very high when the strain goes beyond elastic strain, resulting in an extremely large change in sensor conductivity.

Coordination environment and dielectric contrast effects on luminescence of Eu^{3+} ions in opal films

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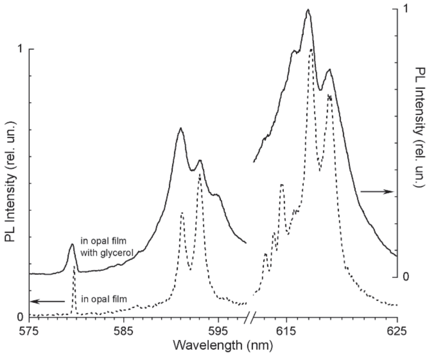
Photonic crystals activated by Eu^{3+}-containing complexes with organic and inorganic ligands are of both fundamental and practical interest, especially, from the point of view of managing their optical properties.

Photoluminescence (PL) spectra of the $C_6H_9EuO_6xH_2O$ salt in pores of opal films, with the globule diameter of 300 nm, were measured by exciting the “hypersensitive” $^5D_1 \leftarrow {}^7F_1$ transition with a 532 nm DPSS laser radiation. Backward scattering geometry with respect to the opal (111) plane was used.

Three emission bands centered at 580 nm, 592 nm, and 617 nm, corresponding to the $^5D_0 \rightarrow {}^7F_0$, $^5D_0 \rightarrow {}^7F_1$ and $^5D_0 \rightarrow {}^7F_2$ transitions in the Eu^{3+} spectrum, respectively [1], were observed in the PL spectrum (dashed curve). Maximum possible number of components of the Stark structure of the transitions $^5D_0 \rightarrow {}^7F_j$ ($j = 1, 2$), equal to $2j+1$, and the high intensity of the $^5D_0 \rightarrow {}^7F_0$ transition indicated a low symmetry of Eu^{3+} centers, not higher than C_{2v}.

An additional impregnation of the salt infiltration area with an aqueous solution of glycerol (85%) resulted in decreasing dielectric contrast from 1.85 to 1.13 and was accompanied by the broadening of emission bands with the spectral intensity redistribution (solid curve). It might be caused by disordering of the ligands in the Eu^{3+} ion coordination environment.



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Photonic band gap and interface effects on the Eu luminescence spectrum in opal films and heterostructures

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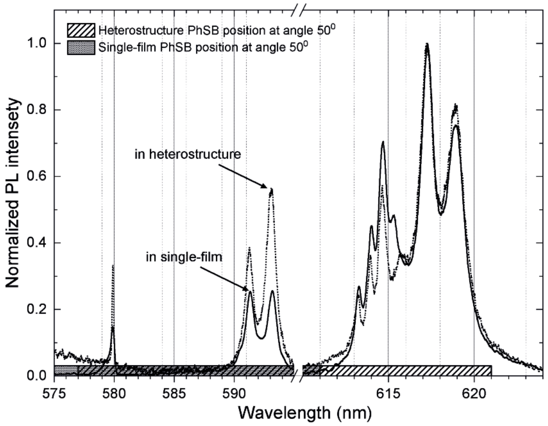
Opal-based photonic crystals (PhCs) offer versatile control of the photoluminescence (PL) spectrum through adjusting photonic stop band (PhSB) parameters and defect incorporation, enabling innovative light sources and sensors. Broad PhSB coverage is crucial for optimal emission control, making dual heterostructures with slight difference in globule size highly favorable option.

Opal-based PhCs were fabricated as films on a glass substrate, composing of silica particles (SPs) synthesized by the Stöber method. A dual heterostructure was formed by depositing a second film layer with similar-sized SPs prepared by the multistage Stöber method. PL spectra of Eu^{3+} containing salt in both single-film and heterostructure were measured under forward scattering geometry using a 410 nm semiconductor laser.

The PL spectra of Eu^{3+} salt in opal films show strong angular dependence of the intensities. However, single-film and dual-film structures exhibit contrasting features, with the latter lacking inhibition of PL bands within the PhSB region (Fig.). Observed disparity can be attributed to the interface between the films, which acts as a defect. This results in the presence of allowed states in the PhSB of heterostructure, which itself is a combination of the individual PhSBs of each film. The impact of the interface on light scattering is also analyzed in this context.



Heat conductivity of PCTFE - TEG and PHTFE - TEG/SiO_2 nanocomposites

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Polymer nanocomposites are currently the subject of intensive research and have broad prospects for practical application. The increased interest in the development and study of their properties is justified by the possibility of obtaining materials with new or improved polyfunctional qualities. The development of new polymer nanocomposites with desired properties and the study of the patterns of their change makes it possible to create materials for obtaining coatings with controlled thermal properties, among which thermal conductivity occupies a particular place. In view of the foregoing, materials based on polychlorotrifluoroethylene and active, both pure and modified with silicon dioxide, thermally expanded graphite deserve special attention.

The purpose of this work is to establish the regularities of the effect of changing the content of components and modifying the surface of the filler on the heat conductivity of composites of the PCTFE-TEG and PCTFE-TEG/SiO_2 systems, as well as methods for obtaining composite materials with a controlled heat conductivity value at a low content of fillers while maintaining the unique properties of the polymer.

Studies of the temperature dependences of heat conductivity in the temperature range 303 ÷ 463 K were carried out with continuous change of the heater temperature in modes close to regular heating using a dynamic λ-calorimeter, which is a modernized heat conductor meter “ИТ-λ-400”.

It has been established that the percolation threshold both in the PCTFE-TEG and in the PCTFE-TEG/SiO_2 systems occurs at concentration values of ~ 0.95%, as evidenced by a sharp jump in heat conductivity. A further increase in the concentration of both TEG and TEG/SiO_2 leads to a certain decrease in the heat conductivity, which in the case of TEG/SiO_2 almost immediately begins to increase again and at a concentration of ~ 2.43% is two times higher than the corresponding values for both pure polymer and composite PCTFE-TEG.

Thus, it was found that the modification of TEG with SiO_2 significantly increases the heat conductivity of the composites.

Injectable composites based on sodium alginate and biogenic hydroxyapatite for medical application

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Today injectable composites based on sodium alginate and hydroxyapatite (including biogenic origin) are very promising for bone tissue engineering and allow reaching hard-to-reach defects using techniques that are minimally invasive.

The aim of the present work was preparation and investigation effect of biogenic hydroxyapatite (BHA) amount on the structure and properties of sodium alginate/biogenic hydroxyapatite (AlgNa/BHA) composites.

AlgNa/BHA composites (BHA content 1, 2, 3 and 10 wt.%) were obtained by mixing of 2% sodium alginate hydrogel and BHA. Previously 2% sodium alginate hydrogel was obtained using sodium alginate, calcium sulfate dihydrate, glycerin and distilled water as a starting materials. BHA was prepared by calcination of cattle bone at 800 °C.

AlgNa/BHA composites were characterized by DTGA (Q-1000 derivatograph, MOM), XRD (X`Pert PRO diffractometer, Malvern PANanalytical), FTIR (IRAffinity-1S spectrometer, Shimadzu) and SEM (Zeiss Ultra Plus microscope, Carl Zeiss Meditec AG). Skeleton density was measured by using a helium pycnometer (AccuPyc II 1340, Micromeritics) according to ISO 12154:2014. Additionally, the equilibrium swelling degree of hydrogels was evaluated after incubating in a thermostat TS-1/80 SPN at 25°C in distilled water for 24 h.

It was demonstrated the incorporation of BHA into a covalently cross-linked alginate hydogel and the formation of composite with a complex porous structure.

Formation of nanostructured porous Nb_2O_5 from Nb thin films

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Recently, a lot of researches have been done on nanostructured niobium oxides, in particular on the transparent semiconductor oxide Nb_2O_5. The areas of its application are catalysis, electronic devices, such as solid-state capacitors, memristors, solar cells, as well as various sensors and biosensors, including optical ones [1].

Nanostructures from Nb_2O_5 can be obtained by various methods, such as hydrothermal and sol-gel methods, pulsed laser deposition, electrodeposition, and liquid anodization in pore-forming electrolytes. Nanostructured niobium anodic oxides have many advantages, such as self-assembled formation, large surface area, controlled pore size and film thickness. The growth and morphology of the anodic oxide film (nanoporous, nanochannelled, nanoveined and nanocolumns) strongly depend on the electrolyte composition and temperature, spinning voltage, and anodization duration [1-3].

A special problem is the preparation of nanostructured anodic niobium oxide films from vacuum-deposited niobium films. The development of a controlled technology for such nanostructures on substrates used in microelectronics and thin-film sensors (silicon, glass) opens up many opportunities for wide application. Obviously, the formed oxide nanostructures should be affected not only by the anodization parameters, but also by the structural features of the niobium films themselves, which depend on the deposition mode and film thickness [3].

This work is devoted to study the formation of nanoporous anodic Nb_2O_5 from niobium films with a thickness of 100 - 300 nm deposited by the magnetron method on sital and glass substrates.

Anodizing was carried out in a two-electrode cell with a platinum wire cathode. A glass capillary pressed against the anodization area on the niobium film served as a container for the electrolyte. The anodizing area 2,25 mm^2 was limited by a positive photoresist mask. A potentiostatic anodizing mode was used in the voltage range of 10 - 40 V. An NH_4F solution in ethylene glycol with a small amount of water was chosen as the electrolyte. It gives opportunity to avoid damage of the substrate during anodization.

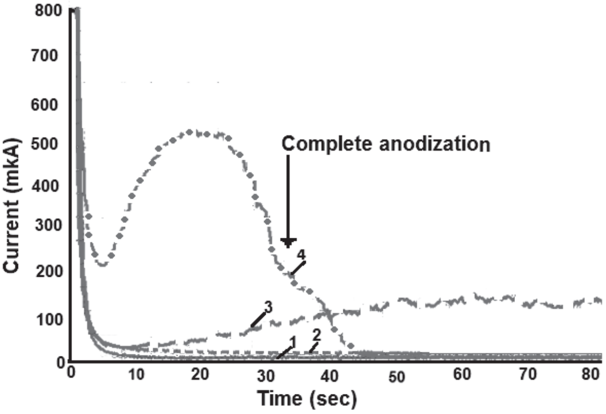

Fig. 1. *Chronampermetric dependences obtained during anodic oxidation of niobium films thickness of 200 nm at voltages of 10 V (curve 1), 20 V (curve 2), 30 V (curve 3), and 40 V (curve 4).*

The chronometric dependences (Fig. 1) obtained during anodization showed that anodic oxidation during the formation of porous Nb_2O_5 films have a minimums current. It is associated with a change in ion and electron currents during the transition from the formation of a dense barrier film to a nanostructured two-layer oxide film consists of barrier layer and porous layer [2]. The minimum becomes deeper with increasing voltage. The rate of transition of the niobium to the oxide increase when forming voltage enlarges. At a voltage of 40 V, the through oxidation time of a 200 nm thick niobium film is less than a minute, and the resulting two-layer oxide film has many cracks and peels.

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Nanosized tin dioxide based semiconductor materials for creation of gas sensors

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Nowadays the synthesis of new oxide nanosized materials is relevant in the creation of high sensitive sensors for detection of toxic and explosive gases in air. Tin dioxide due to its chemical stability remains the most popular among oxide semiconductor materials [1]. An increase in the sensitivity of the semiconductor gas sensors based on tin dioxide can be achieved both by introducing catalytically active additives into the materials of the gas sensitive layers of the sensors [2], and by reducing the sizes of the particles of the nanomaterials [3]. Nanosized SnO_2 has been synthesized by a sol-gel technique and characterized by IR-spectroscopy, DTA-DTG, XRD and TEM methods. Nanosized SnO_2-based sensor materials have been prepared by mixing different quantities of components (tin dioxide and carboxymethylcellulose) in a paste for creation of gas sensors. It is found that the composition of the pastes significantly affects the parameters of the sensors obtained on their base. The obtained data are explained by necessity of the presence of a sufficient number of contacts between the particles of the sensor material, which ensure the electrical conductivity of the sensor. Extreme nature of the temperature dependence of the sensor sensitivity for the synthesized material confirms the contribution of the size effect in the formation of the sensitivity.

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Nanocatalyst based on thermally expanded phlogopite, Pd(II) and Cu(II) compounds for oxidation of CO and SO_2 with atmospheric oxygen

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A common situation is when carbon monoxide and sulfur dioxide are simultaneously present in the waste gases of industrial enterprises. In this regard, research on the polyfunctionality of the Pd(II)-Cu(II)/$\overline{S}$ ($\overline{S}$– different carriers) nanocatalyst and the detection of the influence of SO_2 on its activity are relevant. Natural materials, including polyphase phlogopite concentrate, are effectively studied as carriers ($\overline{S}$) of palladium(II) and copper(II) compounds. The phase composition of the phlogopite concentrate significantly affects the activity of the Pd(II)-Cu(II)/$\overline{S}$ catalyst. We found that high-temperature treatment of natural material leads to homogenization of the phase composition, increase in the content of phlogopite and its swelling. The paper presents the results of the study of nitric acid concentration on the physicochemical properties of thermally expanded phlogopite (TS-Phl) and its acid-modified forms. The samples were modified with 1M, 2M, 3M and 6.0M nitric acid by the reflux method for one hour ($\overline{X}$H-TS-Phl-1, where $\overline{X}$ = 1,0; 2,0; 3,0; 6,0 M HNO_3). Pd(II)-Cu(II)/$\overline{X}$H-TS-Phl-1 catalysts were obtained by the impregnation method, the drying temperature was 110°C. Samples were characterized by XRD, SEM, FT-IR spectroscopy, and pH measurement. Catalysts were tested under conditions of room temperature, relative air humidity of 65-67% in reactions of oxidation of CO (C_{CO} = 300 mg/m^3) and SO_2 (C_{SO_2} = 150 mg/m^3). It was established that only on acid-modified $\overline{X}$H-TS-Phl-1 samples palladium(II) and copper(II) exhibit catalytic properties in the reaction of CO oxidation by oxygen. In the steady-state mode, the degree of CO conversion is greater, the greater the concentration of nitric acid used to modify TS-Phl. Pd(II)-Cu(II)/$\overline{X}$H-TS-Phl-1 samples in the reaction of oxidation of sulfur dioxide with oxygen revealed chemisorption-catalytic properties: the process occurs without establishing a steady state.

Hydrothermally and mechanically induced transformations in the porous and crystal structure of zirconium dioxide

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It is known that polymorphism is characteristic of zirconium dioxide. Different phases are formed depending on the method of its synthesis. Precipitation from aqueous solutions is usually used to prepare of the ZrO_2 in a nano-dispersed and X-ray amorphous state. Its calcinations lead to formation of metastable tetragonal phase and decrease in dispersity due to sintering. The latter limits the use of the ZrO_2 in high-temperature catalytic processes.

We have used successive hydrothermal and mechanochemical treatments (HTT and and MChT, respectively) to synthesize a stable monoclinic modification and create a mesoporous structure that is more resistant to sintering processes. Indeed, HTT at 260-320°C results in the formation of highly crystalline ZrO_2 consisting of a mixture of monoclinic and metastable tetragonal phases, which contains about 40-50% of the first. At the same time, the initial precipitated micro-mesoporous ZrO_2 is transformed into a uniformly mesoporous one. Soft dry milling (300 rpm) transforms the tetragonal component into a monoclinic one (within 0.5-1 h) so that ZrO_2 samples of an almost pure monoclinic phase are formed. Its crystallites are nano-sized: 12-14 nm. Also, the mesoporous structure of hydrothermal samples is almost completely preserved after MChT: milled samples have specific surface area in the range 60 – 100 m^2/g, volume of mesopores – 0.15-0.19 cm^3/g and mesopore diameter 4.0 – 6,5 nm.

The prepared samples do not undergo phase transformations and retain a developed porous structure up to high temperatures, at which they are used as catalyst supports.

Structure and size transformations of argon and nitrogen nanoclusters doped with krypton

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One of the most promising types of advanced nanostructured functional materials are cluster-assembled materials that are deposited using cluster beams. The morphology and properties of such structures can differ significantly from the properties of conventional nanocrystalline composites, and are mainly determined by the structure and sizes of cluster building blocks [1]. In turn, the problem of controlling the properties of substrate-free clusters is nontrivial, and its complexity is aggravated when passing from single-component to binary beams. In this regard, it is extremely useful to study van der Waals clusters of inert and simple molecular gases, which are good objects for testing theoretical models due to the simplicity of intermolecular forces.

In this work, we carried out a comparative electron diffraction study of the structure and size for pure argon and nitrogen clusters, and for clusters doped with krypton atoms. The krypton fraction in gas mixtures varied from 0.1 to 6 mol.%. The cluster sizes were varied by changing the initial temperature and initial gas pressure at the supersonic nozzle inlet and ranged from 3 to 20 nm (from 500 to 40000 molecules per cluster).

It was established that the addition of krypton to the argon jet lead to the intensification of cluster growth while the addition of krypton to the nitrogen jet can lead to either the intensification of cluster growth or its suppression. It was also shown that the growth intensifications were accompanied by opposite phase transformations. In Ar-Kr clusters, an increase in the relative fraction of the hcp phase is observed, while in N_2-Kr clusters, an increase in the fcc phase fraction occurs. The most probable reasons for the presented experimental phenomena are discussed and the mechanisms of cluster formation in binary gas jets are proposed.

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Hybrid solder joints: Effects of Fe nanoparticle-doped flux on morphology and hardness of SAC305 solder joints

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The two most popular methods introducing of nanosized particles into solder joins by flux are based on either addition of nanoparticles (NPs) directly into the solder paste, or the mixing of NPs with flux placed between solder and substrate. In the latter case, the solder joints are prepared in a sandwich form Cu/flux+NPs/solder/flux+NPs/Cu, and the nanosized additions are concentrated at the interface between the substrate and solder. Such hybrid solder joints are expected to have significantly better mechanical properties with lower nanopowder consumption compared to the solder paste mixing process. In a recent study, the authors found that hybrid Sn3.5Ag solder joints prepared by Fe NPs doped flux reveal a higher shear strength and a lower growth rate of Cu_6Sn_5 phase with increasing the NPs additions up to 2.0 wt.% [1].

The present study is focused on the investigations of the mechanical properties of the hybrid SAC305 solder joints with Fe NPs. The nanocomposite fluxes with various content of Fe NPs (0.0 wt.%-2.0 wt.%) were prepared by mechanical mixing for 30 min. The samples were soldered at 543 K for 5 min. A part of the samples was thermally aged for 7 days and 14 days. Subsequently, the variation of hardness across the solder layer was determined by means of nano-indentation tests to obtain a correlation between the distribution of Fe NPs in the solder joints with their microstructure and hardness. Additionally, a comparative analysis of the experimental data with literature has been provided.

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Spin-crossover molecular hexagonal nanocrystal

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Spin-crossover (SCO) complexes are transition metal coordination compounds that undergo reversible phase transitions between low spin (LS) diamagnetic and high spin (HS) paramagnetic states upon exposure to external stimuli. Such molecular spin-crossover can occur for certain first series transition metal ions with $3d^4$–$3d^7$ electronic configurations, and these materials are attractive due to their unique electronic bistability that holds promise for various technological applications [1].

The present study investigates the spin-crossover transition in a hexagonal lattice of finite size consisting of a grid of SCO molecules. The lattice is a standard model for the study of spin-crossover phenomena, and the finite size simulates more realistic experimental conditions. The work addresses to the role of the type of lattice and its finite size in the occurrence of phase transition in the spin-crossover nanocrystal. We used the Metropolis algorithm of Monte Carlo simulations to calculate the system's magnetization for various grid sizes and intermolecular interaction strengths.

Our findings indicate a transition from LS to HS states and vice versa for some grid sizes and intermolecular interaction strengths. We observed the dependence of the transition on the interaction strength by varying this parameter. Additionally, the transition behavior is influenced by the size of the finite lattice, as shown by our simulations.

In conclusion, our Monte Carlo simulations of a hexagonal lattice of finite size have allowed us to observe the transition of different kind from LS to HS states for various grid sizes and interaction forces. These results shed light on the cooperative behavior of intermolecular interactions in SCO systems and suggest potential avenues for further research in this area.

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Multicomponent composite layers as elements for effective multilayered microwave shields and absorbers

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Constructing a multilayered structure as an absorbing coating is an important tool for improving the characteristics of microwave absorbing (MA) and shielding materials. The influencing factors on microwave absorption performances of multi-layered structures are filler types and their spatial distribution in composite layers, filler loadings, stacking sequences and thicknesses, etc. Combining the electrical conductivity and magnetic susceptibility in the composite layers is a promising way due to the synergy of dielectric and magnetic losses. Multicomponent epoxy composites with various content (0-5 wt.%) of nanocarbon (graphite nanoplatelets (GNP), carbon nanotubes (CNT) and magnetic fillers (30wt.% of Fe, Co and Co_3O_4 particles) were studied in a frequency range (1-67) GHz. The observed enhanced microwave permittivity and dielectric loss tangent in these multicomponent composites may be explained by the enhanced contribution of interfacial polarization due to an additional large number of conductive magnetic particles and the formation of more interfaces with accumulated electric charge in heterogeneous structures. The modeling of reflection loss of multilayered composite structures using measured permittivity and permeability spectra showed good microwave absorptive properties. For example, a 4-layered composite structure based on GNP/Co_3O_4/epoxy layers showed a more pronounced reflection loss $|RL_{\min}|$=(30-32) dB (sample thickness is 2.2-2.5 mm) and effective bandwidth $\Delta f_{10dB} \approx 24$ GHz compared with single layers.

Much better microwave absorption properties of the multi-layered structures compared with the uniform single composite layer can be ascribed to the improved impedance matching with free space and the addition of interior interfaces.

The piezoelectric activity in the HfO_2 nanoclusters

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Piezoelectric materials generate electric charge in response to physical stresses (the direct piezoelectric effect) or through deformation under an electric field (the inverse piezoelectric effect). These phenomena are related to the development of piezoresponse force microscopy, sensors, actuators, resonators, electric energy harvesters [1, 2]. It is important to know whether the signs of the piezoelectric coefficient in piezoelectric materials have uniform positive or negative values, or a mixture of local negative and positive responses. For example, it has been recently predicted from first phrinciples that the usual ferroelectric phase of HfO_2 (orthorhombic with space group $Pca2_1$) presents a negative longitudinal piezoresponse. Though, existing experimental measurements of hafnia's piezoresponse suggest a perovskite-like behavior (i.e., a positive longitudinal effect) [3]. Research at the atomic level is needed to elucidate the physical mechanisms governing these phenomena.

In this paper the piezoelectric effects of the HfO_2 nanoclusters are studied by methods of the density functional theory and first-principles pseudopotential based on own program code [4]. The spatial distribution of valence electron density, density of states, and Coulomb potential along transverse direction are calculated. Local force responses from the electronic subsystem, cationic, anionic sublattices of hafnium oxide to multidirectional deformations are discussed.

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The characteristic of mixed cobalt and cerium oxide nanopowder as a precursor to obtain perovskite-type structure

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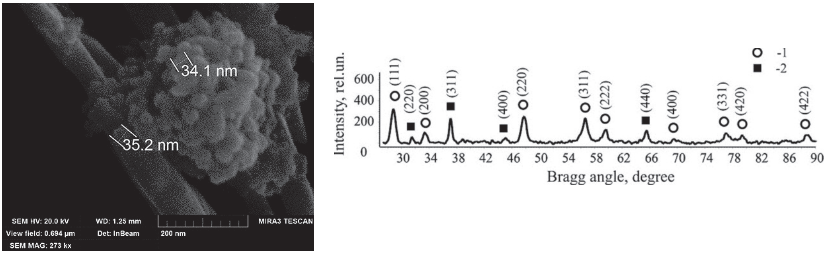
Binary oxides M−Ce−O are good systems for carrying out catalytic processes. The work aims to synthesize and characterize binary nanopowder of cerium and cobalt oxides to create catalytic active materials. The synthesis of the powder was carried out by co-precipitation $Co(NO_3)_2$ and $CeCl_3$ in a weakly alkaline environment with the addition of an auxiliary. The washed and lyophilized precipitate was fired at a T = 600 °C for 3 hours.

The morphology of the nanopowder is shown in Fig. 1a. Oxide particles are homogeneous and do not form aggregates, their average size is 34-35 nm. According to RFA (Fig. 1b), the powders included two oxides: CeO_2 (PDF No. 34-0394) and Co_3O_4 (PDF No. 9-418). For CeO_2 the parameter ***a*** = 0.5233 nm, and the CSR is 11.3 nm. For Co_3O_4, the parameter ***a*** = 0.8050 nm, and the CSR is 18.8 nm. The EDS data confirm the formation of a binary system includes two kinds of oxides. Cerium oxide particles contain wt.%: Ce 68.56; O 22.83; Co 6.34; Cl 2.27, and cobalt oxide particles, respectively, wt.%: Co 57.95; O 33.22; Ce 8.1; Cl 0.73.



a *b*

Fig. 1. *Composite cerium and cobalt oxide's nanopowder: a – SEM image; b – diffractogram. Numbers correspond to: 1 – CeO_2; 2 – Co_3O_4.*

Thus, the binary powder of cerium and cobalt oxides with nanometer-sized particles which are characterized by homogeneity and absence of aggregation, was obtained by a chemical method with subsequent calcination of lyophilized powder at T = 600 °C. Further research will be aimed at determining the catalytic activity of binary powders and obtaining a perovskite-type structure based on them.

Bimetallic NiFe and CoFe nanoparticles deposited on mixed fumed oxides in the reaction of CO_2 hydrogenation

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Fumed oxides SiO_2 and Al_2O_3 with a specific surface area of ~80 m^2/g were proved as the perspective carriers for bimetallic NiFe and CoFe nanoparticles catalytically active in the reaction of CO_2 hydrogenation [1]. One of the important things for the effective CO_2 conversion over the catalyst's surface is the surface basicity of it [2] due to the impact to value of CO_2 adsorption. Therefore, in order to achieve a better catalytic effect, the bimetallic NiFe and CoFe composition were deposited over the surface of mixed bi- (Al_2O_3/SiO_2) and ternary- ($Al_2O_3/SiO_2/TiO_2$) industrial fumed oxides marked as SA96 and AST1 respectively.

The catalytic experiment was carried out on a flow bed glass reactor at atmospheric pressure and a total gas flow rate of 0,1 l/min. The reaction gas mixture of CO_2/H_2 balanced with He in a composition's ratio of 2/55/43 vol.% was applied over the studied nanocomposite catalyst within the temperature range of 25-450 °C. The structure and properties of composites in the oxide and metallic form were investigated with TG, XRD, nitrogen adsorption and TD MS methods.

The results of the catalytic study showed that the application of Co-Fe and Ni-Fe active mass on the surface of fumed carrier SA96 is more promising compared to similar catalysts applied to carrier AST1 due to the absence of carbon monoxide among the reaction products.

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Versatile applications of hydroxyapatite-based composites

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Hydroxyapatite is a mineral of the apatite group with the formula $Ca_{10}(PO_4)_6(OH)_2$. Its structure is formed mainly by calcium and phosphorus atoms. It is included in the bones and teeth of living organisms. In nature it is found in magmatic, calcareous, metamorphic and phosphate rocks. This biomaterial has many favorable properties, including stability, reactivity, low manufacturing costs and high adsorption capacity. Hydroxyapatite has become a versatile biomaterial with applications in many fields. However, it is not a material without flaws. Therefore, the field of research into its modifications, including iron oxides, metal ions, or other organic compounds, is thriving [1].

Modification of the structure of hydroxyapatite with other compounds leads to the formation of a composite - a material made of different components, which in combination give the substance new properties. An interesting alternative that enriches the structure of apatite biomaterial is modification with iron oxides, mainly magnetite Fe_3O_4 and maghemite γ-Fe_2O_3, which are distinguished primarily by their magnetic properties. Another interesting modification of hydroxyapatite is its combination with white clay, which results in good adsorption properties, for example, of uranium, cadmium, nickel and tetracycline ions. Satisfactory results were also obtained in studies on the removal of uranium ions using hydroxyapatite, the structure of which was enriched with silver and calcium ions. The hydroxyapatite compound, combined with graphene oxide and chitosan, has proven its applicability in the adsorption processes of dyes and heavy metals, in this case copper ions. As can be seen, these materials are multidisciplinary in nature, and their potential use is compatibile the idea of sustainable development.

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Synthesis of bulk and supported $CuBi_2O_4$ powders using high-energy ball milling

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Copper bismuthate $CuBi_2O_4$ is *p*-type semiconductor with band gap within 1.5-1.8 eV depending on method of its synthesis. From this point of view, it is a promising material for photocatalytic application under the action of visible light. Its heterostructures with n-type semiconductors are also of particular interest. It is known that the method of synthesis has a significant impact on the physicochemical characteristics of photocatalysts and, ultimately, plays a decisive role in their activity. Usually, $CuBi_2O_4$ is obtained using coprecipitation from solutions or solid-phase interaction of oxides at a temperature of 700°C or higher.

In this work, facile top-down technique, high-energy ball milling, was used for synthesis of bulk and supported onto titanium dioxide $CuBi_2O_4$. Milling at 850 rpm of stoichiometric mixture of Bi_2O_3 with CuO or Cu_2O in air allow to prepare almost pure $CuBi_2O_4$ with crystallite size about 13 nm. When copper and bismuth salts as starting reagents were used, activation of reaction mixtures is observed due to milling. The prepared milled precursors are transformed into $CuBi_2O_4$ as a result of subsequent calcination at 500°C, i.e. 200°C lower than during the thermal treatment of the un-activated mixture. All synthesized samples have band gap within 1.6-1.8 eV.

A milled sample prepared from CuO at 850 rpm was supported to TiO_2 (anatase) in the amount of 5-10% also using a mechanochemical procedure. Due to this, the specific surface of the obtained compositions increased compared to the bulk milled samples - up to 22-25 m^2/g. In turn, this results in dispersion of the deposited $CuBi_2O_4$ phase on the TiO^2 surface, so that it does not form a separate crystalline phase that would be recorded by XRD. Another consequence of such mechanochemical deposition-dispersion is that a one absorption edge was found in the electronic spectra of these compositions. It corresponds to a band gap of 2.95 eV, which is much closer to that of TiO_2. Thus, doping of titanium dioxide with copper bismuth occurs during mechanochemical deposition.

Dynamics and mechanisms of growth of ZnO nanorods on industrial sheet brass

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Material brass is widely used in industry due to its good mechanical properties. However, among the drawbacks is the low wear resistance. To improve the mechanical properties of brass, various types of functional coatings are applied to its surface. ZnO nanorods were synthesized as a transitional layer between the substrate and the functional layer under conditions of plasma surface treatment carried out in a helicon high-frequency discharge [1]. The obtained ZnO structures are randomly oriented nanorods with lengths up to several microns and cross-sectional sizes ranging from 5 to 20 nm. Such a transitional layer provides high adhesion of the desired coating to the brass substrate.

The physics of formation and growth of these nanostructures is complex and multi-level. Their synthesis was previously carried out [2] at relatively high oxygen pressures (~300 bar) without prior plasma treatment. By employing combined regimes of surface cleaning and activation of brass using plasma argon flows, followed by independent heating of prepared samples in an oxygen atmosphere at pressures around ~10^{-2} Pa, the synthesis of well-defined ZnO nanorods occurs on the surface of brass through the diffusion of zinc atoms from within the lattice to its surface.

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N-heterocyclic azo dyes immobilized on silica gel for solid-phase detection of traces of nickel, cobalt and copper by diffusion reflectance spectrometry

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In recent years, chromophoric organic reagents have been widely used to modify the silica surface, which allows one to obtain the corresponding organo-mineral composites for broad application prospects. In this case, N-heterocyclic azo dyes (HR) – 1-(2-pyridylazo)-2-naphtol (PAN) and 1-(2-thiasolylazo)-2-naphtol (TAN) – are of great interest. Previously silicas with HR immobilized were used to metal (M) ions solid-phase determination by light adsorption of MR. It is known, that MR_2 stability, molar extinction coefficient and affinity to hydroxylation surface are higher than ones of MR. So, the sorbent with HR molecules disposition, optimal for MR_2 formation lets improve sensitivity and selectivity of solid-phase determination of M.

Hybrid materials with required location of reagent molecules on the surface were obtained via adsorption of $Zn(PAN)_2$ and $Zn(TAN)_2$ and were deeply investigated by Fourier transform infrared spectroscopy, thermogravimetric analysis in nitrogen and air atmosphere, scanning electron microscopy, and adsorption methods. The best characteristics were shown by $Zn(TAN)_2$ immobilized on silica gel Merk 60 (before and after acid treatment, SG1 and SG3) and $Zn(PAN)_2$ immobilized on Silpearl UV 250 (SP_2). These organo-mineral sorbents were used in further work to study the sorption of M from dilute solutions. The result obtained testify that only Ni(II), Cu(II) and Co(II) were adsorbed. The color of sorbents changed drastically and strongly depended on nature and initial concentration of M in solution. This phenomenon was used for working out visual test and diffusion reflectance spectrometry methods. Detection limits of Ni(II), Cu(II) and Co(II) determination were 2, 15 and 15 μg/l respectively. Methods were successfully used to soil extracts and tap water analysis.

Structural, optical and magneto-optical properties of Mn-doped II-VI based diluted magnetic semiconductor nanoparticles

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II-VI based dilute magnetic semiconductor (DMS) are material in which impurity ions, 3d- or 4f- transition metal (TM) elements replace II ions in crystal lattice [1]. The chemical composition of the DMS is represented by type of (II-VI):TM or ternary solid solutions type of $II_{1-x}TM_xVI$, where x denotes the fraction of impurity ions substitution in the DMS lattice structure. Dopant-carrier exchange interactions in the DMSs give rise to large Zeeman spin splittings of the excitonic or band states and related giant magneto-optical Faraday rotation.

At present, the mechanism that controls the incorporation of a dopant into a nanoparticles has not been fully studied. The developed various theoretical doping models were mainly used to explain the experimental results on the chemical colloidal synthesis of nanostructures of the DMS. In this work, we compare the structural, optical, and magneto-optical properties of Mn-doped CdS, CdTe, and ZnO semiconductor nanostructures obtained by various physical and chemical methods. All the samples were characterized by transmission electron microscopy, scanning electron microscopy, optical absorption, photoluminescence and Faraday rotation spectroscopy. The magneto-optical spectra of nanoparticles exhibit peculiarities typical for bulk DMSs due to the strong spin-exchange interaction between band carriers and magnetic ions and simultaneously manifest some features because of confinement effects in low dimensional structures.

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Porous structure of thermally activated carbon material

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Carbon materials (CM) based on plant biomass are obtained by carbonization and activation of feedstock at high temperatures. CM obtained by this method has a large developed internal surface area. However, the control of thermochemical processes leading to the formation of pores is a common problem nowadays. This problem is especially urgent in the case of obtaining CM for electrodes of electrochemical capacitors application. Moreover, it is not only the size of the specific surface that is important but also the pores size distribution.

The aim of this paper is to study the effect of thermal activation on the development of the CM porous structure. The initial material was obtained by thermal carbonization at 800°C from walnut shells [1]. To improve the structural and adsorption characteristics of the obtained CM, thermal activation was carried out at 400°C for 2 hours.

In order to determine the structural and adsorption characteristics of CM, the analysis of nitrogen adsorption/desorption isotherms obtained at -196°C was carried out using the Quantachrome Autosorb automatic sorbtometer.

The data analysis shows that thermal activation leads to changes in the parameters of the porous structure of CM. In particular, during the activation process, the specific surface area SBET increases from 230 to 431 m^2/g. In this case, the process of thermal activation promotes the development of a mesoporous structure. This is evidenced by the ratio of the mesopore volume V_{meso} to the total pore volume V_{Σ}, which is $V_{meso}/V_{\Sigma} \approx 75\%$ (for the initial sample this ratio is ≈ 11 %). The value of the average pore diameter increases from 2.2 to 4.8 nm.

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Two-electron systems in 2D Heterostructures with ion-covalent bond

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The unique properties of two-dimensional (2D) materials such as graphene [1] and materials with a structure similar to graphene [2] cause interest in connection with the possibility of applying such materials in quantum electronics, sensor technique and quantum computing systems. The study of impurity centers in such materials is one of the fundamental areas of modern nanoscience.

The paper presents the calculation of the energy of singlet and triplet states of two-electron systems such as exchange-coupled pairs of shallow hydrogen-like impurities and D–-centers in 2D graphene-like structures with ion-covalent bond. The calculations were carried out by the variational method with using the Gaussian system of functions. Similar functions were previously used to calculate the energy of the singlet and triplet states of the 2D hydrogen molecule [3]. The parameters of the electron–phonon coupling were determined using the dielectric characteristics calculated in Ref. [2] by the modified method of binding orbitals of binary 2D ANB8–N compounds.

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A solid-phase extraction method using Transcarpathian clinoptilolite for preconcentration of lanthanum from aqueous solution

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Lanthanum is one of the most abundant rare earth elements (REE). La and lanthanides represent a group of very similar rare elements that are hard to be separated. Methods of La determination mostly require a thorough sample pretreatment, which includes preconcentration, separation withdrawal of this REE. There is also a problem of La withdrawal from the technological solutions. One of the ways of solving problems of samples preparation for the analysis is the solid phase extraction method using various sorbents, in particular natural zeolites, which have a lot of advantages in comparison with other ones. The sorptive properties of the Transcarpathian clinoptilolite towards trace amounts of La(III) were investigated under dynamic conditions. Trace amounts of La(III) are sorbed most efficiently from weakly alkaline solutions at pH 9.2. It was established that hydrolyzed cationic and even neutral complexes of La(III) are priority species for sorption on clinoptilolite. The investigation has demonstrated that La(III) sorption on the clinoptilolite is caused by the processes of ion exchange and adsorption on the zeolite surface. Sorption capacity of the clinoptilolite increases significantly with decreasing concentration of La(III) in the solution. This is caused, probably, by the decrease of the amount of $LaOH^{2+}$ and $La_2(OH)_3^{3+}$ with increasing concentrations of La(III) in the solution. The most effecttively La(III) is sorbed by clinoptilolite samples previously calcined at 550–700 ºC. Siloxane bonds are formed in the structure of clinoptilolite at this temperature, that together with the silanol groups are responsible for the sorption of La(III). The maximal sorption capacity of clinoptilolite towards La(III) at optimal conditions is equal 61.7 mg/g. The solutions of mineral acids (HNO_3, HCl) and acidified 1 M NaCl and 1 M KCl solutions are effective La(III) desorbents. The method for La(III) trace amounts preconcentration from the aqueous solutions was proposed in a solid phase extraction mode. Differences in the optimal sorption conditions of La(III), Ce(III), Nd(III), Sm(III) and Eu(III) make it possible to concentrate and separate of the La(III) selectively from solutions containing the other specified REEs of the cerium group.

Fluorescent sensor materials with coumarin dyes and semiconductor colloidal CdTe nanoparticles with sensitivity to microconcentrations of ammonia and acetone in exhaled air

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Today, there are many studies on fluorescent sensors sensitive to ammonia and acetone in the air, including those using nanoparticles and nanostructured materials. It is important to create and research such sensors, which could sense analytes in the region of very low concentrations. This is topical for non-invasive diagnosis of diseases based on the analysis of exhaled air. Our recent study showed the possibility of detecting acetone and ammonia molecules in the air with fluorescent sensors based on silicate matrices, coumarin fluorescent dyes, and CdTe nanocrystals [1]. This work aimed to investigate the sensory properties of such materials to samples of model mixtures of human exhaled air, where such molecules are present in trace amounts.

Experiments showed a 57% increase in the fluorescence of coumarin 7 in an ethanol solution when CdTe quantum dots (size 2.3 nm, luminescence emission λ_{max} = 530-535 nm) were added in a 1:1 ratio. This is explained by the presence of FRET (Förster resonance energy transfer), since there is an overlap of the fluorescence band of quantum dots and the absorption band of coumarin 7. Experimental studies of the fluorescent sensor response of the created nanostructured films under interaction with analyte molecules in model mixtures of human exhaled air were carried out. The fluorescence response of samples with silica gel 60 (specific surface area 500 m^2/g), coumarin 7, and CdTe quantum dots (size 2.3 nm, λ_{max} = 530-535 nm) at 0.5 ppm ammonia was 1%, 1 ppm – 2%, 5 ppm – 6%, and 10 ppm – 14%. The response of samples with Aerosil A-380 (380 m^2/g) and coumarin 4 to 3 ppm acetone was 0.06%, 6 ppm – 0.16%, 9 ppm – 0.24%, 12 ppm – 0.35 ppm, and 15 ppm – 0.43%. It was found that after pumping clean air through the cuvette with the sample, the fluorescence intensity was almost wholly recovered for each sample type.

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Evaulation of Sensor Applications for Atrazine of Gold Nanoparticles synthesized by Using Punica granatum Bark Exrtact

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Au NPs have been widely using industrial areas such as sensor, environmental monitoring, and disease therapy due to their unique optical properties, and very small scale size distributions [1]. Au NPs synthesized via top-down and bottom up approach [2]. Each method have advangates/disanvantages each other. Green synthesis of NPs have advantages such as biocompatible, eco-friendly, cheep, not need high pressure, temperature [3].

In this study, we synthesized Gold (Au) NPs by using *Punica granatum* bark extract. Characteristic peaks of NPs were determined at 569 nm. According to FE-SEM images NPS have spherical morphology with 61 nm. DLS and zeta potential of NPs have been found at 162 nm, and -29 mV, respectively. Functional groups and christianity of NPS were detailed by using FT-IR, and XRD analysis, respectively. As a result, we suggest that, Green synthesized Au NPs might be use for detection of atrazine as colorimetric sensors.

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Extraction and use of nanocellulose from non-wood plant materials in the composition of paper and cardboard

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Cellulose is the most widespread natural polymer on Earth, which is widely used in the production of paper and cardboard, ethers and esters of cellulose, oxycellulose and nanocellulose. Nanocellulose, as a biodegradable material, has unique properties: mechanical strength, transparency and chemical resistance, light weight and low coefficient of thermal expansion, and is used to improve the properties of composite materials [1]. The study described the extraction of nanocellulose from hemp and corn pulp, obtained by environmentally friendly organosolv method of delignification by cooking using a mixture of acetic acid and hydrogen peroxide [2]. A stable transparent nanocellulose gel was extracted from organosolv pulp by acid hydrolysis followed by ultrasound treatment and used for the production of paper and cardboard. The nanosize of nanocellulose was confirmed by AFM and TEM methods [3].

It has been established that the addition of nanocellulose to the fibrous composition or to the surface of paper (cardboard) improves the physical and mechanical properties of food packaging paper and cardboard for flat layers of corrugated cardboard. The changes that occur with the addition of nanocellulose were investigated using SEM and XRD methods. The recommended values of the consumption of nanocellulose for the production of paper and cardboard with indicators that meet the requirements of the relevant standards have been determined.

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Establishing the role of europium activator in the formation of pro-oxidant properties of orthovanadate nanocrystals

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Metal oxide nanocrystals, including rare-earth orthovanadates, have garnered significant attention from scientists due to their valuable properties, making them promising for diverse biological and medical applications. Recent advancements in nanomedicine have unveiled that metal oxide nanoparticles can participate in Reactive Oxygen Species (ROS) production reactions involving electron/hole transfer. Our research has uncovered that orthovanadate nanocrystals exhibit both pro- and anti-oxidant activities, depending on the nanocrystals' size, external conditions, and pre-treatment regimen. Furthermore, when orthovanadate nanocrystals were pre-exposed to ultraviolet light before the experiment, a phenomenon known as "dark" ROS generation was observed.

In this study, we investigate the role of europium activator on the pro-oxidant properties of orthovanadate nanocrystals. By utilizing fluorescence probe molecules specific to superoxide anions and hydroxyl radicals, as well as a non-specific ROS sensor, we examine and compare the efficiency of "dark" ROS generation between doped and undoped nanocrystals. Our findings reveal that in small nanocrystals (2 nm), UV-light pretreatment leads to the reduction of Eu^{3+} to Eu^{2+}. Electrons stored in Eu^{2+} participate in electron transfer reactions with oxygen molecules, resulting in the production of superoxide anions and other ROS. This enhances the overall efficiency of "dark" ROS generation compared to undoped nanocrystals. However, such effects were not observed in larger nanocrystals.

Consequently, activating orthovanadate nanocrystals with europium ions represents a method to enhance the ability for "dark" ROS generation in UV pre-exposed small nanocrystals.

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Composite zinc oxide with zeolite for organic pollutants photodegradation

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Wastewater containing even residues/traces of organic dyes can cause severe environmental pollution, as they affect the organoleptic parameters of surface waters, reduce light penetration, inhibit vital processes, and prevent photosynthesis in water. In addition, some dyes are toxic, mutagenic, and even carcinogenic [1-3].

Traditional purification methods, such as adsorption, ultrafiltration, reverse osmosis, coagulation, ion exchange, etc., do not destroy dye molecules. From the point of view of mineralization of organic pollutants, modern progressive advanced oxidation processes are more effective, but they do not provide the "zero pollution" [1].

In view of this, the photocatalytic method of destruction is the most promising and promising. And photocatalysis using composite semiconductors, including composites of ZnO with zeolite, is a new approach to expand the range of light absorption, as well as to achieve more efficient distribution of charges and increase their service life. In this regard, the aim of the presented research was to develop a new effective composite photocatalyst based on zinc oxide [2,3].

The main tasks of the presented research were the following. Develop synthesis methods and synthesize laboratory series of ZnO composites with zeolite. To investigate the morphology, particle size, phase composition, optical band gap, structural and adsorption characteristics, and acid-base surface centers of the synthesized composites. To study their photocatalytic activity in model processes of photodegradation of organic pollutants using the example of anionic (Congo red) and cationic (methyl blue, methyl green) dyes in static and dynamic modes. To establish the relationship between the structure, composition, structural adsorption, acid-base properties, and photocatalytic activity of the synthesized composites.

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Adsorption capacity of carbon-silica composites towards simultaneous removal of heavy metal ions and drug from aqueous solutions

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Useful adsorbent is characterized by the high adsorption capacity, high selectivity, efficient adsorption kinetics, easy separation from solution after the adsorption process is completed, simplicity of regeneration and low production costs. The purpose of the presented research was to verify whether innovative carbon- silica composites fulfill these expectations. Three composites were selected for the study: primary C/SiO_2, modified iron-enriched C/Fe/SiO_2 and modified manganese-enriched C/Mn/SiO_2. Accordingly, studies were conducted to determine the elemental composition and textural parameters of the selected solids. Subsequently, these composites were used in the adsorptive removal of heavy metal ions (Pb(II), Zn(II)) and a pharmaceutical (antibiotic diclofenac) from aqueous solutions in single and mixed adsorbate systems. Diclofenac is one of the most popular over-the-counter nonsteroidal anti-inflammatory drugs (NSAIDs). Lead, on the other hand, is an absolutely toxic element, and zinc possesses significant threats in excess to living organisms. Measurements of adsorption and desorption capacities were also carried out. Potentiometric titrations and electrophoretic mobility measurements were conducted to comprehensively characterize both the composites themselves and the adsorption layers formed in systems with metals and the pharmaceutical. They allowed the determination of point of zero charge and isoelectric point, two important parameters that characterize solid-solution interface.

Based on the results obtained, it was concluded that the silica-carbon composites used are effective adsorbents that can be applied in the process of simultaneous removal of heavy metal ions and drugs from aqueous solutions.

Effect of preparation conditions on the surface morphology and edge absorption of $ZnGa_2O_4$:Cr thin films

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Phosphors based on $ZnGa_2O_4$:Cr with a spinel structure are used in various luminescent screens with both long and medium afterglow times as the red component. In this regard, the paper investigates the optical absorption edge of $ZnGa_2O_4$:Cr thin films obtained by radio-frequency (RF) ion-plasma sputtering, which is optimal for depositing semiconductor and dielectric films. Thin $ZnGa_2O_4$:Cr films with a thickness of 0.3-0.8 μm were obtained by RF ion-plasma sputtering in an atmosphere of a mixture of argon and oxygen of different percentages on fused quartz (υ-SiO_2) substrates.

The analysis of the obtained micrographs of these films indicates a slight dependence of the size of nanocrystallites forming $ZnGa_2O_4$:Cr thin films on the presence and atmosphere of heat treatment. In particular, the average grain diameter of the unannealed films is 211 nm, when annealed in an argon atmosphere, it increases to 222 nm, and when annealed in an oxygen atmosphere, it increases to 245 nm. As a result of the studies, it was found that, regardless of the composition of the sputtering atmosphere and the heat treatment atmosphere, the fundamental absorption edge of $ZnGa_2O_4$:Cr thin films is formed by direct allowed electron phototransitions. The analysis of the fundamental absorption edge shows that the optical band gap Eg of $ZnGa_2O_4$:Cr thin films is very sensitive to the composition of the sputtering and heat treatment atmosphere. Thus, for films deposited in an argon atmosphere and annealed in oxygen, Eg = 4.55 eV, and for films annealed in argon, Eg = 4.62 eV. An even greater shift is observed when some oxygen is added to the argon spray atmosphere. The addition of 15% oxygen leads to Eg = 4.67 eV, and the addition of 20% oxygen leads to Eg = 4.81 eV.

The Burstein-Moss effect was used to explain the increase in the band gap energy with a change in the concentration of current carriers. As a result, it was found that for films annealed in oxygen $\mu \approx 0.202$ m, for films annealed in argon $\mu \approx 0.414$ m, for films deposited in an atmosphere of 85%Ar + 15%O_2 $\mu \approx 0.470$ m, and in an atmosphere of 80%Ar + 20%O_2 $\mu \approx 0.481$ m. The estimationof the concentration of free charge carriers N showed that for films annealed in argon $N \approx 1.07 \cdot 10^{17}$ cm^{-3}, for films deposited in an atmosphere of 85%Ar + 15%O_2 $N \approx 8.81 \cdot 10^{17}$ cm^{-3}, and for films deposited in an atmosphere of 80%Ar + 20%O_2 $N \approx 5.09 \cdot 10^{18}$ cm^{-3}. We discuss our results.

Synthesis and properties of PVA-$CoFe_{1.97}Ce_{0.03}O_4$ polymer nanocomposite for methylene blue photodegradation

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Currently, organic substances present in water bodies are increasingly attracting the attention of environmentalists and are considered as dangerous pollutants. Traditional treatment facilities usually do not provide the required degree of purification, as they accumulate wastewater from industrial enterprises, agricultural effluents and household waste.

Since a huge number of organic compounds are used that affect the environment and humans, research in the field of using photocatalytic processes has advanced significantly. The development of new efficient photocatalysts is an important task.

In this work, a PVA-$CoFe_{1.97}Ce_{0.03}O_4$ composite was synthesized. The morphology and structure of the starting materials and the composite were characterized using scanning electron microscopy, X-ray analysis, and IR-spectroscopy. Magnetic parameters were measured using a vibration magnetometer. The photocatalytic activity of the obtained materials was carried out based on the results of measuring the absorption spectra.

The particle size is approximately 8-12 nm. In the X-ray pattern of PVA-$CoFe_{1.97}Ce_{0.03}O_4$, it was found that there are extended but easily identifiable peaks. A significant broadening of all diffraction peaks and their low intensity is observed. For the most intense peak at (2θ=40-70), the broadening of the peak to 3.1° full width at half-height is observed, which corresponds to the presence of nanosized PVA-$CoFe_{1.97}Ce_{0.03}O_4$ crystallites. In addition, the presence of cerium cations with a much larger radius is also evident. The X-ray pattern of PVA-$CoFe_{1.97}Ce_{0.03}O_4$ has small ferrite peaks. IR spectra showed the chemical interaction of polyvinyl alcohol and hydroferrite.

The results show that the pphotocatalytic properties of PVA-$CoFe_{1.97}Ce_{0.03}O_4$ composites in the methylene blue composition destruction reaction are 70-98%, depending on the reaction conditions.

Magnetocapacitance Effect in Tunnel Contact $Tb_{22-\delta}Co_5Fe_{73}/Pr_6O_{11}/Tb_{19-\delta}Co_5Fe_{76}$

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Increased interest in the study of magnetic tunnel contacts is due to the effect of tunnel magnetic capacitance (TMC), the value of which reaches several hundred percent in contacts with a barrier nanolayer of MgO. This allows us to talk about the prospect of practical application of the tunnel magnetic capacitance effect in memory elements and other spintronic devices. The TMC effect occurs in magnet/dielectric (semiconductor)/magnet tunnel contacts and its magnitude depends on the spin polarization of electrons in the magnet and the structure of energy levels in the barrier nanolayer. Large values of TMR and TMC in tunnel contacts with the Fe/MgO interface are related to the features of the electronic structure of the Fe/MgO interface, where the efficiency of spin-dependent tunneling is ensured by a good agreement between the crystal lattice parameters of the iron magnetic electrode and the crystal lattice parameters of magnesium oxide. Our work presents the results of research on magnetoresistance and the magnetocapacitive effect in $Tb_{22-\delta}Co_5Fe_{73}/Pr_6O_{11}/Tb_{19-\delta}Co_5Fe_{76}$ tunnel magnetic contacts with perpendicular magnetization of magnetic electrodes and a paramagnetic barrier layer. In tunnel contacts with perpendicular anisotropy of the electrodes, the antiparallel orientation of magnetization radically changes the distribution of the magnetic field in the contact barrier layer and causes the appearance of a high-gradient magnetic field in the direction of magnetization of the contact magnetic electrodes. Under the action of such a field, there is a spatial separation of spin-polarized major and minor electrons, which creates an inhomogeneous distribution of electric charge in the contact barrier layer. As a result, an additional energy barrier appears for major spin-polarized electrons, and an additional effective spin capacitance appears in the contact. Experimental values of tunnel magnetic resistance in $Tb_{22-}Co_5Fe_{73}/Pr_6O_{11}/Tb_{19-\delta}Co_5Fe_{76}$ tunnel magnetic contacts exceed 110%, and values of tunnel magnetic capacitance exceed 115%.

Negative capacitance and dielectric permittivity of nanocomposite films with semiconductor and metal nanoparticles

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Obtaining and investigation of nanocomposite films containing both semiconductor and metal nanoparticles embedded in a dielectric matrix or semiconductor nanoparticles embedded in a combined semiconductor-metal oxide may provide new functionalities, which would be strongly dependent on the matrix structure, composition, native defects etc., governing their electrical and optical properties.

The DC conductivity characteristics of the $SiAl_zO_xN_y$(Si) films at low voltages significantly differ from those of the SiO_xN_y(Si) films. The effect of the conductivity decrease with the increase of electric field at low voltages is observed for the films annealed both in nitrogen and argon atmosphere. At this, the decrease in conductivity with voltage is most pronounced for the $SiAl_zO_xN_y$ films annealed in nitrogen. Increase of the voltage (field) leads to the decrease of the conductivity to a certain value, after which it begins to rise.

To analyze the conductivity in this voltage range, we use the Richardson–Schottky expression for a solid state. Analysis of the experimental data shows that in our case the dielectric constant εr is negative at low voltages. Negative dielectric static constant was observed for some nanostructured materials. It is tightly related to the effect of negative capacitance in the low-frequency (< 1 MHz) region.

A qualitative model based on the peculiarities of electric field polarization of the films was proposed to explain the conductivity decrease with the increase of electric field. The important role is played by the interface traps at the Si nanoparticles – amorphous matrix interfaces that capture electrons. Negative dielectric constant originates from the negative charge trapped at the interfaces near the cathode region. The internal electric field increases the external field. The increase of the charge trapped at the Si nanocrystals – dielectric matrix interfaces explains the decrease of conductivity with the field growth.

Study of the effect of nano-sized zinc particles on formaldehyde emission in high-density chipboard

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According to the Food and Agriculture Organization (2020), the industrial production of wooden boards in the world reached 367 million m^3, the production of fiberboard, chipboard and OSB made up 250 million m^3 of them. Wood composite materials occupy a leading place in the field of construction, so it was interesting to investigate the effect of nano-sized metal particles on their characteristics. First of all, we are interested in reducing the release of formaldehyde, it is used in the composition of resins for better gluing of wood raw materials. According to research conducted by the National Academies of Sciences in Washington in 1980, it was found that free formaldehyde is a carcinogen and leads to myeloid leukemia, cancer of the nasal cavity, damage to bone marrow function, and other negative consequences. Free formaldehyde is released both during the pressing of wood-composite panels and during their further operation.

Since ZnO is used as part of analyzers to determine free formaldehyde, it was interesting to investigate the effect of metallic zinc nanoparticles on the concentration of formaldehyde in samples of chipboards. This study is interesting because depending on the size and degree of oxidation, the metal can have different effects on the final result.

With the help of the electro-spark method of manufacturing nanoparticles, we have the opportunity to obtain nanoparticles with a very small amount of oxide forms. Adhesive dispersion modified with 2%, 4% and 8% colloidal solution of zinc nanoparticles was used for research. The best results were obtained when using glue modified with 8% zinc nanoparticles, which was a reduction of formaldehyde emissions by 48% on the third day after pressing. Since there is information in the literature about the negative effect of zinc on the physical and mechanical properties of wood-composite materials, further research on the effect of a mixture of zinc nanoparticles with other metals, in particular aluminum, is necessary.

Synthesis and antioxidant activity of biocompatible β-cyclodextrin-stabilized aqueous sols of nanocrystalline ceria

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Nanocrystalline ceria (CeO_2 NPs) are well known for their application in various fields of industry, as well as in biology and medicine [1, 2]. Knowledge of synthesis schemes, physicochemical and morphological features of nanoscale CeO_2 is important for assessing their antioxidant behavior. In this study, β-CD@CeO_2 are synthesized via the simple co-precipitation method in alkaline media using unmodified β-cyclodextrin (β-CD) as a solubilizer and stabilizer agent. The properties of obtained NPs are studied using various methods of physical-chemical characterization such as UV−visible spectroscopy, Fourier-transform infrared (FTIR) analysis, transmission electron microscopy (TEM), dynamic light scattering (DLS) and thermogravimetric analysis. The characterization by TEM revealed β-CD@CeO_2 NPs with uniform spherical shape and average diameter of 5 nm. Average hydrodynamic diameter of β-CDs@CeO_2 NPs in aqueous solution according to DLS was 30.2 nm. These small β-CD@CeO_2 NPs have excellent colloidal stability. The reaction of the autoxidation of epinephrine to adrenochrome was used in order to determine the ability of NPs to inactivate superoxide radicals. We have found that β-CDs@CeO_2 have maximum activity at a concentration of NPs of 100 mg/l. Comparison of β-CD@CeO_2 nanoparticles with citrate-stabilized NPs has shown that presence of β-CD has no deteriorating effect on the antioxidant activity of nanoceria making these materials potent both as antioxidant agents and carriers of water-insoluble antioxidant molecules for obtaining of hybrid nanomaterials with improved antioxidant action.

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Antimicrobial properties of clinoptilolite doped with silver and zinc

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The antimicrobial properties of highly dispersed (particle size 100 ∓m) Ukrainian transkarpathian clinoptilolite (CL) composition with transition metal ions such as Ag^+ and Zn^{2+} (CL–Ag 1.05, CL–Zn 1.1, CL–Zn 2.2, CL–Ag 1.05–Zn 1.1) were studied. The concentration of metal ions in the compositions are: Ag^+ – 1.05 mg/g, Zn^{2+} – 1.1 and 2.2 mg/g.

Silver– and Zinc–containing zeolite materials have been prepared on the basis of clinoptilolite using ion-exchange reactions between zeolite and salt of a transition metal in a solid phase extraction mode. Compositions of zeolite with listed above zinc ions concentrations have been shown antimicrobial activity against gram-negative bacteria *E.coli* (20-40% survival) and yeast *C. albicans* (about 30%). Compositions of zeolite with silver ions in different concentrations have been shown significant antibacterial (survival of *E. coli* 0.1-1.2%) and antifungal (survival of *C. albicans* 0.2-1.2%) activity. The combination of zinc and silver ions in the composition based on clinoptilolite slightly increased the antimicrobial effect, delaying the growth of *E. coli* in the range of 0.04-1.1% and the yeast *C. albicans* from 0.1 to 1.0%.

Effect of temperature on the parameters of ion-selective electrodes obtained using different types of nanostructured materials – a comparative study.

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Solid contact ion-selective electrodes (SCISEs) are useful and often chosen measuring devices in potentiometry. Due to this, it is important to improve their construction to make the obtained results more accurate, precise and reproducible. One of the more frequently modified element of these electrodes is a solid contact (SC), which ensures the stability and reversibility of the potential [1]. In addition, it provides good ion-electron conductivity, faster charge transfer, which in turn improves other analytical parameters of electrodes, i.e. the membrane resistance and electrical capacitance of the double layer [2].

In the presented poster, it will be discuss the effect of temperature on the performance of potassium ion-selective electrodes, in which different nanostructured materials, i.e. perinone polymer, poly(3-octylthiophene) (POT) and multiwalled carbon nanotubes (MWCNTs) were used as the solid contact. SCISEs were prepared by covering glassy carbon disc electrode (GCE) with a layer of solid contact material and then depositing a membrane cocktail by the drop casting method. The control electrode was an unmodified membrane coated disc electrode.

For all prepared electrodes, the effect of temperature on parameters such as the slope of characteristic, range of linearity, limit of detection, stability and reversibility of the potential, long-term stability (E0) and selectivity towards Mg^{2+}, Na^+, Ca^{2+} ions was studied.

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Factors influencing the characteristics of porosity of ceramic materials

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In recent years, there has been a rapid increase in interest in the study of porous ceramic composite materials due to their excellent properties, such as high permeability, high temperature stability, wear resistance, high selectivity, corrosion resistance, and others. Due to their unique properties, ceramic membranes (separation of liquid and gaseous phases) have recently been increasingly used in industry, squeezing polymer membranes, in particular, in the process of industrial wastewater treatment. The use of ceramic materials involves the appropriate degree of their porosity, which can be achieved by using pore generating agent, varying the sintering temperature of membranes, using different methods of forming membranes and a wide range of pressing pressure, etc. Usually, the following materials are used as pore generating agent: carboxylic acids, carbonates, carbon materials (technical carbon, graphite), etc. In [1], macroporous bioactive glass ($CaO–SiO_2–P_2O_5$ system) was obtained using the sol-gel method, using granulated stearic acid as a pore generating agent. To prepare inexpensive microporous ceramic matrices, the authors [2] used: a mixture of Spanish clay, chamotte and starch. As pore generating agent, calcite was used in the amount of 15 – 20 wt.%. Studies [3] demonstrate the use of calcium carbonate as pore generating agent in a ceramic membrane based on kaolin, zeolite, and silica xerogel composites. It was established that the volume fraction of connected pores depends on the content of calcium carbonate. Research shows that the type of pore generating agent affects the porosity of ceramic materials, and by varying its content, the desired porosity and strength of the materials can be achieved.

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Electric charge accumulation at the interface of supramolecular clathrate MCM-41<CH_4N_2S<$CoCl_2$>>

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One of the biggest challenges for humanity today is the task of developing efficient technologies for accumulating and storing electricity. The electrochemical systems in use, which are divided into lithium-ion batteries and carbon supercapacitors, are unable to meet the rapid growth in energy consumption despite constant improvement and increase in their efficiency. Their main disadvantages are insufficient energy capacity, inability to be miniaturized and incorporated into microelectronics, and harmful environmental impact. Therefore, fundamental research in this area has become extremely relevant, which will allow us to offer a radically new approach to solving the problem of electricity storage. All studies are actually related to the development of the concept of quantum energy storage as an alternative to existing electrochemical ones. In this context, it is worth highlighting the work on the creation of a quantum supercapacitor, the energy intensity of which can approach the energy intensity of, for example, burning gasoline [1, 2].

To realize this concept, it is necessary to form nanostructured materials that, due to the large area of heteroboundaries and high dielectric constant, would accumulate an electric charge at the interface. Based on the experience from previous studies [3, 4], we have formed the supramolecular clathrate MSM-41<CH_4N_2S<$CoCl_2$>>, which demonstrates the ability to accumulate an electric charge at the interface. This is evidenced by the results of impedance and current-voltage studies. To understand the physical mechanisms of the observed phenomena, X-ray diffraction studies and studies of the structure of impurity energy levels were also carried out by measuring the currents of thermally stimulated discharge.

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Creation and some practical application of hybrid TiO_2 and SiO_2 sol-gel nanocomposites

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Multifunctional hybrid TiO_2 and SiO_2 nanocomposites (films, powders) with new, unusual, properties are attracting a lot of attention as the latest nanomaterials for use in various areas of opto- and nanoelectronics, catalysis, biosensorics, fuel cells etc. Significant progress in this direction was achieved thanks to the application of controlled sol-gel synthesis, which opened up new technological possibilities for the creation of such materials.

The hybrid TiO_2 and SiO_2 sol-gel films with a high concentration of dyes, having a dimer fluorescence output of 36 times more than that of solutions have been created. The results of the tests obtained hybrid films showed the possibility of creating on their basis components of integral optics (elements of optical memory, planar waveguides) [1].

Tests of proton conductivity of the composite membrane Nafion/TiO_2 has highlighted the benefit of doped titania nanocomposites introduction on the conductivity in the temperature range up to 240 °C, that maintained at 10^{-5}-10^{-2} S/cm, compared to the commercial Nafion membrane. It may be a prerequisite for effective behavior in conditions close to operating conditions of fuel cells.

It was shown that obtained TiO_2 nanocomposites significantly improve the main operational parameters of laccase-based electrodes when compared with controls. The developed bioelectrodes were tested for phenol analysis in real communal wastewater samples spiked with these analytes, demonstrating the high accuracy of the assay [2].

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Viscoelastic properties of polymeric and nanocomposite proton conductive membranes for fuel cells

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For successful operation in fuel cells proton conductive membranes must have a number of characteristics including mechanical strength.

We synthesized polymeric and nanocomposite proton conductive membranes based on acrylic monomers and sol-gel systems by UV-polymerization in the presence of 2 mass % of photoinitiator and determined their viscoelastic properties by DMA (Table 1). Feed compositions for membrane syntheses were as follows: SSNa – acrylonitrile (AN) : acrylic acid (AA) : potassium styrene sulfonate (SSNa) : ethyleneglycole dimethacrylate (EGDMA) = 44 : 14 : 20 : 20 mass %; SSNa/SG – to the same feed composition 10 mass % of sol-gel precursors (TEOS and MAPTMS) were added.

Table 1. Viscoelastic properties of the membranes

Membrane	T_g (°C)	tan δ_{max}	E′ (MPa) (25°C)	E′ (MPa) (200°C)
SSNa	176	0.31	4393	130
SSNa/SG	179	0.32	3928	122

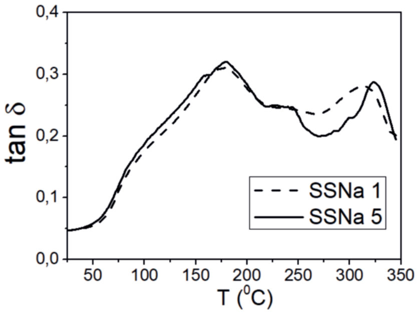

Fig. 1. tan δ_{max} *vs temperature*

The introduction of silica makes the structure of the composite more rigid, leads to an increase in Tg, a decrease in the values of the modulus of elasticity and the loss modulus for the membrane. This can be interpreted as a weakening of intermolecular bonds and a decrease in the packing density in the polymer matrix.

The features of nanostructure formation in lithium aluminum silicate glass-crystalline materials

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Nanostructured glasses and vitreous materials based on them are one of the promising nanomaterials [1]. During the synthesis of nanostructured glass-crystalline materials, the main aspect is the provision of volumetric uniform finely dispersed crystallization, in particular, due to the implementation of the liquation mechanism of nucleation. The appearance of secondary delamination, as a stage of heterogeneous nucleation of crystal centers, is associated with the formation of stabilized clusters – heterophase fluctuations that form a self-organizing nanostructure [2].

The features of nanostructure formation in the developed lithium aluminum silicate glass-crystalline materials at the initial stages of nucleation and their influence on the formation of a self-organized sitalized structure were analyzed [3]. The influence of the thermal background of the developed glasses on their structure during heat treatment was determined. The mechanism of phase formation in the glasses of the $K_2O – Li_2O – RO – RO_2 – Al_2O_3 – B_2O_3 – P_2O_5 – SiO_2$ system was determined, consisting in the flow of volumetric finely dispersed glass crystallization due to the intensive formation of lithium metasilicate nucleators (T=550÷580°C) in the form of spherulites; the formation of crystals of lithium metasilicate or β-eucryptite (T=630÷650°C) and their recrystallization into stable lamellar crystals of disilicate (T≈820°C) of β-spodumene columnar-flat prismatic habit (T=850°C), which are strongly connected. The developed glass-crystalline materials form a dissipative sitalized structure by the mechanism of phase separation under conditions of low-temperature heat treatment, which allows to ensure their high operational properties and can be recommended for structures to protect special equipment and devices.

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Structuring and viscoelastic properties of polyurethanes, doped with aerosil nanoparticles and activated by xanthene dyes

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Among the main problems found in the polymer solid-state dye lasers, there are degradation of the dye organic molecules in the polymer matrix and negative consequences of the dye aggregation processes on the material stability and optical characteristics. One of the methods, allowing diminishing these effects is incorporation of different inorganic dopants into the polymer medium, in particular, aerosil nanoparticles. Nanoparticle introduction into the polymer host was shown to improve the dye photostability and luminescence intensity [1].

However, the development of laser elements, operating under conditions of powerful radiation, requires polymers of high elasticity, which ensures their strong beam resistance. Most polyurethanes possess high polarity and elasticity, but the insertion of organic dyes and inorganic nanoparticles can significantly affect the chemical structure, dynamic and viscoelastic characteristics of these matrices.

This work contains the investigations of the structure, dynamic and viscoelastic properties of the dye-activated and aerosil-doped polyurethanes by means of the IR-spectroscopy, dynamic-mechanical analysis and electron paramagnetic resonance methods for different nanoparticle concentrations and dye functional groups. In the presence of dyes, the self-association of urethane groups within the polyurethane rigid segments prevails and the interactions of these groups with the flexible oligoether components decrease. This promotes the mobility growth of the flexible parts. The obtained data are consistent with the drops in the glass transition temperature and modulus of elasticity for dye-doped polyurethanes.

In conclusion, the presence of both dye and aerosil nanofiller has a positive effect on the polymer mechanical properties, which ultimately improves the stability of the corresponding laser elements as a whole.

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Silica based inorganic–polymer hybrid materials for remove toxic ions from wastewater

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Environmental pollution has become one of the most severe problems, which is harmful to human health and ecological systems. Various methods such as chemical precipitation, membrane filtration, ion exchange, electrochemical processes, chemical coagulation and adsorption have been utilized to remove heavy metals from wastewater. Among these methods, adsorption is known to be the most efficient method. A large number of natural and synthetic materials have been used for the adsorption-based removal of heavy metals from wastewater. These materials include zeolites, clays, biosorbents and silica.

This work is devoted to the synthesis and study of the sorption properties of silica gel with adsorbed copolymer 5-(4`-nitro)-phenylazo-8-methacryloxyquinoline with methyl methacrylate (3:1), poly(aminostyrene) and poly(oxystyrene) modified with boc-S-benzyl-L-cysteine on Cu (II), Cd (II), Pb (II) and Fe (III) ions.

The fact of adsorption of the copolymer and polymers on the silica surface was confirmed by the methods of IR spectroscopy and thermogravimetric analysis. The amount of copolymer in the synthesized composite according to the thermogravimetric analysis is 25%.

From the analysis of CEM-photo it was established that the copolymer on the silica surface is mainly in the form of convex agglomerates and does not significantly affect the structure of the surface of the silica gel. By comparing the sorption properties of the modified and the original silica, it is found that as a result of the modification, its sorption properties are improved with respect to the Cu (II), Cd (II), Pb (II) and Fe (III) ions.

Synthesis And Sorption Properties Of Hybride Composite Materials Based On Saponite And Copolymer 5-(4`-Nitro)-Phenylazo-8-Methacryloxyquinoline:Mma

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Recently, numerous approaches have been studied for the development of cheaper and more effective technologies, both to decrease the amount of wastewater produced and to improve the quality of the treated effluent. Adsorption has become one of the alternative treatments, in recent years, the search for low-cost adsorbents that have metal-binding capacities has intensified. The adsorbents may be of mineral, organic or biological origin, zeolites, agricultural wastes, biomass, and polymeric materials. For this purpose, it is advisable to use natural porous minerals, in particular saponite clay.

This work is devoted to the synthesis and research of the sorption properties of polymer-inorganic composites based on adsorbed copolymer 5-(4`-nitro)-phenylazo-8-methacryloxyquinoline with methyl methacrylate (3:1) on the saponite surface of the Tashkiv deposit to ions Pb(II), Cd(II), Cu(II), Fe(III). The fact of immobilization of copolymer on the saponite surface was established by comparative analysis of the IR spectra of the modified and the original saponite. The amount of adsorbed polymer in the synthesized material according to the thermogravimetric analysis is 24.65%.

Using the results of low-temperature adsorption-desorption of nitrogen and scanning electron microscopy, changes in the morphology of the saponite surface after adsorption of poly[8-oxyquinolinemethacrylate] by the selected methods are shown.

The sorption characteristics of the synthesized composites with respect to Cu(II), Pb(II) and Fe(III) ions were investigated in static mode. It was established that as a result of the physical adsorption of the copolymer on the saponite surface, its sorption capacity for Cu(II) ions increases by 3.47 times compared to the original carrier, for Pb(II) ions - by 1.5 times, and for Fe(III) ions – 6 times, and for Cd(II) ions – 10 times.

Facile and environmentally friendly synthesis of transition metal phosphides based nanocomposite electrocatalysts for hydrogen evolution from water

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Transition metal phosphides and their nanocomposites are considered to be one of the most promising Pt-free hydrogen evolution reaction (HER) electrocatalysts. At the same time, obtaining of nanocomposite electrocatalysts based on d-metal phosphides is often a complex and multi-stage process, and also requires the use of environmentally hazardous phosphorus compounds. We have proposed a universal approach to obtaining nanocomposite electrocatalysts for hydrogen evolution from water based on d-metal phosphides (Co, Ni, Mo, Fe, V) and N, P-doped carbon. The approach involves the pyrolysis (at 900ºC in an inert atmosphere) of H_3PO_4-doped polyaniline together with the salt of the corresponding metal. The proposed approach has advantages such as the simplicity of its implementation, the low cost of the initial reagents and the absence of toxic compounds among them.

The formation of phosphides in the obtained composites has been confirmed by X-ray phase analysis, regardless of the type of d-metal (except for vanadium, where nitride phosphide was formed). It has been found that FeP, MoP, and V_5NP_3 are the sole metal-rich crystalline phases in their respective hybrid materials. However, in the case of Co- and Ni-containing composites, a coexistence of two phases is observed (Co_2P as the dominant phase along with CoP; Ni_2P as the dominant phase along with $Ni_{12}P_5$).

The ability of all the obtained nanocomposites to exhibit electrocatalytic activity in the HER has been determined in 0.5 M H_2SO_4 and 1.0 M NaOH aqueous solutions. However, the type of phosphides in the composite materials, which serve as the main active sites in HER, significantly influences the efficiency of electrochemical hydrogen evolution from water. It has been demonstrated that the most effective electrocatalyst in acidic electrolyte is based on Ni_xP_y (with a Tafel slope, b~60 mV/dec and an overpotential at 10 mA/cm$_2$, η_{10}~150 mV), while in alkaline electrolyte, the catalyst based on MoP shows the highest efficiency (b~84 mV/dec and η_{10}~126 mV). Based on the determined b values (55-109 mV/dec) for the synthesized catalysts, it can be suggested that the hydrogen evolution proceeds via the Volmer-Tafel mechanism.

2D magnetic Freedericksz transition in a rectangular cell of a ferronematic filled with spindle magnetic nanoparticles

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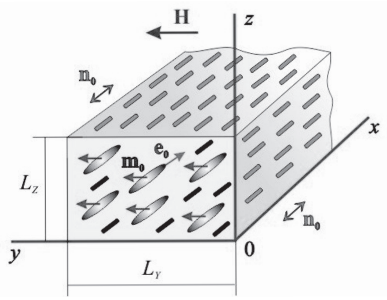
We theoretically investigated the magnetic field-induced Freedericksz transition in a rectangular cell filled with a ferronematic (FN). As the latter, we considered a suspension of hematite spindle-like magnetic nanoparticles in a nematic liquid crystal [1]. The main feature of this magnetic impurity is that magnetic moments of the elongated spindle nanoparticles are oriented perpendicularly to their main axes.



The original texture of the rectangular ferronematic cell is shown in the figure. We suppose that the diamagnetic susceptibility of the nematic matrix is positive. We also assume that planar boundary conditions for the nematic director **n** are specified on cell walls (parallel to *x* axis) and on surfaces of the nanoparticles (parallel to main axes). As a result, in the absence of a magnetic field, the initial director $\mathbf{n}_0$ and the unit vector $\mathbf{e}_0$ of the average orientations of the nanoparticles main axes are lie along the x axis.

The magnetic field **H** is directed along the y axis. This field interacts both with magnetic particles (dipole interaction) and with nematic matrix (quadroupole interaction). In the weak field regime, the dipole mechanism dominates and the cell is magnetized along the field direction (or along the unit vector $\mathbf{m}_0$). Due to the additional coupling interaction between nanoparticles and nematic matrix, which is characteristic of FN, the initial uniform orientational state of the cell is stabilized. As the field strength increases, the quadrupole mechanism is activated, which tends to orient the nematic director also along the field. At the some critical field, 2D orientational deformations of the cell arise. We found this critical Freedericksz transition field and determined its dependence on material parameters of the nematic matrix and the magnetic nanoparticles, as well as on cell sizes.

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Nanomaterials on the base of acid-activated bentonite clays and its applications for environmental protection

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Acid activation of bentonite clay is a common method of obtaining porous sorbents for organic and inorganic substances, acid catalysts. At the initial stage of acid activation, exchangeable cations are replaced by hydrogen ions with the formation of H-bentonite. Already at the early stages of activation, a significant amount of exchangeable ions is removed, and the release of structural cations from the crystal lattices of clay begins. Then, depending on the acid concentration, structural cations are washed out in the following sequence: $Mg^{2+} > Fe^{2+} > Fe^{3+} > Al^{3+}$ [1].

Nanomaterials on the base of the natural clay mineral of Cherkasy deposit bentonite were carried out by nitric and hydrochloric acids treatment. Nitrogen sorption-desorption isotherms for all samples have a waveform and belong to type II isotherms according to the IUPAC classification. In the range of values of $p/p0 > 0.35–0.4$, well-defined hysteresis loops are observed on the isotherms, which indicates the presence of a well-developed structure of H3-type meso- and macropores characteristic of such samples. In acid-activated bentonite, as a result of the partial dissolution of its oxide structure, the porosity changes significantly, and the specific surface area increases by more than three. The X-ray diffraction spectrum of acid-activated bentonite samples undergoes significant changes only in the region of small reflection angles. At the same time, there is both a decrease in the relative intensity of reflexes and an increase in the reflection angles. Longer acid treatment leads to disruption of the structure of the bentonite phase.

Feature of purification of contaminated water from radionuclides uranium, cesium, and strontium by acid-activated bentonites was presented in a wide range of concentrations. It was established that acid activation of bentonite clay significantly increases sorption characteristics for cesium ions.

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Structure and physical properties of multicomponent films based on the Fe-Si-B system

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There were investigated by the methods of X-ray diffraction analysis, electron microscopy, magnetic measurements, and plotting the temperature dependences of electrical resistance (ER) the conditions for the formation of metastable structures and phase transformations in multicomponent films $Fe_{73}Si_{15,8}B_{7,2}$-$(Cu, Nb)_4$ (composition 1) and films $Fe_{78,5}Si_6B_{14}$-$(Ni, Mo)_{1,5}$ (composition 2) obtained by three-electrode ion-plasma sputtering.

In the freshly deposited state, in films of composition 1, an amorphous structure was recorded, characterized by a blurred halo corresponding to the CSR size $L \approx 1.6$ nm. In films of composition 2, a nanocrystalline structure with a CSR size of $L \approx 12$ nm is fixed. At 843K, the beginning of the decay of metastable structures is observed with the appearance of a supersaturated solid solution of α-Fe. The activation energy of the relaxation processes of the initial metastable structures was estimated from the temperature dependence of reaching the maximum value of the relative change in electrical resistance (R/R_0), assuming that the maximum values of R/R_0 for a single-phase interval, achieved at different heating rates, correspond to the same degree of relaxation of the structure. The values of activation energy calculated by the Kissinger method are 10400 ± 1200 K. The obtained value is four times lower than the values of activation energy and the average diffusion coefficient in the $Fe_{40}Ni_{40}P_{14}B_6$ alloy quenched from the liquid state (43000 K), determined kinetic parameters.

This difference is explained by the two-dimensionality of the films under study as compared to quenched from the liquid state foils. The coercive force (HC) of freshly deposited films of compositions 1 and composition 2 is twice as high as the HC of pure iron films. After heating films of composition 2 to 893K, HC decreases by 1.2 times, and in films of composition 2 by 1.5 times, which is explained by the establishment of the optimal ratio between particles of nanocrystalline α-Fe and amorphous phase residues.

The effect of cobalt ions on the recharging of nanoparticles of cobalt ferrous ferrite and lepidocrocite in suspensions

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The development of methods for obtaining nanosized particles of metals and their compounds, including iron and cobalt, remains relevant due to their unique magnetic, antibacterial, antifungal, anticancer, catalytic, etc. properties. Both surface charge and ζ-potential are important characteristics that determine the stability of nanofluids based on these nanoparticles, their use in wastewater remediation processes, and allow us to draw additional conclusions concerning the mechanisms of their formation.

We obtained nanosized particles of cobalt ferrous ferrite, and lepidocrocite in a presence of cobalt (II) chloride in $Fe_0(St_3)$-H_2O-O_2-$CoCl_2$ system [1]. The cobalt ferrous ferrite particles exhibited irregular shapes with sizes ranging from approximately 20 to 60 nm. We determined the electrokinetic potential of the particles using the microelectrophoresis method in the presence of cobalt (II) chloride as a non-indifferent background electrolyte or sodium chloride.

In the presence of NaCl background electrolyte, we observed a characteristic pattern of particle recharging. In the presence of non-indifferent $CoCl_2$ electrolyte, for both cobalt ferrous ferrite and lepidocrocite phases, both cobalt ferrous ferrite and lepidocrocite phases exhibited positive ζ-potential values across the measured pH range of 5-10 without recharging. The obtained ζ-potential values showed no significant variations throughout the entire pH range, likely attributed to the adsorption of Co^{2+} ions on the particle surfaces, compensating for changes in ζ-potential caused by pH fluctuations.

The slight changes in the ζ-potential range suggest a minor compression of the diffuse part of the electric double layer, indicating that the electrokinetic dispersion factor is not the primary determinant in this case. Consequently, we conclude that other stability factors, primarily hydration, play a more significant role in maintaining the colloidal stability.

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Cerium titanate thin films: synthesis and characterization

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Development of new semiconductive materials with unique physicochemical properties is important task of chemistry and physics. Metal titanates present the solid complex structures containing the common bonds between the metal ions ([-M-O-Ti-]) that are responsible for the differed on bare metal oxides electronic and surface properties.

In this research, three-layered films with Ce:Ti=1:1 ratio were synthesized by sol-gel method. The different treatment temperatures of the films' layers were applied to find out the optimal conditions for cerium titanate crystallization. It is shown that the preliminary treatment of interlayered coatings at 300°C leads to crystallization of CeO_2 (10-15 nm) and anatase (2-6 nm), whereas CeO_2 (10-15 nm), Ce_2Ti_2O7 (16-21 nm) and anatase (4-9 nm) are formed at 600°C. The XPS data indicate that the films' surface contains in 3-4 times higher atomic content of Ti than Ce that are present in different oxidation states (Ce^{3+} and Ce^{4+})

The effect of phase composition on the band gap energy values and the potentials of the conduction and valence bands is shown by photoelectrochemical investigation. The band gap energy of the films contained CeO_2&TiO_2 and CeO_2&$Ce_2Ti_2O_7$&TiO_2 corresponds 2.9 eV and 3.0 eV, respectively, whereas TiO_2 is characterized by 3.2 eV. The cathodic shift of the conduction band potentials is observed for cerium-contained films compared to TiO_2. Photocurrent quantum yield at λ=400 nm is increased in 2-4 times for CeO_2&$Ce_2Ti_2O_7$&TiO_2 compositions compare to CeO_2&TiO_2.

The higher activity of electrocatalytic hydrogen evolution process is fixed for CeO_2&TiO_2 films compare to CeO_2&$Ce_2Ti_2O_7$&TiO_2 ones that is connected to the electronic structure of the crystalline phases.

Electrical and electrodynamic properties of polymer composites with nanocarbon filler

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The work presents the results of complex investigations of electrical and electrodynamic properties of polymer composites (PCs) based on polychlorotrifluoroethylene with nanocarbon fillers. As fillers thermoexfoliated graphite (TEG) and multiwalled carbon nanotubes (MWCNTs) have been used.

PCs have been obtained by a two-stage method, in the first stage of which the nanocarbon filler has been dispersed in an alcoholic medium (ethyl alcohol). At the second stage, the necessary amount of powdered polychlorotrifluoroethylene (spherical aggregates with a diameter of $d \sim 200$ nm) has been added to the dispersion of ethyl alcohol - nanocarbon. The mixture, with constant stirring, has been heated to a temperature not higher than 640 K until the alcohol was completely removed. Bulk specimens for the study of electrical and electrodynamic properties have been made from powdered PCs by the method of thermal pressing.

In the work, studies of the concentration and temperature dependences of the conductivity on direct and alternating current for PCs with different nanocarbon fillers have been carried out. Also, the concentration and temperature dependences of the real and imaginary components of the complex dielectric constant have been analyzed. The frequency dependences of the attenuation coefficient of electromagnetic radiation (EMR) and the standing wave coefficient for PCs with filler content from (2.5 to 5) % mass in the temperature range from 293 K up to 373 K have been also studied in detail.

Conducted studies have shown that electrical transport in the investigated PCs occurs both due to direct contacts between filler particles and contacts through thin polymer layers. The reproducibility of the conductivity value after thermal cycling indicates the absence of irreversible changes in the microstructure of PCs upon heating and a high level of polymer-nanofiller interphase interaction. High stability of electrodynamic characteristics in the temperature range of (293 – 373) K has been also established. A slight improvement in the shielding characteristics has been revealed, mainly due to an increase in the EMR absorption coefficient at heating studied PCs up to temperature of 373 K.

Nanofilled fluoropolymers for tribological purposes

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Fluorine-containing polymers are one of the best materials used in friction units of machines and mechanisms. Due to their unique properties (low coefficient of friction, high level of wear resistance, wide range of working temperatures, high chemical resistance, etc.), such materials are increasingly intensively displacing traditional materials for tribological purposes as metals and their alloys. Among the disadvantages of fluoropolymers should be attributed their low level of physical and mechanical properties, which is improved by filling with reinforcing fillers, preferably nanosized.

Polytetrafluoroethylene, polyvinylidenefluoride, and a copolymer of tetrafluoroethylene and ethylene were used as fluoropolymers in this work. Micro- and nano-sized amorphous silicon dioxide (silica gel) are used as fillers [1].

The filling took place both according to the traditional method of mechanical combination of the original components of the composition, and with the help of in situ combination in the process of synthesis of the filler

According to the obtained results, the materials obtained by in situ combination of initial components have a 10-20% better level of physico-mechanical, thermophysical and tribological properties than those obtained by standard methods. This happened due to the change in the morphology of the filler and its better distribution in the volume of the polymer matrix, as well as the creation of fillers with a main particle size of up to 100 nm [2,3].

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The Comparison of Intercalation of Li Atoms in SnS_2 Anode of Battery and $TaSe_2$ Anode of Battery: ab initio Calculation

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Motivated by the broad need to develop battery-based energy storage technologies, ion intercalation into materials suitable for these applications has been pursued intensively in recent years. Layered transition metal dichalcogenides featuring a Van der Waals interlayer coupling are capable of hosting ions in its various interstitial sites, making transition metal dichalcogenides an important class of electronic materials for ion intercalation studies [1]. In all these studies, however, the process of Li ion intercalation and its effect on the electrical transport in the thin crystal were not studied in detail [2-3]. In order to minimise the disadvantages in the manufacture for anode materials, it is necessary to use in advance a computational experiment, which is based on quantum calculation from the ab initio.

Applying the methods of the functional of electronic density and ab initio pseudopotential, we carried out computational experiments on atomic models that reproduced the 2-D layered structure of SnS_2 and 2-D layered structure of $TaSe_2$ with intercalated Li atoms. We have obtained the spatial distribution of the density of valence electron, the total energy, the energy barriers of migration of Li atoms in the interlayers of SnS_2 and of $TaSe_2$. Such a transfers was investigated at various degrees of the interlayers spatial SnS_2 and $TaSe_2$ of metal atoms. The comparison distributions of the density of valence electrons, the energy barriers of migration of Li atoms in the intermediate layer SnS_2 are compared and migration of Li atoms in the intermediate layer $TaSe_2$ are compared.

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The effect of defects of various genesis on the properties of carbon nanotubes

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Unusual electrophysical properties of carbon nanotubes cause their extensive research in various directions. The electronic properties of individual CNT particles and the composite or material consisting of such structures differ: they depend on the amount of contact between neighboring particles and the presence and composition of impurities in them. Therefore, it can be assumed that in such structures and composites contact phenomena play the main role in determining certain properties.

Optimizing the properties of materials is widespread in materials science because it contributes to the improvement of the properties in the desired direction.

Mechanical deformation and defects are affecting the electronic structure, concentration of charge carriers, electrical, emission, and other properties of CNTs. Defects occur both in the process of synthesis (growth and gas impurities) of CNTs, and in the event of external influences, especially radiation exposure. They deviate the shape of CNTs from a straight line, change the conditions of current flow, affect the concentration of charge carriers, the Fermi energy, and electrical conductivity.

Edge dislocations in CNTs almost double the interlayer distances in the dislocation core, which leads to a downward shift in the energy diagram of dimensional quantization levels, causes them to “capture” free electrons, and thus opens conduction channels for charge carriers that are inside the CNTs, which causes an order of magnitude increase in radial electrical conductivity and the appearance of quantum oscillations during deformation.

Each of the topological defects of graphene layers of different genesis (growth and radiation) deviates the shape of CNTs from a straight line and forms a topological disorder that reduces electrical conductivity and increases the thermo-EMF coefficient. The combined effect of defects of different genesis, or the irradiation dose, reduces the curvature of the shape of nanotubes, which indicates the interaction of topological defects and their "healing" as a result of the recombination of knocked-out the carbon atoms with vacancies.

Organic nanostructures for the creation of sensitive elements of explosive substances

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In the modern world, the threat of military conflicts is constantly increasing, as a result of which the problem of detecting ultra-low quantities of explosives at a distance or in difficult conditions is becoming an urgent problem. The detection of traces of explosives is actively researched by scientists [1]. A serious danger is created by explosive substances, in particular RDX (hexogen), PETN (penthrite), NG (nitroglycerine), TNT (trinitrotoluene), and NMH (octogen), most of which contain nitro groups. Therefore, many known detection methods are not aimed at finding specifically explosive substances, but at groups containing nitrogen [2].

On the basis of known liquid crystal materials with a wide temperature range of mesophase existence and a stable spiral pitch, new liquid crystalline mixtures based on E7 nematic and CB15 cholesteric impurity, doped with single-double and multi-walled nanotubes were created. The concentration of nanotubes is up to 0.7%. Obtained spectral characteristics of mixtures doped with nanotubes, which are characterized by a minimum transmission at a length of 600 nm, and shifts to the long-wavelength region with an increase in the concentration of substances containing nitro groups. These mixtures can be used as a sensitive element of sensors for detecting explosive substances. A model of an optical sensor for the detection of nitro groups during the storage of explosive substances has been developed.

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Dielectric properties of heterogeneous polymer systems with nanosized metal fillers

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The influence of fillers of different nature in the process of obtaining polymer composite materials (PCM) is given considerable attention, since the choice of the type of filler in PCM makes it possible to obtain systems with predetermined dielectric and physical-mechanical characteristics. Given the lack of a single theory of the influence of the type of filler on PCM characteristics, the study of the properties of such systems is of considerable theoretical and practical interest.

A linear flexible polymer - polyvinyl chloride (PVC) with a Fikincher constant of 65 was chosen as the object of research. As a filler, nanodispersed copper with characteristic dimensions of 31÷39 nm was used, obtained by two different methods: the electrochemical method and the method of electrical explosion of the conductor. Samples for research were obtained in the P-mode in the range of filler concentrations from 0.05 to 5 volume percent. The concentration and frequency dependence of the real component ε' and the value of dielectric losses tgδ was performed in the frequency range from 100 Hz to 100 kHz using a measuring capacitor cell.

According to the results of experiments conducted on systems formed with different filler content, its concentration and production method affect the processes of structure formation in PCM, which is reflected in a significant change in the entire complex of physico-mechanical and dielectric properties of polymers. The characteristic dependences between the values ε', ε'' and tgδ, the content and type of filler in the system and the frequency of the external field acting on it are established.

As a result of the conducted research, the peculiarities of the concentration and frequency dependence of the dielectric constant value, dissipative energy losses of PCM with metal filler obtained by various methods were established and analyzed. It is shown that the electrical relaxation in such systems is nonlinear in nature. It has been established that the effectiveness of the filler depends on the content and method of its production.

Development of the High-Voltage Electrodischarge Method for Obtaining Carbon Nanomaterials from Carbon-Containing Gases and Liquids

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Electrodischarge processing of carbon-containing gases is widely used to obtain carbon nanomaterials of various structures and purposes. This method has a number of disadvantages, the main of which is that when a certain power of the electric discharge is reached and/or its constant increase, the productivity grows more slowly or stops growing altogether, which leads to an increase in specific energy consumption per mass unit of the output product. Also, with an increase the length of the working gas gap, in which the gas is processed by plasma, the power of the electric discharge installation for obtaining nanomaterials can be increased. This effect is shown in [1]. However, the discharge gas gap cannot be more than 30-40 mm due to the fact that the breakdown voltage of a gap will be 60-80 kV, which can damage the equipment and is unsafe. The instability of the process also increases due to fluctuations in the length of the plasma column caused by the flow of gas inside the reactor.

Therefore, the **aim** of this work is to find a way to increase the productivity of carbon nanomaterials at a constant specific power consumption of high-voltage installations for the electric discharge treatment of carbon-containing gases without increasing the length of the interelectrode gap.

The **main idea** of the work is that in order to increase the productivity of carbon nanomaterials at a constant length of the interelectrode gap, it is necessary to increase the density of the treated substance in the reaction zone during the electrodischarge processing. This can be achieved either by increasing the pressure of the carbon-containing gas or by using a carbon-containing liquid. These two methods will be described in this work.

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The influence of the thickness of films with ferrite nanoparticles on the characteristics of adjustable microwave composite filters

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Magnetically adjustable microwave filters consisting of a bulk non-magnetic dielectric cylinder with a high Q-factor and a composite film containing nano-sized particles of nickel ferrite have been manufactured. $BaTi_4O_9$ was used as the non-magnetic component of filters and a composite consisting of photopolymer matrix including ferrite particles.

Nanosized particles of nickel ferrite were synthesized by the citrate sol-gel method and characterized by XRD, TEM method. Ferrite particles were mixed with Permabond UV-630 photopolymer and applied to the ends of dielectric cylinders and exposed to ultraviolet light. Filters with films 50, 80, 100, 200 nm thick were manufactured. The resulting structures were investigated using an Agilent N5230A PNA-L network analyzer to obtain their transmission spectra.

X-ray diffraction patterns showed the formation of single-phase spinel after heat treatment at $T = 1173$ K. The average diameter of the particles was 85 nm. Despite the small volume of ferrite films there are steep field-driven peaks on the spectra of the filters. The external magnetic field changes the resonance frequency and peak absorption.

According to classical electrodynamics, the frequency shift should be proportional to the volume fraction of the ferrite component. The frequency shift of the obtained filters increases with the increase in the thickness of the ferrite film from 0.6 MHz for a 50 nm film to 26 MHz for a 100 nm film. Increasing the film thickness to 200 nm practically did not affect the frequency shift. The reason must be investigated.

The described heteromaterial filters can be used as a new smart adjustable component base for classical ferrite devices (filters, circulatiors, generators, etc.).

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Effect of supporting layer on electrical characteristics of field-effect transistor based on reduced graphene oxide film

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Graphene is considered to be a promising material for various fields of practical application. The unique properties of graphene as a gapless semiconductor are due to the conical shape of the electronic spectrum of the hexagonal structure of the sp^2-bonded carbon monolayer [1]. In particular, the Fermi level position and, as a result, the ambipolar conductivity of graphene can be controlled by an external electric field. This property of the carbon monolayer is used to create a new type of field-effect transistors (FETs) with graphene as a conductive channel material [2]. The efficiency of graphene FETs significantly depends on the quality of the supporting dielectric layer and its interface with the graphene film [3]. Therefore, the study of various types of supporting layers and the peculiarities of using reduced graphene oxide (RGO) film may be promising for simplifying the technique of manufacturing graphene FETs.

In this work, RGO-based FETs with SiO_2 and a porous silicon layer as the supporting dielectric were created. The porous silicon layer was additionally subjected to thermal treatment. The quality of the supporting layers was researched using thermal activation spectroscopy and volt-farad characteristic measurement. The electrical properties of the FETs based on RGO film were studied in both DC and AC modes. A significant influence of the supporting layer and silicon substrate on charge carrier transfer processes in the RGO-based FETs was found.

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Influence of helicon discharge plasma on the IR characteristics of AlN films on flexible polymer substrates

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Thin films AlN synthesized on flexible polymer substrates in a helicon-arc ion-plasma reactor demonstrate effective blocking of IR radiation [1,2]. The spectral characteristics of these films are determined by their composition, structure and its perfection, and also depend on their thickness. In the synthesis of AlN films by vacuum-arc discharge deposition with the addition of chemically active nitrogen gas, the technological conditions of their production have a significant impact on the blocking properties of the films. An important step in the synthesis of AlN is the activation of the film surface by the plasma component of the gas immediately before the formation of the nitride coating in an RF helicon discharge with ultra-high density plasma (up to ~10^{12} cm^{-3}) and high energies of ion flows (up to ~30 eV), which are accelerated in the self-consistent electric fields of the plasma. AlN synthesis is carried out on the surface of the substrate through the chemical reaction of Al atoms and ions with the excited atomic and partially ionized nitrogen component.

In the helicon-arc unit, two plasma sources operate simultaneously: helicon and vacuum-arc. This allows for effective influence on surface processes on the substrate. The addition of a helicon plasma flow to the substrate increases the fraction of the ionic nitrogen component, which intensifies the processes of AlN synthesis and changes the structure of the film, in particular, leads to its texturing. The effect of an additional helicon plasma flux on the structure of AlN films and their spectral characteristics in the infrared range (2-25 μm) was investigated. A change in the structure of these films under the influence of an additional flux of helicon plasma and a change in the characteristics of the Reststrahlen band were found.

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Photoluminescence efficiency of the composite system Si - nanocrystalline CdTe

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Upon incorporation of nanocrystalline (NC) CdTe into Si, an increase in the photoluminescence (PL) of Si was found due to the formation of a heterojunction, which ensures the injection of charges into the bulk of Si.

The dependence of the PL intensity of the “porous Si (PSi) – CdT NC” composite system on the morphology of the PSi surface and the conditions of deposition of a colloidal solution of CdTe NC on the porous surfaces of n-type Si wafers oriented in the (100) direction was studied. PSi layers were formed by electrochemical etching with the formation of pores with a diameter of 2.5 μm, a depth of 20–30 μm, and a density of 10^6 cm^{-2} and by chemical etching with the formation of smaller pores with a larger diameter and lower density.

The measurements showed that, during the deposition of CdTe NC in PSi with a small pore diameter (2.5 μm), the radiation efficiency per unit surface area turned out to be lower than for a matrix with larger pores i.e. NC penetration occurs more efficiently in pores with a large diameter. This is probably due to the incomplete filling of pores due to the difficulty of penetration of CdTe NC into smaller pores due to the presence of an adsorption layer of a stabilizer on the NC surface, which is used in the colloidal synthesis of NC in order to increase the resistance to aggregation and sedimentation. The reason for the incomplete filling of small pores can also be the appearance of an electrostatic field due to the presence of a charge on the surface of CdTe particles. This may be due to insufficient exchange of charge carriers between the components of the system. The possibility of removing the stabilizer shell from the surface of CdTe NC is being studied, which leads to an increase in the number of embedded NCs in PSi pores. Another positive effect of the removal of the shell may be the elimination of the reason for some decrease in the radiation yield from CdTe NC. To achieve this goal, 5–10% isopropyl alcohol, which dissolves the surface layer of thioglycolic acid, was added to the colloidal solution of CdTe nanocrystals during precipitation. The use of this technique made it possible to increase the efficiency of the PL of the PSi–nanocrystalline CdTe system, in which the PSi layer was formed by electrochemical etching.

Radiation functionalization of low density polyethylene and polyvinyl chloride composites with methylene blue dye

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The degree of crystallinity, dynamic moduli of elasticity and shear at a frequency of mechanical stresses ~1 MHz, spectra of Raman light scattering (RMS), photoluminescence (PL) of pure low-density polyethylene (LDPE), polyvinyl chloride (PVC) and its composites with the dye methylene blue (MB) after radiation functionalization by electrons with energy Ee = 1.8 MeV and absorption dose of 10 MRad, 1 MRad were studied.

From the reconstruction of the Raman spectra, it was established that the introduction of the MB modifier leads to the cross-linking of LDPE macromolecules through side groups, which is accompanied by their destruction. The PL spectra show the formation in LDPE and PVC due to the crosslinking of polyene structures, which is significantly enhanced by the introduction of MB and electron irradiation. With an increase in the content of MB, there is a restructuring of the conjugated systems, which are mainly responsible for improving the dynamic elastic and shear modulus.

Features of reactive sintering of HfB_2-SiC-C ultra-high temperature ceramics with enhanced thermal shock resistance

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The presented work discusses the features of reactive (1) and non-reactive sintering of HfB_2-SiC-C ceramics, which is a promising material for solar energy systems, as well as leading edges, nose cones and nozzles of rocket engines.

Hot pressing of HfC-B_4C-Si powder mixture leads to the formation of new phases of hafnium diboride and silicon carbide according to the following reaction:

$$HfC+B_4C+Si \rightarrow HfB_2+SiC+C. \quad (1)$$

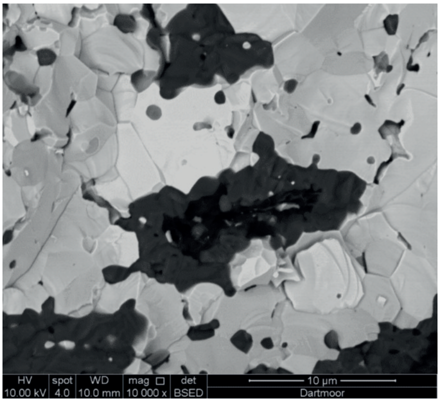

Fig. Scanning electron microscopy (secondary electrons) of a grafite inclusion in the matrix HfB_2-SiC

The reaction took place for 4 min at the temperature of 2120 K. The porosity of final samples did not exceed 1%. Non-reactively sintered samples contained 10-15% of pores, moreovere, their compaction kinetics differed significantly from the reactively sintered ones.

The main issue with ceramics is their low crack resistance, which was improved by the introduction of carbon shown in the figure. The manufactured samples exhibited crack resistance and microhardness values of 7 MPa·$m^{1/2}$ and 21GPa respectively.

Green synthesis of cobalt ferrites using different types of plant extracts

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Materials with a spinel structure have long been of interest because they can be used as magnetic materials, pigments, catalysts, and refractories. They can exhibit different properties depending on the synthesis method. Various methods can be used for the synthesis of spinel nanoparticles with a large surface area, such as sol-gel, co-precipitation, hydrothermal, combustion, microemulsion, sonochemical method, etc. In this research, we have used the method of green chemistry for cobalt ferrite obtaining. Green chemistry is a technique applied for nanoparticles synthesis and involves using of plant extract as an effective reducing and chelating agent. This paper describes the synthesis of cobalt using different types of plant extracts as an effective reducing agent. In particular, the extracts from follow plants were used: Gingko Biloba leaves, Physalis fruits, and Rosa canina fruits. The powders were characterized by XRD, SEM, EDS, and IR spectroscopy. Crystallite sizes of the samples are obtained by Scherer and Williamson-Hall methods and were found around 10 nm. The spinel structure of magnetic nanoparticles has been confirmed by XRD and IR spectroscopy. The tetrahedral and octahedral structure is confirmed by two corresponding peaks in the IR spectra, and few peaks in the range 1300-3700 cm^{-1} that show surface functionalization of magnetic nanoparticles. SEM and EDS proved the surface morphology and elemental composition respectively. Nanoparticles of $CoFe_2O_4$ obtained by an environmentally friendly method can be used as a magnetic adsorbent for water purification.

Compute synthesis of the crosslinked polymers based on glycidyl ethers of quercetin using a ReaxFF force field

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The increasing use of polymers in various fields highlights the need for new functional polymers. Traditional synthesis methods, involving trial and error testing of various small molecules, are costly, time consuming, and unreliable. Therefore, computer modeling methods such as ReaxFF and empirical potential come to the rescue. ReaxFF can detail chemical reactions, including the formation and breaking of bonds during simulation. [1].

In this work, the synthesis of cross-linked polymers based on glycidyl ethers of quercetin (GEQ): poly(7,4'-diglycidyloxy-3,5,3'-trihydroxyflavone) (I), poly(7,4',3'-triglycidyloxy-3,5-dihydroxyflavone) (II) and poly(7,3,4',3'--tetraglycidyloxy -5- hydroxyflavone) (III) with a desired set of properties that were obtained previously is reported [2]. The process involves an amine-epoxy ring-opening reaction and proton transfer, linking DETA and GEQ molecules into dimers, trimers, etc., in a system of 10 DETA and 20 GEQ.

Necessary note, the obtained crosslinked polymers in the result computer simulating synthesis had low densities. For I, II and III the densities were equaled 0.261 g/cc, 0.398 g/cc, and 0.371 g/cc, respectively. Therefore, for the obtained polymers, a geometry optimization (by the Fast Internal Relaxation method) and an annealing procedure (three cycles in the temperature range of 298–598 K) were carried out [1]. After the annealing procedure, the densities of the crosslinked polymers for I, II, and III were consisted of 1.301 g/cc, 1.283 g/cc, and 1.287 g/cc, respectively. The glass transition temperatures of the synthesized polymers, determined for the stated densities, were 466K, 449K, and 420K for I, II, and III respectively, as per the previously described procedure.

Through computer simulation of network polymer synthesis using the ReaxFF force field, it's found that the calculated data align well with previous experimental results.

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Metastable metal – semiconductor alloy films for next-generation technologies: an atomic scale study by means of advanced TEM techniques

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Natural materials have practically exhausted their potential in frontier technologies. Doping semiconductor materials to concentrations well above the equilibrium one opens a new avenue for designing high-performance materials for solar cells, ultrasensitive photodetectors, sensors, optical modulators, light emitters and lasers, and thermoelectric generators. Moreover, nanosized condensed films provide ample opportunities to obtain metastable phases that cannot be reached in bulk. In this respect, there is a quest for nanosized metamaterials and structures with unique properties for next-generation technologies of energy conversion and storage.

To tackle the problem, we investigated the mechanism of the metastable phase formation in Bi – amorphous Ge binary system down to the atomic level.

The *a*-Ge/Bi/a-Ge layered films with the size varied in the range of 30 – 300 nm formed by sequential condensation of components in a high vacuum for throughout thickness characterization of the dissolution process. Cross-section lamellae cut from annealed at different temperatures Ge/Bi/Ge layered films were used for advanced TEM characterization of the metastable alloys. The thickness of samples varied in the range of 30 - 300 nm and the overall composition in the range of 5 wt% - 50 wt% of Bi. The films were annealed between 20 and 300°C.

Morphology, nanostructure, and distribution of chemical elements in the samples were systematically investigated through film thickness down to the atomic scale using high-resolution imaging, diffraction, and EDX techniques in a TEM.

The concentration of Bi in the metastable Bi-Ge alloy was determined as a function of annealing temperature, film thickness, and overall composition of the layered film. As a result, the terminal concentration of Bi in the metastable Bi-Ge alloy was established for each configuration studied. The activation temperature of the dissolution process was determined also.

As a result, the type of the Bi-Ge metastable solid solution was identified and fully characterized.

Nanocomposites based on N,P-doped carbon and nickel phosphides as multifunctional electrocatalysts for oxygen reduction, oxygen and hydrogen evolution reactions

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Phosphides of some transition metals directly and in the composition of carbon composites are currently considered as promising platinum-free electrocatalysts toward important reactions of hydrogen evolution (HER), oxygen evolution (OER), and oxygen reduction (ORR). We have shown the possibility of obtaining nitrogen and phosphorus co-doped carbon nanocomposites with nickel phosphides particles (Ni_xP_y/N,P-C) - as HER, ORR and OER electrocatalysts - by pyrolysis of polyaniline doped with phosphoric acid together with $NiCl_2 \cdot 6H_2O$.

Based on the data of X-ray phase analysis, it was found that an increase in the pyrolysis temperature leads to the formation of nickel phosphides with a lower phosphorus content in the composition of the composites. The dominance of $Ni_{12}P_5$ and the presence of NiP occurs in NixPy/N,P-C(800) formed at 800ºC; the absence of NiP in Ni_xP_y/N,P-C(900) and NixPy/N,P-C(1000) obtained at pyrolysis temperatures of 900 and 1000ºC, as well as a sharp increase of Ni_2P when the composite formation temperature increases from 900 to 1000ºC.

It was found that the activity of the obtained nanocomposite catalysts in the HER increases in 0.5 M H_2SO_4 in the order NixPy/N,P-C(1000) < NixPy/N,P-C(800) < Ni_xP_y/N,P-C(900), and in 1.0 M NaOH – Ni_xP_y/N,P-C(1000) < Ni_xP_y/N,P-C(900) < Ni_xP_y/N,P-C(800). The electrocatalyst Ni_xP_y/N,P-C(900) has the highest functional characteristics in HER in acidic electrolyte (Tafel slope, b ~ 58 mV/dec; overpotential at 10 mA/cm^2, η_{10} ~ 150 mV), and in alkaline – Ni_xP_y/N,P-C(800) (b ~ 100 mV/dec; η_{10} ~ 176 mV).

At the same time, the activity of electrocatalysts in ORR and OER (in an alkaline electrolyte) is the opposite to that found for in HER, which may be due to different sites that are involved in these processes. The obtained Ni_xP_y/N,P-C(900) and Ni_xP_y/N,P-C(1000) are characterized by high values of the half-wave potential in the ORR (~ 830-850 mV vs RHE), and oxygen reduction on them occurs mainly by the 4-electron mechanism. In OER, the mentioned catalysts provide values of the overpotential of oxygen evolution at a current density of 20 mA/cm^2 ~ 370-400 mV and are characterized by the value of b ~ 161 mV/dec.

The influence of morphology and dispersion on the emission properties of materials based on lanthanide complexes

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It is well known that dispersion and morphology have a decisive influence on the properties of nanomaterials. If some regularity has already been determined for nanopowders of metals and oxides, there are few studies for coordination compounds. Coordination compounds of lanthanides are widely used as precursors for luminescent materials. Depending on the electronic structure of the central ion, compounds can emit in the visible or IR range of the spectrum. In this work, the synthesis of mono- and heterometallic, monomeric and metallopolymer complexes of lanthanides with unsaturated β-diketones was carried out. Copolymers based on styrene, vinylcarbazole and methyl methacrylate were obtained. The composition, structure, morphology, dispersity and spectral-luminescence properties of all synthesized compounds were studied.

The study of the synthesized compounds by classical physicochemical methods of analysis (IR, DRS, luminescence spectroscopy) demonstrated different optical properties for similar systems. In this regard, a thorough study of the dispersion and morphology of the synthesized powders and films was carried out. The relationship between the dispersion, morphology and luminescent properties of the synthesized lanthanide coordination compounds was established. The highest emission characteristics are characteristic of aggregatively and kinetically stable systems with an ordered structure.

Green synthesis of silver and gold nanoparticles

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The development of nanotechnologies is constantly moving forward, and the development of new methods of synthesizing nanoparticles of precious metals by replacing raw materials with the aim of optimizing and reducing the cost of final products is an urgent task of modern science. AgNPs and AuNpcs are characterized by high electrical and thermal conductivity, chemical stability, catalytic activity, optical properties. Nanoparticles of precious metals are used in the food, cosmetic and pharmaceutical industries. The use of plant extracts as sources of reducing substances for the synthesis of nanoparticles of noble metals attracts attention due to the environmental friendliness and practicality of this method. Disadvantages of this method are the presence of secondary compounds and metabolites, temperature limitations characteristic of enzymes. The choice of method depends on the field of further application of the obtained AgNPs\AuNpcs. Therefore, the purpose of this study is a comparative analysis of gold and silver nanoparticles obtained by "green synthesis" and when aminopolycarboxylic acids are used as reducing agents. For the study, water-alcohol-glycerin extracts of *aloe vera, matricaria chamomilla, Avena sativa*, *Urtica dioica* produced by the company "Vilarus" were taken. The starting solutions consist from extract 4.0%, glycerol 10%, ethyl alcohol 20%, sodium benzoate 0.08%, water >20%. Structural analogues of ethylenediaminedisuccinic and ethylenethiaminetetraacetic acids were used as chemical reducing agents. The conducted studies showed high efficiency of both natural extracts and polycarboxylic acids. However, the extracts are characterized by a higher reducing ability at lower concentrations and, accordingly, a higher stability of the synthesized nanoparticles. The use of natural extracts expands the range of practical applications of the obtained AgNpcs.

Ab initio study of structural and elecronical properties of β-Ga_2O_3 nanoclusters

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We present results of ab initio density functional theory studies of energy spectrum and ground stage parameters of small β-Ga_2O_3 nanoclusters (5 to 45 atoms). Calculations were performed using ultrasoft pseudopotentials in the basis of plane waves, similar to previous studies of semiconductors [1]. To describe the exchange-correlation energy of the electrons, a generalized gradient approximation with Hubbard corrections (GGA+U) in Perdew, Burke and Ernzerhof parameterization was used. Optimization of the nanocluster structure was performed using conjugate gradient method. No symmetry restrictions were used during structure optimization.

In order to determine the most stable structure for the small clusters Ga_2O_3 nanoclusters (5 to 45 atoms) we examined a number of isomers. Among them were ring structures, chain structures, sphere structures, all of which satisfy the assumption of the presence of translational symmetry in the studied atomic systems.

To analyze the stability of β-Ga_2O_3 clusters we calculated binding energy per one formula unit of Ga_2O_3. Analysis of the energy values shows that for β-Ga_2O_3 nanoclusters built from one to three formula units the most energetically favorable are chain-like structures. All such structures have approximately the same binding energy. With increase of formula units in the researched systems the shift to ring structures (four to six Ga_2O_3 formula units) and then to compact sphere structure (seven to nine formula units) was observed. Among the structures in the form embedded clusters more stable are those in which the interatomic distance between the outer and inner shell is greater.

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Tribology Properties of Coatings Based on MAX Phase $Ti_2(Al, Sn)C$

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Improving the durability of engine tribo-couplings that operate under high-temperature and dry friction conditions is an urgent task. The nanolaminate MAX phases of Ti-Al-C system and their corresponding coatings hold promise for this application. Alloying with different elements can further enhance their tribological properties. The purpose of this study is to investigate the impact of Sn concentration on the tribological properties of Ti-Al-C coatings at two temperatures: 20°C and 500°C.

The Ti-(Al, Sn)-C coatings were deposited into polished stainless steel samples using the vacuum arc method. MAX phase cathodes, namely Ti_2AlC, $Ti_2(Al_{0.75},Sn_{0.25})C$, and $Ti_2(Al_{0.5},Sn_{0.5})C$, were employed in the deposition process. The composition and structure of the coatings were examined through XRD, SEM, and EDX analysis methods. To investigate the mechanical properties, a microhardness tester was used. The wear resistance was evaluated by subjecting the coated plates to reciprocating motion against a hardened steel ball ShKH15.

Tribological tests revealed that Ti-Al-C coatings exhibited a friction coefficient (μ) ranging from 0.4 to 0.5. The wear specific rate (w) increased from 6.47×10^{-5} mm^3/Nm at 20 °C to 3.28×10^{-4} mm^3/Nm at 500 °C. On the other hand, $Ti_2(Al_{0.75},Sn_{0.25})C$ coatings displayed a coefficient μ within the range of 0.35 to 0.65, and a value of w slightly decreased from 2.14×10^{-5} mm^3/Nm at room temperature to 1.94×10^{-5} mm^3/Nm at 500 °C. An increase in the tin concentration did not result in an improvement in the tribological properties of the coatings. Therefore, incorporating a small amount of tin into the MAX phase Ti_2AlC enhances the wear resistance of the resulting coatings.

Raman scattering in $Pb_3(P_{0.5}V_{0.5}O_4)_2$ nanocrystals grown in pores of opal matrix in the temperature range 290 K – 470 K

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Lead phosphate crystal is an attractive acoustooptic material for fabrication of nanocomposites, that undergoes a ferroelastic phase transition from a high-temperature rhombohedral phase to a low-temperature monoclinic phase at 453 K [1, 2]. There may be a modification of its properties when fabricating lead phosphate nanocrystals regularly arranged in opal matrix. In this paper, opal-based nanocomposites with inclusions of the $Pb_3(P_{0.5}V_{0.5}O_4)_2$ nanocrystals are characterized by using Raman spectroscopy technique within the 290 K – 470 K temperature range.

The nanocomposite was prepared by the procedure based on capillary forced impregnation of opal matrix with the lead phosphate melt with the following crystallization. To investigate the processes in volume of sample its surface layer was mechanically removed to a depth 0.5 mm.

Nonpolarised Raman spectra, excited by a 532 nm DPSS laser radiation, were measured by using the spectrometer based on a double monochromator DFS 12 equipped with a photon counting system. The samples were heated by resistance furnace in air atmosphere.

Comparison of the nanocomposite spectrum measured at room temperature with that obtained for single crystal earlier [2] testify to the crystalline state of substance in opal pores. Analysis of the ratio of the Raman spectral intensities of bands at 833 cm^{-1} and 938 cm^{-1}, corresponding to the valence vibrations of VO_4 and PO_4 groups, respectively, points to the stoichiometry maintenance. No new Raman bands that could indicate the formation of a new crystalline phase were detected. Temperature behavior of the Raman band parameters was analyzed in the framework of the phase transition theory.

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Azo-compounds based on 2- and 3-aminopiridine: photoinduced E→Z isomerization and diffraction efficiency index in thin films

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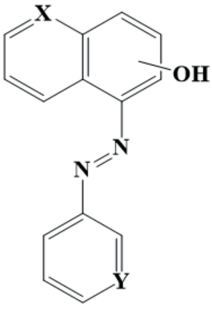
Polymers and composites containing azo- chromophore groups are a class of optical materials extensively investigated in the past decade while it combines the virtues of photoisomerization and photo-orientation and nonlinear response to a strong optical field. For example, azobenzenes can be used in in optical information storage devices, as optical switches and sensors, in polarization holography [1], and in photonics, etc. One of the best matrixes for this deal is polymethylmethacrylate (PMMA) that provide high optic transparency and low light scattering loses. One of the ways of photophysical properties regulation is introduction of heterocyclic fragments into photochromic molecule instead of classic aromatic system.



X = N, CH
Y = N, CH

Azo-compounds synthesized by 3-aminopyridine diazotization and further coupling with α-naphthol/β-naphthol/8-hydroxyquinoline were obtained with a good yield. A commercially available azo dyes, i.e., Sudan I and 1-(2-Pyridylazo)-2-naphthol, were used to study the influence of the pyridine nitrogen position (*ortho-* or *meta-*isomer) or its absence on the polymer composite diffraction characteristics.

Thin films of a polymer composite containing 5% (wt.) of azo compounds and 95% (wt.) of PMMA were formed from a DCE solution. It is shown that the diffraction efficiency increases with the transition from thin films (~1 μm) to thicker ones (~2.5 μm). The diffraction efficiency values for the parallel polarization of the recording beam are greater than for the perpendicular one.

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Percolation threshold in the annealed ultrathin SiO_x films by 2D Monte Carlo simulations

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A superlattice approach is an efficient solution for fabricating nanocomposite structures composed of Si nanopaticles embedded in a SiO_2 matrix for nano- and optoelectronic applications [1]. In this approach, a superlattice containing alternating understoichiometric Si oxide (SiO_x, $x < 2$) and SiO_2 layers with nanometer thicknesses is first created. A high-temperature anneal of such superlattice induces phase separation of SiO_x and formation of Si nanoparticles, the sizes and positions of which are defined by the initial SiO_x layer thicknesses and locations, respectively. Various Si morphologies, from isolated spherical quantum dots to fully percolated two-dimensional networks, can be obtained by varying the initial SiO_x stoichiometry [2]. Understanding the formation mechanisms of different Si structures is needed for obtaining nano-Si/SiO_2 composites with required characteristics.

In this work, the kinetics of phase separation in ultrathin SiO_x films is modeled using the 2D Monte-Carlo simulation method. The separation of Si and Si oxide phases by redistribution of oxygen atoms between the neighboring $Si–Si_aO_{4–a}$ tetrahedral complexes composing the SiO_x microstructure is considered. The net direction of oxygen redistribution corresponds to the decrease of the penalty energy of the participating complexes, which is taken into account by applying the Metropolis algorithm. As a result, the dependence of the morphology of the Si nano-structures formed in Si oxide matrix on the initial SiO_x stoichiometry is obtained. Nearly spherical isolated Si quantum dots form at $x > 1$. Progressive increase of excess Si content leads to the formation of elongated Si particles, their merging and finally fully percolated Si networks at the percolation threshold $x \sim 0.7$.

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Discrete spintronics devices for recording electromagnetic radiation

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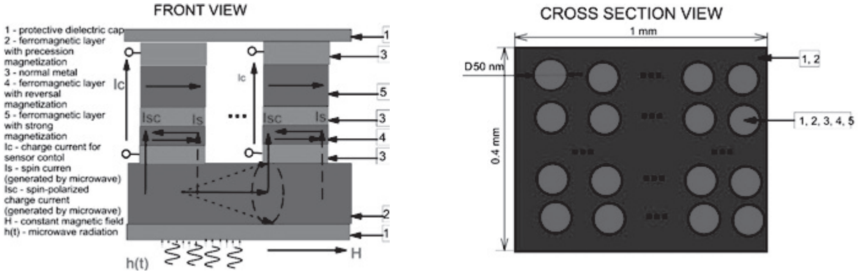
The paper proposes an intelligent high-frequency electromagnetic field sensor that uses the phenomenon of ferromagnetic resonance. The device is a multilayer structure (Fig. 1), which uses a number of phenomena caused by the spin properties of electrons, which cause the existence of a spin current.



a) *b)*

***Fig. 1**. Electromagnetic field spin sensor: a) – front view (1 – protective layer; 2 – magnetic layer with a weak coercive force, where precession of the magnetization vector occurs; 3 – non-magnetic metal; 4 – freely remagnetized magnetic layer (in the plane of the sample); 5 – magnetic layer with fixed magnetization in the plane of the sample); b) cross section and its geometric dimensions (1, 2 – protective layer and outer ferromagnetic layer, 3, 4 and 5 – nanoscale spin valve structures).*

Highly sensitive sensors can significantly expand the field of application of Internet of Things devices and other cyber-physical systems, where electromagnetic field emitters with different radii are used. The use of fundamentally new methods of digital signal processing will significantly expand the possibilities of application, protection against interference and the possibility of functioning in the conditions of complex electromagnetic conditions of sensor networks of various levels of topological complexity and control technologies. Based on the analysis of literary sources, it was concluded that it is possible to combine several phenomena related to the application of spin at once: generation of spin current, generation of spin-polarized current due to the reverse spin Hall effect, remagnetization of a ferromagnetic layer with a small coercive force, reverse remagnetization due to the passage of direct current in the opposite direction to the spin-polarized current. The researched method of detecting the external electromagnetic field has a number of advantages compared to traditional detection methods that use conventional antennas made of conductors: hardware losses due to thermal current and secondary radiation of the antenna are significantly reduced; potentially increases detection speed and accuracy.

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Heat transport in Si_xGe_{1-x} nanocomposites with different atomic configurations

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Understanding thermal transport properties in materials used for green energy transition is essential to improve device conversion efficiency. For example, silicon-germanium alloys are widely used as active elements of thermoelectric converters [1]. In the latter, the figure of merit, the quantity that defines the device's efficiency, is inversely proportional to the thermal conductivity of the compound. Hence, thermal management in thermoelectrical converters is one of the critical issues for their further improvement.

In binary compounds such as silicon-germanium alloys, the tailoring of the thermal properties can be ensured by the "smart" distribution of one component into another. Paths for such engineering can be based on spatial modulations with different local concentrations of substituting elements (Si or Ge). However, there is still a lack of information about the impact of the atom arrangement in such alloys on thermal transport properties.

Thus, the main goal of our study is to investigate the configurational dependencies of Si_xGe_{1-x} samples on heat conduction, keeping the same concentration of the composite components. To this aim, we used equilibrium molecular dynamics based on the Green-Kubo method [2]. This approach allowed us to evaluate thermal conductivity for different distributions of Ge atoms. The obtained results will be used to understand better the features of heat transport in Si-Ge nanocomposite systems.

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Screen-printed carbon electrode modified with carbon nanotubes as a simple and fast tool for determination of trace concentrations of lead ions

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Electrochemical sensors are attractive analytical devices because they combine high sensitivity and simplicity with low instrumentation cost. Currently, a major challenge in electroanalysis is the development of miniaturised and portable electrochemical sensors made of alternative and inexpensive materials. These devices require only small volumes of samples and reagents, which is highly desirable from an economic and environmental point of view. A good solution to address this challenge is screen-printing technology as an established method for the preparation of portable chemical sensors. Screen-printed electrodes (SPEs) are widely used and the range of materials from which they are made continues to expand. One of these materials are carbon nanotubes. They improve electrode properties important in voltammetric measurements, for example, increase the surface of the working electrode. Also they exhibit good chemical stability and excellent electrical conductivity. In our work, we proposed use of screen-printed carbon electrode modified with carbon nanotubes as a simple and fast tool for determination of trace concentrations of lead ions. Today, there is quite a bit of lead in our environment, used mainly in batteries, formerly as a fuel additive. Metallic lead as well as lead compounds show high toxicity. Salts and oxides of this element are poisons that accumulate in the body, causing disorders of the nervous system, in extreme cases leading to brain damage and death, so analytical techniques to monitor its content in various samples are being sought.

Hydrogenation and hydrolysis properties of MgH_2 composites with additions of RMO_3 perovskites

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MgH_2–based composites with nanoparticles of perovskites and graphite were synthesized by the reactive ball milling method. These composites can have a dual use (similar to the MgH_2-$Zr_3V3O_{0.6}H_x$-C composites [1]) – for hydrogen storage and hydrolysis generation. Ferrites of rare earth metals, $Dy_{0.5}Nd_{0.5}FeO_3$ and $TbFe_{0.5}Cr_{0.5}O_3$, were synthesized by the sol-gel method (particle size of 80-300 nm) and used as catalytic additives. The effect of these complex oxides on the hydrogenation of magnesium during milling and improvement of hydrogen sorption-desorption kinetics is shown. The phase-structural composition of the composites was determined by powder X-ray diffraction. Thermal desorption from these composites occurs in two stages and at temperatures above 300 °C. The activation energy (E_a) of hydrogen desorption was determined by the Kissinger method, based on the analysis of thermodesorption curves at different heating rates. Ea for the composite with $TbFe_{0.5}Cr_{0.5}O_3$ is 123 kJ/mol, and for the composite with $Dy_{0.5}Nd_{0.5}FeO_3$ - 147 kJ/mol. The synthesized nanocomposites were tested as materials for generation of hydrogen by hydrolysis in pure water and in magnesium chloride solutions. The duration of ball milling increased the reaction rate and the yield of hydrogen in hydrolysis reactions. During the hydrolysis of the synthesized composites in pure water, the volume of hydrogen released was 320-350 ml/g. The degree of conversion significantly improved with the addition of $MgCl_2$, the yield of the reaction reached 90% after 30 min of hydrolysis.

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Optical investigations of the magneto-electric effect manifestations on individual magnetic domains ferrite garnet films

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Results of investigations of the magneto-electric effect (MEE) manifestations in the region of an individual magnetic domain, which is in a state close to collapse (H||k, where k is a light wave vector) are presented in this paper. The effect of an electric field (E||k) and a bias magnetic field on the domain walls (DW`s) of a cylindrical magnetic domains (bubbles) has been experimentally studied. The studies were carried out by the magneto-optical method based on the Faraday effect using a polarizing microscope [1,2]. Ferrite-garnet film with a developed <111> surface, grown by liquid-phase epitaxy on a gadolinium-gallium substrate with the composition $(TmBi)_3(FeGa)_3O_{12}$, was chosen for the study. The thickness of the film was about 7 μm, and the thickness of the substrate was about 600 μm. Investigated of the electric-field dependences of domain diameter (d) for fixed values of the external magnetic field. The results of visually observed changes in the domain diameter showed that an abrupt change in the domain diameter in an gradient electric field was observed for a cylindrical domain in a state close to collapse. Our results indicate the manifestation of a direct relationship between the curvature of the domain wall and the degree of its response (sufficient for visual observations) to external action by a gradient electric field. The jump in the domain diameter, which is sharp in shape, is probably associated with the defective structure of the film and the pinning of the DW on defects. For an ideal situation of a defect-free film, the change in diameter would occur linearly with increasing electric field value.

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Effect of acid-base characteristics of zeolites of different framework types on their catalytic properties during isobutanol dehydration

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Reducing the consumption of non-renewable natural resources, including crude oil and gas, by replacing them with renewable bio-raw materials is a very essential challenge of modernity. Given the rapid development of isobutanol (2-methylpropan-1-ol, i-BuOH) production by fermentation of non-food biomass of plant origin in the last decade, i-BuOH is one of such renewable bio-raw materials. Four butene isomers (1-butene, trans-2-butene, cis-2-butene and isobutene), which are used in industry to produce various polymers, fuel additives, etc., can be obtained by dehydration of the bio-alcohol.

The purpose of the work is to establish the effect of nature and strength of acidic sites of FER, MFI, FAU and BEA zeolites on their catalytic properties in the process of i-BuOH dehydration. The acid-base characteristics of zeolite samples were investigated by IR-spectroscopy of adsorbed pyridine, potentiometric titration, and temperature programmed desorption of NH_3 and CO_2 probe molecules with mass spectrometric control. It was found that a larger quantity of strong acid sites with desorption activation energy of ~ 125 kJ/mol on the surface of FER and MFI zeolites contributes to the formation of linear isomers of butene, and can be attributed to Brønsted acid sites. Whereas, the predominance of strong Lewis acid sites on the surface of FAU and BEA catalysts leads to the formation of isobutene and other by-products.

Effect of tungsten doping on photo- and electrocatalytic properties of titania films

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Doping with metal ions is well known strategies to increase the photocatalytic activity of titania based materials. Tungsten has been chosen as one of the promising agent employed to improve not only charge separation but also adsorption processes due to high surface acidity of W^{n+}/TiO_2 photocatalysts.

Mesoporous nanoscale TiO_2 and TiO_2/W^{n+} (0,1% до 10%) films were synthesized by the sol-gel method using titanium tetraisopropoxide, $(NH_4)_{10}W_{12}O_{41}\cdot 11H_2O$, nonionic triblock copolymer Pluronic (P123) as a templating and acetylacetone as complexing agent at pH=3-4 (adjusted by $HClO_4$), and deposited on glass and steel substrates via dip-coating procedure. The structural and optical properties, phase composition of the synthesized films and powders, obtained after precursors gelation were investigated by XRD, Raman and UV-Vis spectroscopy. Band gap energy and the position of flat band potentials were estimated by direct photoelectrochemical measurements. XRD patterns of W^{n+}/TiO_2 powders showed anatase (20-25 nm) and rutile (35-40 nm) nanocrystalline phases. The lower degree of anatase to rutile transformation was observed for tungsten doped films compared to pure titania. The most effective in the photoreaction of Cr^{6+} ions reduction to Cr^{3+} in the presence of EDTA as an electron donor under UV irradiation were TiO_2 films with a content of 5-7% W^{n+}. When the dopant concentration was increased to 10%, the activity decreased, but remained higher than to pure TiO_2. Electrocatalytic properties of TiO_2 and W^{n+}/TiO_2 electrodes were investigated in process of oxygen electroreduction. The potential of oxygen reduction changes with the film composition.

Synthesis and properties of Cu/TiO_2 photocatalytic films and powders

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Modification of nanosized TiO_2 with ions and atoms of transition metals, in particular silver and copper, is widely used to obtain composite materials with high photocatalytic and bactericidal activity. Due to the difference between the ionic radii of Ti(IV) and the modifier ion, the unit cell of TiO_2 is slightly deformed, the band gap of TiO_2 decreases, and the photocatalytic activity increases under the influence of visible light. As we showed earlier, the content of up to 7% of Cu^{n+} ions in the structure of films and powders leads to acceleration of photocatalytic reactions of water denitrification, reduction of Cr^{6+} ions to Cr^{3+}, etc. Bactericidal activity arises from the release of ions from the surface of metal NPs upon contact with water or biological fluid. The release of ions from the surface of NPs (or their oxides) critically depends on their localization in the TiO_2 structure, which is related to the method of synthesis. The purpose of this work was to compare the structure, photocatalytic and bactericidal properties of modified samples of porous Cu-TiO_2 films and dispersions depending on the concentration of copper in a wide range (from 0.1 to 30%) and the nature of the pore former at the sol-gel synthesis stage - 1) pluronic or 2) PEG in the presence of terpineol. It is found that in an aqueous environment, metal ions are released from the surface of sol-gel powders synthesized using method 1, which determines the ability to decontaminate effluents from organic toxic substances. Copper-containing crystalline films and Cu-TiO_2 dispersions have a high redox photocatalytic effect in relation to heavy metals and their adsorption removal. In the case of using method 2, stable oxide phases of the dopant are formed in the TiO_2 structure, from the surface of which metal ions are not desorbed. The studies have shown a high bactericidal activity in relation to *Escherichia coli (E. coli)*. The desorption of Cu^+, Cu^{2+} ions from the surface of the composites quantitatively correlates with the bactericidal properties of the obtained powders.

A model for several-step electrical percolation in random mixtures and composites

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Numerous experimental studies of electrical properties of random mixtures and composites reveal more complicated types of transition from a non-conducting to a conducting state than that predicted by the classical percolation theory; typical examples are two-step, several-step, and smeared percolation. This fact evidences the significance of specific features of a percolating system — its microstructure and physico-chemical mechanisms in it — for the formation of its electrical conductivity and permittivity. A consistent theory is therefore required to (1) incorporate the relevant quantitative characteristics, often uncertain, of the system into a single model; (2) account for feasible variations of those as the system's composition is changed; and (3) exploit a reliable technique for homogenization of the model.

We suggest that requirements (1)-(3) can be met by treating a real system in terms of a model dispersion of hard-core–penetrable-shell particles. The details of such a model in application to composite solid and polymeric electrolytes are given in [1,2]. The shells are electrically inhomogeneous (for instance, layered); their conductivity profile accounts for the dominant mechanisms in the real system. The dispersion is subject to certain rules of dominance for its overlapping components. The homogenization is internally closed and carried out using the compact group approach; the results for the conductivity are rigorous in the static limit.

In this report, we demonstrate the capability of the indicated model to predict and quantitatively describe a several-step electrical percolation in random system. The effect is accompanied by a drastic increase in the dielectric constant near the percolation thresholds. The results obtained are validated by comparing them with experimental data.

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Chemical and electrochemical nanofabrication of polyaminothiazole/graphene oxide composites

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Conducting polymers (CP) are similar to metals and semiconductors due to their electrical and optical properties while preserving the useful properties of polymers – easy and inexpensive synthesis, elasticity, etc. Materials based on CP are versatile because their properties can be easily modified by surface functionalization and/or doping. One of little studied CP is poly(2-aminothiazole) (PAT), which contains S and N in a 5-membered thiazole ring. PAT has interesting sorption properties [1]. It is known that 2-aminothiazole is a biologically active compound with antimicrobial, antitumor properties [2]. In addition, graphene-based coatings functionalized with PAT have been reported to show potential applications in corrosion protection and antistatic coatings [3]. Therefore, optimizing the conditions for the synthesis and studying the physicochemical properties of PAT and its composites is a promising and actual task. In this work, we studied the conditions of chemical synthesis of PAT and its composites with graphene oxide (GO) in an aqueous solution under the action of inorganic oxidants, as well as electrochemical deposition on electrode surfaces of various natures – Pt and optically transparent SnO_2. The globular structure of obtained polymer with a globule size near 0.4-0.6 μm was shown by scanning electron microscopy. For PAT/GO the globules are smaller. According to the FT-IR spectra of PAT and PAT/GO composite, the polymerization of aminothiazole occurs through the amino group. To confirm the results of IR-spectroscopy, a quantum-chemical calculation using the semi-empirical PM7 method was carried out. The electrochemical activity of polymer films was examined. Increasing effective parameters of charge transport for surface films obtained in the presence of GO were detected.

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The proton transfer in the system "polystyrene matrix-dye-gold nanochip" under conditions of temperature variations

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Excited-state intramolecular proton transfer (ESIPT) is a four-level photochemical process [1] observed in some luminescent molecules. This process can be influenced by external factors, such as an electromagnetic field. Since high-conductive nanostructures might create enhanced local electromagnetic fields, it is worthwhile to investigate how they will affect ESIPT when irradiated at the localized surface plasmon resonance (LSPR) frequency.

To investigate this process, we compared the luminescence of the multidomain dye HTTH [2], which was applied in the polystyrene matrix onto nanochip with gold nanostructures and onto glass plate, before and after the heating (80°C, 1 min) and cooling (4°C, 1 min) cycles to enhance diffusion of dye molecules to the nanostructures. We found that the initial luminescence on the glass plate was significantly higher than on the nanochip. Additionally, changes were observed in all spectra after thermal treatment.

From the spectra normalized by the highest peak (443 nm), we found that the initial samples exhibit nearly identical spectra in the low-energy peak region (540 nm), indicating similar conditions for the ESIPT phenomenon in both samples. However, after heating and cooling, the intensity of the low-energy peak decreases to a much greater extent in the spectrum of the sample with the nanochip. This finding highlights the significant influence of gold nanostructures on the ESIPT phenomenon in HTTH multi-domain dye when luminescence and LSPR overlap.

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Microindentation hardness and structural properties of $Ag_7(Si_{1-x}Ge_x)S_5I$ superionic conductors based ceramics

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The crystal structure of Ag_7XS_5Hal (X = Si, Ge; Hal = Cl, Br, I) compounds was first investigated by Kuhs et al. [1]. Due to their high ionic conductivity, superionic conductors are of great interest in the field of solid-state electronics given the increasing demand for electrochemical energy storage. Compounds with the structure of argyrodite are promising superionic materials that are suitable for the fabrication of electrochemical sensors and solid-state energy sources based on them, such as photoanodes, supercapacitors, all-solid-state batteries, etc. [2]. The microstructure of ceramic samples of the composition $Ag_7(Si_{1-x}Ge_x)S_5I$ was studied by scanning electron microscopy. The composition of the samples was determined by an energy dispersive X-Ray method. Microhardness measurements were carried out using a PMT-3 microhardness tester with a Vickers diamond indenter in the load range of 0.05-2 N.

By indexing the obtained powder patterns, the formation of $Ag_7(Si_{1-x}Ge_x)S_5I$ solid solutions was determined. Established that $Ag_7(Si_{1-x}Ge_x)S_5I$ solid solutions crystallize in a face-centered cubic cell (SG F-43m). The microstructural investigation of the $Ag_7(Si_{1-x}Ge_x)S_5I$-based ceramics shows a narrow distribution of crystallite sizes and close values of the average crystallite size in the range of 2.52-2.70 μm. The chemical composition of the investigated ceramic samples is homogeneous and close to the specified composition. For $Ag_7(Si_{1-x}Ge_x)S_5I$-based ceramics, the presence of a direct size effect was established - the microhardness H decreases with increasing values of the applied load P.

The characteristic of microhardness dependence on composition at different loads with a nonlinear decreasing trend and correlation with porosity value was determined.

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Molecular assembling polymer/inorganic nanocomposites for energy conversion, storage, and conservation devices

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The ever-expanding field of energy conversion, storage, and conservation demands new materials that meet stringent requirements in terms of cost, environmental impact, stability, efficiency, and simple synthesis. Nanocomposites based on functional polymer/inorganic supramolecular structures demonstrate their effectiveness in electronics as high-Q capacitors in the radio frequency range and sensors for external physical fields; exhibit great promise in energy storage devices, where they are explored as quantum batteries and spin capacitors possessing spin electromotive force. New developed approaches for obtaining composites with tailored optical and electrophysical properties consist of assembling polymer/inorganic clathrates intercalated with nanoparticles and Li^+ ions on ceramic or polymeric surfaces as well as in spatially confined molecular crystal lattices of MoS_2 or GaSe. Combination of radical and non-radical reactions provides *in situ* formation of the assemblies of a “host – guest” complex architecture wherein grafted polymeric brushes can be host and guest simultaneously. Precise control over composition, brush length, and packing density further enhance the ability to manipulate functional properties, paving the way for applications of the synthesized materials in energy conversion and storage.

This research presents a comprehensive investigation of the energy storage properties of polymer-containing composites and coatings. The study shows synthesis technique and highlights potential avenues for utilizing these synthesized materials in energy storage and related applications.

The Effect of Y Doping on the Electronic Structure of ZnO: First Principles Simulation

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Zinc oxide (ZnO) is a widely used semiconductor with versatile applications in gas sensors, TCO, displays, transistors, and solar elements. ZnO doping has attracted scientific interest for its ability to modify the band gap. While Al, In, and Ga doping in ZnO is extensively studied for n-type systems, research on other III elements like La, Y, and Sc is limited. However, these elements show potential as alternative TCO materials. A recent study [1] investigated the impact of surface morphology on the optical and electrical properties of Y-doped ZnO thin films (ZnO: Y). The researchers found that increasing the Y concentration to 4.7 wt. % in ZnO: Y films caused a blue shift in the absorption edge. However, higher concentrations resulted in a redshift.

In this work, we present the results of first-principle calculations of the band structure and optical properties of ZnO: Y with different impurity concentrations to establish the doping effect on ZnO's electronic and optical properties. For DFT calculations, the GGA (PBEsol) exchange-correlation functional was used with Hubbard corrections implemented in the CASTEP package. In our work, we consider the 2×2×2, 3×3×1, 2×2×3, 2×2×4, 3×3×2, and 3×3×3 supercell in which Y replaced one Zn atom, corresponding to dopant concentrations of 6.25%, 5.56%, 4.17%, 3.125%, 2.78%, and 1.85%, respectively.

The calculations revealed that as the concentration of Y impurity increases, the lattice parameters of the material also increase. The investigation into the electronic properties demonstrated that the Fermi level of the doped ZnO moves upward into the conduction band, indicating its behavior as an n-type semiconductor. Moreover, the bandgap expands as the Y concentration rises, resulting in a blue shift of the absorption edge in ZnO: Y. The influence of point defects, particularly oxygen and zinc vacancies, on ZnO: Y’s electronic structure was also considered to account for the experimental data. It was discovered that the presence of Zn vacancies leads to a reduction in the band gap. These findings hold significance in the future development of ZnO: Y for experimental purposes.

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Atomic and electronic structures of interfaces in “K_2O-P_2O_5-MoO_3-Bi_2O_3 glass - $KBi(MoO_4)_2$ crystals” glass-ceramics

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Oxide glass ceramics are composite materials perspective for various applications, in particular, in electronics, optical thermometry and biomedicine. The properties of oxide glass-ceramics are largely determined by processes in the "interface/interphase region", which has an atomic structure different from the structure of both crystalline and glass components. The mutual diffusion of component atoms can be effectively modeled in calculations using the molecular dynamics (MD) methods. Further application of the electronic structure calculation methods to the obtained atomic structures (when coordinates of atoms optimized in MD approach are input parameters of ES calculations) allows to calculate the most important micro- and macro-characteristics of the interphases layers.

In this report we present results of the computational studies of atomic and electronic structures of interfaces in “$KBi(MoO_4)_2$ crystal / K_2O-P_2O_5-MoO_3-Bi_2O_3 glass” glass-ceramic composite material. The atomic structures of interface layers of composites were calculated by MD methods implemented. The calculations were performed for ~20x20x45 Å three-dimensional periodic cells, which contained 300-500 atoms of composites. The electronic structure calculations were performed in the DFT approximation using the band-periodic plane wave pseudopotential method, for which the cells of smaller size ~12x12x12 Å were used. Calculations of the excited electronic states energies and optical absorption spectra of particular oxyanionic molecular groups of interface regions were performed by the TD-DFT method.

Relationships between atomic and electronic structures of interface (interphases) layers and optical characteristics of studied composites are discussed.

Hydroxyapatite nanocomposite catalysts supported on carbonaceous materials for Guerbet condensation of 1-butanol

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The development of catalysts for the production of industrially important substances using raw materials of non-petroleum origin like non-food biomass is one of the promising areas of research. The process of producing higher alcohols from (bio)alcohols via the Guerbet reaction is generally accepted to be a sequence of reactions: dehydrogenation of initial alcohol, followed by aldol condensation, dehydration, and hydrogenation of the unsaturated aldehyde. Hydroxyapatite catalysts can be used for this purpose due to the balanced acidity and basicity of the surface [1]. A dispersion of active components on a support with a larger surface area is proposed in order to increase productivity of catalysts for the selective conversion of short-chain alcohols into higher ones [2].

This work presents the results of the investigation of catalytic properties of the supported catalysts containing hydroxyapatite (HAP) and carbonaceous materials (CM) during Guerbet condensation of 1-butanol in the flow mode. The effects of the nature of carbonaceous materials as a catalyst carrier on the acid–base characteristics and catalytic properties (activity and selectivity) are considered. HAP/CM systems exhibit catalytic activity in the process of 1-butanol condensation with carbon chain elongation. The distribution of 1-butanol conversion products depends on the carbon carrier nature. The yield of 2-ethylhexanol is up to 21% can be achieved over HAP/activated coconut charcoal.

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The Systems Polyamide-Carbon Nanotubes

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The energy of covalent bonds in a free ε-aminocaproic acid (ACA) dioligomer molecule and when it is incorporated into an intermolecular complex with a graphene-like surface was calculated by the density functional theory method using the B_3LYP exchange-correlation functional, the 6-31G(d,p) basis set, and the Grimme dispersion corrections [1]. As a polyamide fragment, the ACA dioligomer was used, which is formed by the condensation of two ACA molecules, and a polyaromatic molecule with a gross composition of $C_{48}H_{18}$, which is commensurate with the dimer of the considered amide, was chosen as the graphene-like plane. It was believed that the energy of a covalent bond is numerically identical to the energy effect of the reaction of its homolytic cleavage with the formation of two radicals in the doublet state. The analysis of the results of quantum chemical studies shows that the bond between nitrogen and carbon atoms (−HN−CO−) in the amide group of the free ACA dioligomer molecule turned out to be the strongest and its energy is 447.1 kJ/mol. In the formed nanocomposite polyamide–fragment of a graphene-like plane, the energy of all investigated covalent bonds significantly increases compared to the free ACA dioligomer molecule.

The experimental study of PA6, PA 6.6 and PA 12.12 nanocomposites showed an increase in strength characteristics compared to the initial polymers with the same preliminary thermomechanical treatment, a change in the degree of crystallinity, an increase in the maximum oxidation temperature of high-molecular (crystalline) areas of polymer materials, etc. with a low content of carbon nanotubes.

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Synthesis of carbon and gold nanoparticles in metal-alkanoate matrix: a study of structural properties and electrical behavior

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The focus of this work is on studying the structural and electrical properties of ionic metal-alkanoate composites consisting of a cadmium octanoate matrix in combination with various types of nanoparticles. Specifically, carbon and gold nanoparticles were chemically synthesized within the smectic A phase of ($Cd^{+2}(C_7H_{15}COO)^{-2}$, brief - CdC_8), which served as a well-ordered nanoreactor. The size and shape of the nanoparticles were precisely controlled during the synthesis, resulting in highly stable and organized nanocomposites. The structural properties of these nanocomposites were studied using the transmission electron microscopy (TEM) technique, which allows an understanding of the nanoparticle locations and estimation of the sizes and dispersion of the synthesized nanoparticles.

The electrical characteristics were studied at different temperatures corresponding to different phases of the material. Since our samples have a layered structure of smectic A, we examined the electrical properties parallel and perpendicular to their cation-anion layers. We compared the electrical properties of both pure matrix and nanocomposites with gold and carbon nanoparticles to find out their role. Notably, the nanocomposites exhibited anisotropic conductivity, highlighting the structural anisotropy of the material. Based on the experimental data, a simple model of the charge transfer process is proposed.

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Rapid-hardening nanoengineered cementitious composites with enhanced operational properties

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The development of rapid-hardening nanoengineered cementitious composites with high operational properties is based on the principles of directed control of the processes of early structure formation at the nano-, micro- and macro-scale levels due to the establishment of regularities in the selection of component and particle size composition, changes in the energy and physico-chemical parameters of the surface of nanoparticles with the provision of nucleation effects, adsorption modification, self-reinforcement, self-autoclaving, photocatalysis.

A fundamentally new concept of creating ultra rapid-hardening nanoengineered cementitious composites with enhance operational characteristics has been introduced, which involves the use of nanomaterials with an extremely high surface area-to-volume ratio and a large proportion of surface or interfacial atoms. The synthesis of nanocomposites of various types (N-C-S-H-PCE, Ca-Al LDHs) with a huge specific surface and metastable characteristics, which determines their extremely high surface energy and reactivity during the formation of the structure of cementitious systems in the early stages, was carried out [1, 2].

This work shows that by controlling physico-chemical processes at the nanoscale level, it is possible to adjust the technical characteristics of the material as a whole to obtain nanoengineered cementitious composites of a new generation with fundamentally new properties and functions that provide long-term high mechanical, technical and environmental characteristics of buildings and structures, in including in extreme operating conditions. At the same time, ultra-high-strength cementitious composites will provide significant prospects for the development of advanced technologies for the creation of fortification and protective structures and objects.

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Mechanisms of structural functionalization of the α-form of polyamide-6 with methylene blue

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It is shown that the structural functionalization of PA-6 with the MB dye leads to the rearrangement of the electronic and vibrational structure, the degree of crystallinity, and the mechanical properties, which contributes to the increase of electrical conductivity in the percolation region caused by the strengthening of tunnel transitions. In Fig. 1. the dependence of electrical conductivity of PA-6 on the content of MB is given.

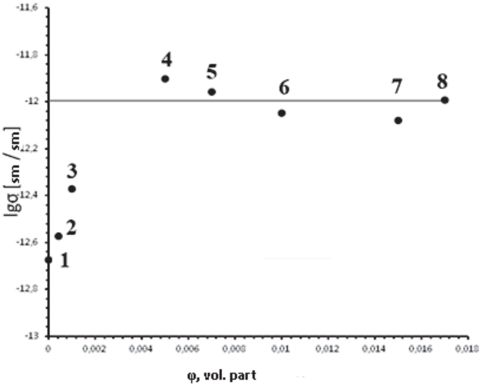

Fig. 1. *Dependence of electrical conductivity (in a logarithmic scale) of bulk PA-6 with the α-form of the crystalline phase on the concentration of MB 0 (1), 0,001 (2), 0,002 (3), 0,005 (4), 0,007 (5), 0,01 (6), 0,015(7), 0,017 vol. part (8) (T=293ºK)*

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Hierarchical Sn-beta zeolites as selective catalysts for Baeyer-Villiger oxidation of D dihydrocarvone with H_2O_2

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The conversion of biomass-derived terpenes and terpenoids into high value-added compounds opens the way to sustainable and environmentally friendly chemical synthesis. Baeyer-Villiger oxidation of D-dihydrocarvone with hydrogen peroxide allows to obtain lactone (4-isopropenyl-7-methyl-2-oxo-oxepanone), which is used for production of flavouring substances. Due to developed mesoporosity in hierarchical Sn-beta zeolites, promoting accessibility of catalytically active Sn Lewis acid sites (LAS) for reactants, these materials can be promising catalysts in the aforementioned reaction. The crucial role of Sn LAS in this material is to activate the carbonyl group of the ketone, making it more reactive towards the attack of an oxidant molecule [1].

Hierarchical (micro-mesoporous) and conventional (microporous) Sn-beta were prepared via a two-step post-synthetic method involving dealumination of commercial Al-beta (Si/Al=12.5) and conventional Al-beta (Si/Al=15), respectively, by nitric acid followed by wet impregnation in the absolute ethanol, containing anhydrous tin(IV) chloride. According to UV vis spectroscopy, most of the tin atoms in the obtained samples are localized in the zeolite framework in tetrahedral coordination and formed Sn LAS.

In oxidation of D-dihydrocarvone with H_2O_2 (30 wt% solution, 1,4-dioxane as a solvent, 90°C, 24 h), the higher selectivity towards corresponding lactone for hierarchical Sn-beta with Si/Sn=30 (89 % at 75 % conversion of ketone) compared to conventional Sn-beta with the same tin content (47 % selectivity) can be explained by lower Sn LAS strength localized on the external surface of hierarchical beta zeolite.

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Energy transfer processes in composites based on CdS QDs, Ag NPs and dyes

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Recently, there has been a growing interest in research related to the creation of new efficient laser media based on composites. Composites consist of semiconductor quantum dots (QDs) and laser-active dye molecules or noble metal nanoparticles (NPs).

The conditions for achieving fluorescence enhancement of composites will depend on many parameters, such as size, shape, structure and concentration of nanoparticles, chemical and spectroscopic properties of phosphor molecules, dielectric permittivity of the matrix. These parameters determine the spectrum of the plasmon resonance band of introduced nanoparticles, as well as the degree of influence of NPs on the probability of absorption, radiation, and non-radiative energy transfer processes.

The present study is devoted to the study of the influence of dyes with different absorption spectra on the spectrum and intensity of luminescence of CdS QDs and dyes, as well as the influence of silver NPs on the luminescence of CdS QDs.

The dependence of the contour of the fluorescence spectrum of CdS QDs on the type of dyes (methylene blue and acridine yellow) and the influence of the concentration of the dye on the intensity of their luminescence in the composite of CdS QDs / dyes was investigated. The influence of Ag NPs on the luminescence enhancement factor of CdS QDs and the dependence of this phenomenon on the concentration of silver nanoparticles in the CdS QD/Ag NP composite was studied.

It was found that at low concentrations of the dye, an increase in the luminescence intensity of the methylene blue dye is observed, which is explained by the mechanism of energy transfer from the CT (donor) to the dye (acceptor) by the Förster mechanism (FRET). However, at a high concentration of the dye, quenching of luminescence is observed, which is explained by the transition of part of the dye molecules into aggregates that do not luminesce. [1]

In the composite of CdS NCs with silver NPs, the luminescence of CdS NCs is enhanced due to the excitation of surface plasmons of silver NPs and, as a result, due to an increase in the local electromagnetic field. As the experiment shows, the luminescence enhancement factor of CdS NCs in the composite with silver NPs shows a concentration dependence. The increase in the luminescence intensity of CdS NPs is replaced by the quenching of their luminescence, remaining, however, greater than the initial value. We believe that this can be explained by taking into account the fact that metal NPs in a state of plasmon resonance participate in two processes - they absorb and scatter light.

The dominance of one of these processes depends on the distance between CdS NPs and silver NPs. As the distance between the particles decreases, absorption prevails over scattering. As the concentration of silver NPs increases, their density increases and they mainly absorb plasmon energy, which leads to a weakening of the luminescence enhancement effect of CdS NPs.

The investigated nanocomposites had stable characteristics and can beused as biological markers in nanomedical and biological applications.

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Facilitating photodegradation of organic contaminants using synthesized ZnO nanosheets

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The primary organic contaminants of wastewater, antibiotics and dyes, contribute significantly to environmental pollution. These pollutants not only compromise the integrity of aquatic life but also pose substantial risks to the health and vitality of humans and other living beings. Their concentration in water could potentially trigger cancer, induce genetic mutations and cause respiratory harm. Thus, the exploration and development of methods to purify organic contaminants is of significant interest. In this regard, photocatalysis emerges as a noteworthy solution, given its benign conditions, straightforward procedure, and eco-friendly characteristics. ZnO has earned considerable acclaim as a photocatalyst for pollutants degradation due to its superb transport capabilities, affordability, and non-harmful properties.

Our findings reveal that ofloxacin and methyl orange maintain considerable stability under UV light exposure, with no self-degradation observed. Moreover, following the mixture of the antibiotic and dye with ZnO in a lightless environment, their concentration remained unchanged, implying that the adsorption process could be disregarded. ZnO displayed remarkable photocatalytic efficacy in the degradation of contaminants under UV light exposure, achieving complete elimination of ofloxacin within 1 h and methyl orange within 2 h, respectively. The photodegradation of ofloxacin and methyl orange using ZnO under UV light treatment adhered to the first-order reaction, and the rate constants were subsequently determined.

Therefore, the results we have obtained underscore the superior photocatalytic effectiveness of the created ZnO in the photodegradation of ofloxacin and methyl orange under UV light exposure, showcasing its potential for environmental preservation.

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Nanocarriers based on xanthan and eumelanin natural polymers for metal nanoparticles encapsulation

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Natural polymers are well known for their biocompatibility, non-toxicity, biodegradability as well as their binding ability to drugs, inorganic and metal nanoparticles. Among them, the heteropolysaccharide xanthan and polyphenolic biopolymer eumelanin, which is an anticancer drug, play an important role as a templates for metal nanoparticles (MeNPs) encapsulation. MeNPs, stabilized in natural nanocarriers or natural drugs, can be used for controlled imaging-guided tumor chemotherapy. In the present work, the xanthan and eumelanin samples, of natural microbial origin, were used as templates for a simple and effective *in situ* synthesis of cobalt and silver nanoparticles in an aqueous medium.

The processes of borohydride reduction of cobalt and silver salts to metal nanoparticles in xanthan and eumelanin nanostructures respectively were studied depending on the concentration of salts and given matrices using photography, UV-Vis and FTIR spectroscopy, TEM. It was shown that the corresponding matrices provide high stabilization of Co and Ag NPs in an aqueous medium. The resulting CoNPs/Xant composition consisted of swollen xanthan coils ~47-97 nm in size containing small amorphous CoNPs ~1.3-9.8 nm in diameter. The morphology of the AgNPs/EMel composition is mainly represented by various EMel nanostructures containing silver metal nanoparticles of ~1.5-12 nm in size. However, in single large EMel structures the size of AgNPs can reach ~50 nm.

Photocatalytic degradation of ciprofloxacin in ultraviolet light using TiO_2

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Removal of antibiotics is very difficult due to its intractability and complex structure. Among the effective cleaning methods, advanced oxidation methods are distinguished. AOPs include: ozonation, Fenton's reaction (homogeneous process), radiation-stimulated catalytic reaction, electrochemical processes, ultrasonic treatment, liquid-phase catalytic peroxide oxidation, photolysis, photocatalysis [1]. The photocatalysis process is a green and inexpensive way to clean wastewater from antibiotics. For the degradation of the antibiotic to CO_2 and H_2O, it is necessary that the redox potential should be greater than that of the alkaline radical [2]. TiO_2 is most often used as a photocatalyst because this catalyst has good optical and electronic properties, chemical stability, reusability, non-toxicity and low cost. In addition, this photocatalyst allows you to oxidize antibiotics to CO_2 and H_2O. As a modification of TiO_2 uses, a combination with other semiconductors based on metal oxides, doping with metals and non-metals, sensitization with dyes, modification with MOF. Under the influence of light, MOFs behave like semiconductors and therefore can be considered as a potential photocatalyst for highly efficient antibiotic degradation due to their extremely high thermal and mechanical stability and excellent structural characteristics [3].

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Emission Spectroscopy of Underwater Discharge Plasma in the Synthesis of Metal Nanoparticles

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The process of electric erosion, which caused by gas discharge between metal electrodes immersed in a liquid, is one of the most interesting methods for generating metal nanoparticles. These methods have gained special attention due to their potential use in sterilization, treatment, and the production of materials for various fields such as medicine and agriculture.

This work focuses on the diagnostics of such a kind of underwater discharge plasma using optical emission spectroscopy. The investigation of plasma discharges in liquid between metal granules is carried out directly in the discharge chamber of the installation developed for synthesizing colloidal substances with metal nanoparticles. Four discharge modes have been examined, including discharges occurring in deionized water or electrolyte, as well as the same cases with the presence of air bubbles. The correlations between electrical parameters, plasma parameters, and the discharge liquid media have been investigated.

The electrical parameters, such as voltage, current, and power supplied, have been determined by analyzing the resulting wavelength during discharge burning.. The plasma parameters have been determined from the registered emission spectra. Specifically, the excitation temperature has been obtained by the Boltzmann plot technique based on the emission intensity of metal atomic spectral lines. Meanwhile, the electron density has been calculated from the full width at half maximum of spectral lines, broadened due to the Stark effect.

Synthesis of silver and gold nanoparticles and their binary systems by galvanic replacement in an ultrasonic field

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Galvanic replacement (GR) is one of the effective methods of decorating metal and semiconductor surfaces with metal nanoparticles and nanostructures. In particular, GR in the ultrasound field (sonogalvanic process) in solutions which containing reducible metal ions and surfactant synthesizes stabilized metal nanoparticles within the solution's volume [1,2].

This study aimed to determine the conditions for the synthesis of silver (AgNPs) and gold (AuNPs) nanoparticles colloidal solutions, and the binary system (AgAu)NPs in aqueous solutions of metal precursors and surfactant in an ultrasonic field using magnesium as a sacrificial metal.

It has been discovered that the shape of AgNPs and AuNPs is affected by the concentration of metal ions and the duration of sonogalvanic synthesis in both stationary and pulsating ultrasonic fields. The ratio of silver and gold precursors in the solutions has the biggest impact on the concentration of these metals in the (AgAu)NPs binary system. Kinetic regularities of sonogalvanic synthesis of nanoparticles have been established.

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Hierarchical TS-1 zeolite supraparticles prepared by spray-drying method

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Spray-drying (SPD) technique is a well-known reproducible and scalable way to produce fine particles (usually few micrometers size). When the sol of the nanoparticles (NPs) is used for the SPD, the hierarchical particles known as suprapraticles are formed.

Here we report an application of SPD technique to make zeolite TS-1 (MFI type) supraparticles from primary 110 – 130 nm TS-1 NPs, prepared by low temperature aging (90°C) of tetraethoxysilane, titanium isopropoxide and tetrapropylammonium hydroxide aqueous solution.

The proposed approach has following benefits:

1. Synthesis of hierarchical TS-1 zeolite supraparticles (HTS) do not need either long-time hydrothermal treatment (possibly, similar process takes place directly during SPD stage) or application of secondary long-chained or gemini-type surfactants.
2. The TS-1 HTS of 2 – 10 micrometers size possess large surface area (up to 560 m^2/g) and biporous structure combining the micropores (1-1.2 nm) intrinsic to the zeolite NPs and secondary mesopores (40-50 nm). It is favorable for catalytic applications, particularly, for reactions of bulky molecules, which are not able to enter inside the zeolite micropores.
3. The TS-1 HTS demonstrate up to 100 % conversion and 90 % selectivity it styrene conversion to styrene carbonate, which is superior to 250 nm TS-1 particles, prepared by a standard procedure.
4. The TS-1 NPs sol pretreatment and SPD procedure conditions allow to get TS-1 HTS formed by either individual or «glued» particles.

About the lattice formation in the structure of islands of electron-hole liquid in some single-layer dichalcogenides

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Recently, electron-hole liquid (EHL) in dichalcogenides of transition metals (DTM) has been under intense research [1]. In 2D systems, EHL should be formed in the shape of individual islands. As a result of carrier recombination processes, the island has a finite radius, the size of which depends on the recombination speed and radiation intensity. Currently, there is almost no investigation of EHL droplets in DTM, and the interaction between islands has not been considered until now. The studying EHL in low-dimensional structures remains relevant, in particular for applied purposes [2].

The stochastic theory of the formation of spatial structure of EHL under light irradiation was composed in [3] for 2D semiconductor systems using the kinetic approach applied to excitonic liquid [4]. Using this methodology, we performed simulations in the case of homogeneous irradiation of the DTM layer (namely, MoS_2 and $MoTe_2$). The kinetic equation for the number of particles in the island was solved together with the equation for the diffusion of excitons outside the island, taking into account the spatial distribution of the pumping.

The pumping was assumed to be in the shape of a strip, the thickness of which varied from the value, at which the formation of islands was possible along the line of the strip only, to thicker strips, where the formation of several rows of EHL islands is possible. The parameters of the locations of the islands were estimated depending on the geometry of the system and the pumping intensity.

The ordered arrangement of EHL islands in the layer of a dichalcogenide is an example of the new type of lattice in a 2D structure.

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Photocatalytic activity of nanosized TiO_2/WO_3 composites synthesized by mechanochemical method in the decomposition of metronidazole

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One of the promising methods of decomposition of drugs, which contaminate water sources, is the photocatalytic destruction of these substances on heterogeneous catalysts, among which TiO_2 is one of the most popular. However, this catalyst has a number of disadvantages, so the intensive search of the systems with improved characteristics on the base of complex oxides composition (including TiO_2) and the methods of their synthesis attracts the attention of the most scientific lab [1].

The mechanochemical synthesis (MChT) of the samples TiO_2/WO_3 with a molar ratio of 1: 1 in medium, such as air, water, ethanol, was realized in this study.

It was shown that MChT permits to obtain the samples with larger specific surface area and total pore volume than the initial oxides mixtures. It was established that the treated system TiO_2/WO_3 = 1:1 (water) demonstrates there the significantly higher photocatalytic activity (K_d) and the degree of metronidazole photodegradation (G) under the action of UV light than the modified system TiO_2/WO_3 = 1: 1 (air, ethanol) or the initial TiO_2/WO_3 = 1: 1.

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Photothermal transformation in silicon based nanomaterials

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Photothermal methods are promising for the study of various nanostructured materials with different morphologies. Such methodologies are based on the photothermal transformation effect: excitation of thermal fields in material due to its irradiation with visible light. The most significant advantages of these methods are the possibility to perform measurement contactless, which is crucial in applications to nanostructured materials.

During the talk, we will analyze the applications of the photothermal approaches for the investigations of thermal transport properties of silicon-based nanomaterials like porous silicon, silicon nanowires arrays, multilayered structures. Specifically, we will focus on the applications of the Raman approach [1] as well as gas-microphone [2] and piezoelectric [3] photoacoustic techniques for characterization of such materials.

We will show the advantages of the complimentary use of these approaches for the study of thermal transport anisotropy of the mentioned above systems. Specifically, thermal conductivity tensor was measured in silicon-based nanostructured materials. The strong anisotropy in the heat propagation was demonstrated in the case of porous silicon and silicon nanowires arrays.

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Hierarchical zeolites and nanocomposites – effective catalysts for cyclic carbonate synthesis from styrene under CO_2 pressure

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The structure and chemical composition of zeolites affect their chemical nature of the surface, adsorption, acid-base properties, determining their use in heterogeneous catalysis (chemical and petrochemical industry, fine organic synthesis), separation of gas mixtures and gas sorption, ion exchange. Zeolites, which have several levels of pores that exist in an orderly manner in the material, and the presence of pores of a larger diameter improves access to smaller pores, are classified as hierarchical. Cyclic carbonates are widely used in the chemical industry, in particular as monomers of biodegradable polymers, electrolytes of lithium batteries, precursors in organic synthesis, aprotic polar solvents. The development of zeolite hierarchical catalysts for the heterogeneous-catalytic liquid-phase production of cyclic carbonates is a promising direction.

CeO_2-containing materials show a fairly high activity in the first stage of the reaction of obtaining cyclic carbonate from styrene – (oxidation of styrene with hydroperoxide of tert-butyl alcohol to the corresponding epoxide) - conversion of styrene up to 77%. Provided that the second-stage catalyst (zeolite with basic properties or Bu_4NI is present in the reaction mixture, the styrene epoxide formed in the first stage was almost quantitatively transformed into the corresponding cyclic carbonate. In the absence of an additional catalyst of the second stage, the epoxide was partially converted into a cyclic carbonate, most of the epoxide was further oxidized to ketoalcohols or diketones. Modification of CeO_2-containing materials with magnesium oxide led to a decrease in the conversion of styrene, but increased the selectivity for cyclic carbonate, which was manifested in a significant decrease in the number of products of deep oxidation of styrene. Such a change in catalytic properties can be caused by an increase in the basicity of the catalyst. The development of research can be the optimization of the oxidation process of olefins (for example, styrene) with oxidants of various nature with the participation of "softer" catalysts (for example, titanosilicate zeolites of various types). The selection of heterogeneous catalysts for the second stage of the process – the formation of cyclic carbonates from epoxides under CO_2 pressure can be focused on Cs-exchangeable forms of zeolites (or other alkali metals) as well as titanosilicate zeolites.

Nano- and microplastics pollution in Ukraine

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According to US National Oceanic and Atmospheric Administration, microplastics are synthetic organic polymer particles with a size less than 5 mm [1,2]. But there is not clear definition of nanoplastics. There are two views on which particles can be called nanoplastics [3]. According to the first point of view, nanoplastics are organic polymer particles with sizes from 1 to 100 nm [4]. This is consistent with the common definition of nanoparticles. But there is also another point of view, according to which the size of nanoplastics is in the range from 1 to 1000 nm [3].

Nano- and microplastics pollution is a significant ecological problem. The disintegration of plastic waste is a main source of these pollutants in water, but there are many other sources, including wastewater after treatment, tire wear, paint failure, industrial processes, textile washing, personal care products, at-sea losses, etc. [2,3]. In Ukraine, the problem of nano- and microplastics is still not given sufficient attention due to the fact that in Ukraine in general, plastic packaging gained popularity much later than in Europe or the USA. But currently, there is a huge amount of unprocessed plastic waste in the country, which is a potential source of micro- and nanoplastics.

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Magnetic properties of Laponite/magnetite composites

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This work discusses structure and magnetic properties of magnetite Fe_3O_4 (M) prepared by the Elmore method and Laponite® based magnetic composites (LapM). For *in situ* preparation technique, the LapM composites were obtained from mixtures of Lap platelets and iron Fe^{2+}/Fe^{3+} salts using co-precipitation reaction in the alkaline environment. For ex situ preparation technique, the LapM composites were obtained by mixing of M with Lap platelets in aqueous suspensions. The synthesized magnetic materials were studied by Roentgen-phase analysis, IR spectroscopy and Quantum Design PPMS DynaCool vibrating sample magnetometry. *Table 1* presents the main characteristics of the studied magnetic materials.

Table 1.

Main characteristics of the studied materials at T=300 K

Samples	**M (Fe_3O_4) #1**	**LapM in situ, #2**	**LapM in situ, #3**	**LapM ex situ, #4**
Concentration of Fe (wt. %)	70.56	50.3	39.7	39.2
Lattice constant, nm	0.8368(8)	0.8345(5)	0.8366(8)	0.8353(3)
Particle size, nm	9	9	15	11
Magnetization, emu/g, H= 2000 Oe	57.7	42.6	19.7	28.5

The magnetization loops, *M(H)*, were measured at temperatures T=3÷380 K in magnetic fields up to 4 kOe. The temperature dependences of the magnetization, *M(T)*, were measured in ZFC-FC mode in magnetic fields of 0.1, 0.3, and 1 kOe. The *M(H)* and *M(T)* data confirm the transition of all samples to the superparamagnetic state at T>300 K. In this case, the coercivity of the samples tends to 0 Oe being 225÷270 Oe at T=3K. The data obtained indicate the presence of deep integration of the M and Lap components in the investigated LapM materials.

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New hybrid nanosystems based on curcuminates

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Due to their high biological activity and wide spectrum of application, curcuminoids attract the attention of researchers. Curcumin, as their main representative, is used in complex therapy of autoimmune, infectious, neurodegenerative and oncological diseases. Its advantage is non-toxicity, low working concentrations, a wide range of practical applications from biological activity to fluorescent properties. Poor solubility in water and rapid clearance prevent curcuminoids from realizing their potential. Quite simple ways to eliminate these shortcomings are the modification of the diferuloylmethanate molecule - the synthesis of Schiff bases to obtain complexes based on them. Currently, the therapeutic effect of a number of complex compounds of curcumin with transition metals has been studied, which indicates the efficiency of this approach.

The purpose of this study is the synthesis of modified curcuminoids, mono- and heterometallic complexes based on them. A new strategy is the study of hybrid systems based on them, obtained by grafting curcuminoids onto the surface of inorganic and polymer matrices. At the same time, an important task is to establish the relationship between composition   structure   properties.

A new curcuminoid based on alanine was synthesized, its composition, structure and properties were determined. New mono- and heterometallic metal complexes of 3d- and 4f metals were obtained. Hybrid systems were obtained by grafting metal curcuminates onto the surface of halloysite nanotubes. Spectral-luminescent properties, dispersion and morphology of all synthesized compounds were studied. It is shown, that hybrid systems based on curcuminoids are characterized by high dispersion and stability, which allows them to be proposed as precursors of functional materials.

Multicomponent nanostructured adsorbents for arsenic compounds removal

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High arsenic level in natural water is typical for China, Taiwan, Vietnam, Bangladesh, India, Iran, Ghana, Hungary, USA, Mexico, Chile, Argentina, etc. [1-3]. In these countries, arsenic concentration in groundwater can often reach 40 mg/l, which is 4000 times higher than the maximum allowable arsenic content (10 μg/l) in drinking water [1,2]. Excessive and prolonged consumption of arsenic-containing drinking water may cause a lot of health consequences due to mutagenicity, teratogenicity and carcinogenicity of arsenic compounds [4].

There are a lot of arsenic removal methods, but adsorption is the most commonly used treatment method [1]. Multicomponent adsorbents are often significantly effective then based on single component. The arsenic removal of activated carbon modified by iron(III) oxyhydroxide is 51% more than unmodified carbon [1]. Multicomponent adsorbents based on zeolites or different oxides are also effective for arsenic removal. So, multicomponent nanostructured adsorbents are very perspective materials for arsenic compounds removal.

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Green approaches in synthesis of $Z_nM_xO_y$ (M = V or Mo) from oxides

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Complex mixed oxide systems $Z_nM_xO_y$ (M = V or Mo) have attracted considerable attention as effective catalysts, anode materials and promising rare-earth-free phosphors due to its high absorption and emission properties and low cost of raw materials. The traditional synthesis of mixed oxide systems $Z_nM_xO_y$ is either energy-consuming or leads to water pollution. Our goal is to develop a green low-temperature synthesis of $Z_nM_xO_y$ without water pollution.

The raw materials for the syntheses used ZnO and V_2O_5 (MoO_3) that was treated: i) mechanochemically on a Pulverisette-6 planetary ball mill in an aqueous medium during different times; ii) barothermaly in steel autoclave in water medium; iii) ultrasonically in water medium at room temperature. Synthesized samples were characterized by XRD, BET, SEM, TEM, FTIR, TPR-H_2 and DTA. The key role of water in the formation of ZnM_xO_y systems from poorly soluble oxides was shown. Based on the results of the SEM and TEM methods, a topochemical mechanism for this reaction was proposed. XRD data shows the formation of $Z_nMoO_4 \cdot 0.8H_2O$ and $Zn_3V_2O_7(OH)_2 \cdot 2(H_2O)$ phases in all cases. DTA shows a loss of crystalline water in the temperature range 150-350 °C with the formation of Z_nMoO_4 and $Zn_3V_2O_8$ confirmed by XRD analysis. The TEM and SEM images of Z_nMoO_4 show a structure of short needle-shaped particles and $Zn_3V_2O_8$ have the morphology of thin nanoplates. The PL spectra of zinc pyrovanadate obtained by alternative syntheses have intense broadband emission from 400 nm to 700 nm. So, alternative syntheses with mixture ZnO and V_2O_5 (MoO_3) in water medium makes it possible to synthesize nanostructured complex mixed oxide systems at room temperature, avoiding environmental pollution.

Magnetron nanocoatings on chitosan films: XRD characterization

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Metallic thin coatings with nanometer thickness on the surface of polymeric films are important for the development of novel materials in various fields: organic electronic devices, medicine, smart packaging and protective films. The characterization of the coatings and their interaction with the substrate is essential. One of the methods necessary for such characterization is XRD phase analysis, which gives information about the crystal state of the coatings. Ti, TiN, TiO, Mo, MoN, Zn, ZnO coatings on chitosan films were deposited by magnetron sputtering. Coating thickness was 10-30 nm.

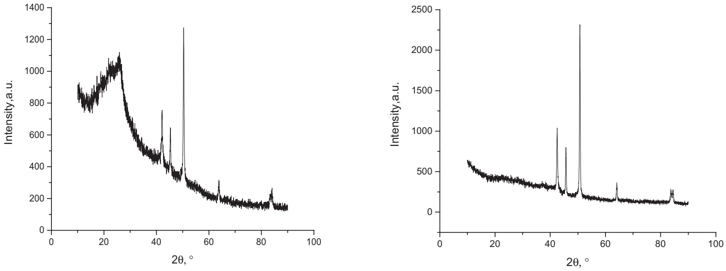

Fig. 1. XRD pattern of Zn coating on chitosan (left) and glass (right).

XRD studies of coatings on the chitosan films deposited during 3 min reveal no crystal phases in the coatings, but this is may be due the low thickness, when it is not sufficient for detecting the X ray diffraction patterns due to little number of crystal planes taking part in the XRD pattern formation. When the deposition time is longer than 9 min, embrittlement of the chitosan substrates is too intense, so we used deposition in the same condition on a glass substrate as a reference samples. The crystal composition, crystal state of the coatings strongly depend on their elemental composition and do not depend on the substrate.

Microwave absorbing performances of hybrid composites based on nanocarbon and magnetic nanoparticles with negative permeability

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This results of the study of segregated polymer composites based on ultra-high-molecular-weight polyethylene (UHMWPE) filed with hybrid filler - nanocarbon and magnetic nanoparticles. As nanocarbon particles we use graphite nanoparticles (GNPs) and Fe, Fe_3O_4 and Co_3O_4 as magnetic component. Shielding of the reflection and transmission spectra in the frequency ranges 40 – 360 GHz of such segregated polymer composites (SPCs) as a function of the content of electroconductive filler particles have been studied.. The enhanced EMI shielding efficiency of 237 dB is obtained for (GNPs-Fe)/UHMWPE SCM at 5wt.% of the filler content. SE_A values were found to be much higher than SE_R for all types of developed SCPs materials. It indicates a leading role of absorption factor in the overall EMR decay which may be explained by the significant role of EM-waves multiple-reflection inside a composite specimen with segregated structure. The phenomenon of negative imaginary permeability has been revealed for all types of with the influence of of type and content of fillers, frequency on the imaginary permeability has been investigated. As we know, a positive imaginary part of permeability manifests by convention the magnetic energy loss. Contrarily, a negative value denotes the magnetic energy radiation out of the investigated material. Up to now the discussion about the nature of negative imaginary permeability is a hot topic [1,2]. We hypothesize that the source of that radiated energy is in the motion of charges under the ac electric field. Such motion of charges produces an ac magnetic field. Motion of charges is fed on the electric field energy so this energy loss appears as an increased imaginary part of permittivity. In the considered CMs a negative imaginary permeability is accompanied by an essential increase in the positive imaginary permittivity which can be treated as the total energy loss due to the prevailing dielectric loss.

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How does the fullerene C_{70} feel the presence of a dye with donor electrons?

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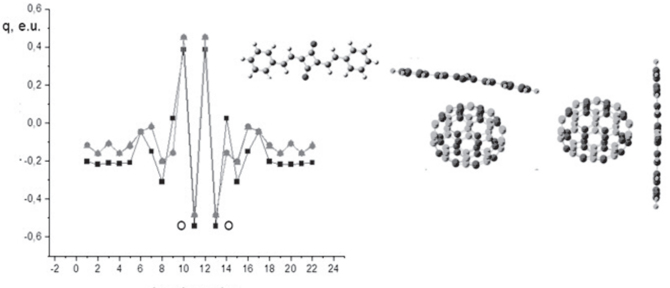
The improvement of the efficiency of organic solar cells is an important scientific challenge [1, 2]. Maximum power conversion efficiency for elements based on C_{60} and dyes has been reached the level of around 15 %. This percentage could be increased if the fullerene C_{60} molecule is substituted with the C_{70}molecule because of its advantages when compared to the C_{60} molecule: allowing a broader absorption spectrum and more efficient photo-current generation.

Here we report about charge redistribution on fullerene C_{70} when interaction with squaraine dye, shown in fig.1, a for two locations around fullerene. The first location is parallel to the longest diameter of C_{70} (fig.2, a) and the second one is perpendicular to it (fig.2.b).



a *b* *c*

Fig.1. *Optimized geometry of squaraine dye and atomic charges in initial state (black squares) and in the complexes b (blue triangels) and c (red traingles).*

It can be seen in fig. 1,a that charge distribution on the π-conjugated chain of the dye changes: equalized charges in the initial state became alternated (1-6, 17 – 22 atoms). Oxygen atoms got less negative charges in the complexes, proving the charge transfer onto fullerene.

Molecule of C_{70} fullerene has 30 atoms with negative charges and 40 atoms with positive charges. In complex with squaraine dye 31 atoms have negative charges and 39 – positive charges for perpendicular location. In case of parallel location amount of positively and negatively charged atoms is the same as in pure fullerene despite of slight redistribution between the atoms. Additional negative atom on C_{70} molecule appears on the side close to the dye.

Obtained results of charge distribution in complexes of C_{70} with dye point on that orientation of C_{70} molecules is important for the effective charge transfer in the solar elements.

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PS@PNIPAM core@shell nanoparticles: tuning of LCST

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Amphiphilic nanoparticles of the "core-shell" type are intensively used as carriers of small molecules, in particular for intracellular delivery of anticancer drugs [1,2]. Thermo-responsive PNIPAM-based NPs used in biomedical field usually are obtained in a form of nanosized gels dispersed in water. The inherent lower critical solution temperature (LCST) of PNIPAM-based "shell" is ~32°C [3] what is a sufficient drawback for NPs intravenous administration due to aggregation of NPs [4].

In the presented study nanoparticles with polystyrene in the "core", and the outer "shell" formed by a layer of (N-isopropylacrylamide-co-acrylamide/ N, N-dimethylacrylamide) copolymers with different starting ratio of monomers were investigated. LCST of PNIPAM-based "shell" of NPs was tuned by copolymerization of NIPAM with hydrophilic monomers (e.g., acrylamide (AA) or N,N-dimethylacrylamide (N,N-DMAA)) to ~38-40°C. The effect of the molar ratio of the copolymer components as well as outer "shell" thickness on the thermal sensitivity of the nanoparticles dispersion was found. It was determined that the increase in the content of acrylamide units in the poly(NIPAM-co-AA) copolymer shell cause the increase of the "coil-globule" transition temperature.

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Hierarchical zeolites as selective catalysts for epoxidation of cyclic olefines with H_2O_2 and organic peroxides

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Epoxides are quite important materials which have wide use as precursors for production of different valuable polymers, in particular, cyclic carbonates [1]. Mild oxidation of olefines is one of the important methods to produce epoxides. Ti-containing zeolites are known to be effective catalysts for olefin epoxidation process [2]. However, in process involving “bulky” cyclic olefines molecules, such as cyclohexene or cyclooctene, the activity of microporous "zeolites" is extremely low, due to their diffusion and steric limitations [2]. The creation of materials with a developed external surface (hierarchical zeolites), and a high concentration of active centres on the external surface is aimed at significantly improving the catalytic activity of these materials.

In the work, a number of Ti-containing hierarchical zeolites were obtained using Gemini-type surfactants as structure-directing agents. Such materials are characterized by a developed external surface and a high proportion of active centres available for bulk molecules. A high selectivity of activity in relation to the target product was revealed in the case of Cs-AlBEA in the styrene oxidation with hydrogen peroxide at a temperature of 100 ^{0}C (Fig. 1). Such materials are also expected to be active and selective catalysts for the oxidation of cyclic olefins with hydrogen peroxide under milder conditions.

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Influence of annealing duration on the structure and magnetic properties of Co-Pt thin films

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CoPt-based magnetic thin films are attractive materials for different spintronic, permanent magnets applications and exchange coupled composites [1]. The formation of ordered magnetic phases in Co/Pt based thin films at low temperatures when bulk diffusion is frozen may require a longer annealing duration [2].

In present study, Pt(14 nm)/Co(13 nm)/Ta(3 nm) were sputter deposited on SiO_2/Si substrate and annealed in high vacuum at the temperatures of 450 °C and 550 °C with annealing duration from 30 minutes to 8 hours. X-ray diffraction was used to analyze the effect of annealing duration on structure of the post-annealed stacks. Chemical composition and magnetic properties were determined by SIMS chemical depth profiling and VSM magnetometry.

Despite the fact that the disordered *A1*-CoPt remains the main phase in the stack composition, a long heat treatment time leads to complete homogenization of the stack structure and an increase in the coercive field.

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Morphology, structure and optical properties of “nanocellulose+$K_3Tb_{1-x}Eu_x(PO_4)_2$” composites

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Growing field of optoelectronic devices usage requires new efficient eco-friendly materials. Nano/microcrystalline cellulose and its derivatives have been considered recently as a basic component of “paper” electronics. The physicochemical properties of cellulose-based materials can be significantly improved by adding of some fillers e.g., oxides. The interaction between this natural polymer host and filler determines many useful features of the cellulose-based composites. Unfortunately, a little attention has been paid to such interaction due to its high complexity.

Here, we report morphology, structural, and optical (luminescent) properties of cellulose composites containing $K_3Tb_{1-x}Eu_x(PO_4)_2$ luminescent oxides.

Composites were made from bacterial nanocellulose or commercial microcrystalline cellulose and noted oxide, taken in the form of micro/nanopowder, as a result of mixing aqueous suspensions of micro/nanocellulose and oxide with subsequent ultrasonic treatment and drying in air.

The data on optical properties of “cellulose+$K_3Tb_{1-x}Eu_x(PO_4)_2$” composites were analyzed together with corresponding data for starting oxide micro/nanopowders and suspensions of initial cellulose. It was found that visible luminescence of composite films can be excited from ultraviolet to blue spectral region. The cellulose-related luminescence band with maxima near 570 nm was observed when excitation took place at 440 nm, while only weak Tb^{3+}-related emission was found for this excitation wavelength. The Eu^{3+} - related luminescence was observed for excitation at 473 nm. The studied composites can be considered as a multi-colored luminescent material suitable for use in 3D printing devices.

Magnetocapacitance effect in tunnel contact with perpendicular anisotropy of magnetic electrodes

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In this report, we want to consider the features of the magnetocapacitive effect in tunnel magnetic contacts with perpendicular magnetization of magnetic electrodes. Great interest in magnetic tunnel junctions is caused by the fact that not only a large value of tunnel magnetoresistance is obtained by the fact that in recent years in tunnel contacts with interfaces of the Fe/MgO type, a significant change in the capacitance in the magnetic field has been experimentally registered.This effect is called the magnetic tunneling capacity (MTC) effect, and it is considered one of the most promising effects that may have practical applications in memory cells and other spintronic devices. In contact tunnels with perpendicular anisotropy, the antiparallel orientation of magnetization radically changes the distribution of the magnetic field in the contact barrier layer and causes the appearance of a high-gradient magnetic field in the direction of magnetization of the contact magnetic electrodes. Under the action of such a high-gradient field, there is a spatial separation of spin-polarized major and minor electrons of electrons in the interface region, which creates an inhomogeneous distribution of electric charge in the contact barrier layer. As a result, an additional energy barrier for major spin-polarized electrons appears near each of the magnetic electrodes, and an additional effective capacitance, called spin capacitance, appears in the contact barrier layer. This additional spin capacitance can significantly reduce the total capacitance of the tunnel magnetic contact. The value of such additional spin capacity is proportional to the value of the spin polarization of electrons in the magnetic electrodes and the value of the magnetic field gradient with antiparallel orientation of their magnetizations. The mechanism of tunnel magnetic capacitance described by us is not only fundamentally different from the mechanism of tunnel magnetic capacitance in tunnel contacts with Fe/MgO interface boundaries, but also, in our opinion, has a better prospect for practical use. The large values of TMR and TMC in tunnel contacts with Fe/MgO interfaces are related to the features of the electronic structure of the Fe/MgO interface, where the effective spin-dependent tunneling effect is ensured by a good agreement between the crystal lattice parameters of the iron magnetic electrode and the crystal lattice parameters of the magnesium oxide nanolayer. In tunnel magnetic contacts with perpendicular magnetization of the electrodes, such matching of the grid of the magnetic electrode and the barrier nanolayer is not a strict necessity, which allows to simplify their manufacturing technologies. We conducted experimental studies of magnetoresistance and magnetocapacitive effect in tunnel magnetic contacts $Tb_{22}Co_5Fe_{73}/Pr_6O_{11}/Tb_{19}Co_5Fe_{76}$ with perpendicular magnetization of magnetic electrodes and a paramagnetic barrier layer. At room temperature, the value of tunnel magnetic resistance exceeds 110%, and the value of tunnel magnetic capacitance exceeds 115%.

Ceramic membranes based on silicon carbide

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Ceramic membranes based on silicon carbide (SiC) have many advantages over ceramic materials made from aluminum oxide, silica, titanium oxide, and silicon dioxide. These advantages include thermal and improved chemical stability, and high mechanical properties. SiC ceramic membranes are used to separate gases and liquids, namely for wastewater treatment, in the energy, gas purification, food and pharmaceutical industries [1].

In recent years, research has been conducted on reducing the temperature and maintaining high porosity of sintering SiC ceramic membranes. This was achieved by adding mullite, silicon dioxide, zirconium, alumina, zeolite and glass. Alumina reduces the sintering temperature from 2200°C to 1350-1500°C, and liquid glass - to 800°C [2].

We synthesized a series of membranes based on silicon carbide with the addition of sodium tetraborate, aluminum oxide, sodium and ammonium carbonate. The physicochemical properties of ceramic membranes were studied using diffraction methods of analysis, scanning electron microscopy, and transport and mechanical characteristics were determined.

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Functionalization of montmorillonite clay composite by grafting with organic compounds

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The functionalization of the surface of natural clay minerals allows an opportunity for obtaining new materials with controlled properties and a winde range sphere potential technical and environmental applications. Various inorganic (metal oxides and oxyhydroxides) and organic (polymer, surfactant) compounds are used for this purpose.

The main objects of this study were natural montmorillonite (MMT) from the Cherkasy deposit (Ukraine) and a composite based on MMT. The highly porous MMT composite was synthesized according to the method described in [1], considering the ratio HDTMA/CEC = 5/1 mass ratio. Surface functionalization of the studied samples was carried out with the help of chemical modification. For this aim we are used organic compounds containing active acid groups (-COOH) and basic groups ($-NH_2$).

The successful surface modification of MMT and MMT composite confirmed X-ray phase analysis and IR spectroscopy. Titration methods determined the content (wt.%) of grafted functional groups. For all modified samples, the content of amino groups was 2.5 wt.%, and for carboxyl groups - 2.9 wt.%.

In this work we also considered the possibility of using the obtained materials as adsorbents for treatment polluted waters from copper ions. The results indicate an increase in the sorption capacity of the synthesized materials to Cu (II) ions compared with the pure samples in the range of initial concentrations 0.1-10 mgL^{-1}.

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An improved plasma chemical method for fabrication of AgNPs-GO nanocomposite with functional properties

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As an innovative approach, graphene oxide-silver nanocomposite (GO-AgNPs) was fabricated by the usage plasma-chemical method. Graphene-based powders were obtained by the method of controlled detonation gas synthesis. The method involves extracting the finished graphene and subsequent thermal and mechanical activation in the vortex layer device. The carbon material obtained by this method is graphene with a content of the crystalline phase of graphite up to 32%. The average size of crystallites L of graphene sample is 168 Å. Physicochemical properties, antibacterial and cytotoxicity activity of both nanocomposites were subsequently studied comparing with free silver nanoparticles (AgNPs) and pure GO. The processed graphene samples are characterized by the presence of a certain amount of graphene oxide. The synthesized nanocomposite GO-AgNPs was characterized using UV–vis methods, powder X-ray diffraction. The surface morphology of synthesized nanoparticles was studied using scanning electron microscopy. It was detected, that syntheses Ag/GO composite exhibits properties such as good optical sensitivity to trace heavy metal ions, adsorption affinity, and catalytic activity for the removal of organic compounds. Thus GO-AgNPs can be considered a multifunctional nanocomposite that can be applied in various fields such as biomedical treatment and environmental remedy.

Effect of heating rate on the yield of the Ti_3AlC_2 MAX-phase

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The MAX-phases attract considerable attention as advanced materials due to their unique properties [1]. Now several ways are being proposed for their synthesis [2]. Most of them are complex procedures and require high pressures and temperatures. These approaches typically are featured by the sluggish interdiffusion between the sintered components, resulting in multiphase products. The synthesis of mono-phased stoichiometric carbides (MAX-phases) is fronted with crucial technological limitations. In this report, we notify about a simple approach to produce a high percentage of the MAX phase in the sample without high pressure. The structure of the synthesized MAX-phases is studied by XRD, SEM and NMR techniques. The influence of the heating rate on the formation of the MAX phase was established. The powder mixture was heated up to the final sintering temperature of 1435 °C with 40, 100, and 120 K/min rates. The sample, heated at 40 K/min, contained ~70 wt.% MAX-phases Ti_3AlC_2 and ~30 wt.% TiC. In the sample heated at a rate of 100 K/min, the amount of the Ti_3AlC_2 phase increases to ~88 wt.%. A further increase in the heating rate to 120 K/min changes the phase composition of the sample. The composite containing ~96 wt.% of MAX-phase Ti_3AlC_2 was successfully synthesized using the proposed method. This method is featured by the short time in duration, also. The proposed process is realized by a high heating rate (up to ~10^2 K/min), which inhibits unwanted phase formation and limits elemental loss due to the short-time process.

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Silica filler coated with ZnO nanoparticles for UV protection of polymers

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It is well known that polymers are most useful materials in modern world. Textile, automotive, electronics as well as space technologies are difficult to imagine without polymers and their compositions [1]. But degradation of polymers is observed under the influence of external factors, in particular UV radiation. ZnO is successfully used in ultraviolet protection of materials [2].

In this paper, composites based on high-disperse pyrogenic silica containing zinc oxide nanoparticles in the surface layer were studied. Such type fillers with ultraviolet protection properties are of considerable interest. Zinc oxide particles was obtained by impregnation of silica with an alcohol solution of zinc acetate followed by temperature treatment at 600°C. The zinc oxide content was 0.02, 0.2, 2 and 10 mmol per 1 g of silica. According to spectrophotometric studies of aqueous dispersion of silica coated with 10 mmol/g ZnO shows a transparency in the range of 400-900 nm, which is significantly reduced in the UV region with a maximum near 376 nm. X-ray analysis shows that only 10 mmol/g zinc oxide amount sample have diffraction peaks at $2\theta = 32^{o}, 34^{o}, 47^{\circ}$ and 56^{o} which are characteristic of the crystalline structure ZnO.

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Cobalt and Co/Mn nanocomposites with SiC and TiC for the Fischer-Tropsch catalysis

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A catalytic conversion of a gas blend named syngas ($CO + H_2$) into the mixture of liquid hydrocarbons, occurring at elevated temperatures and pressures in the presence of metal catalysts is known for a century as the Fischer-Tropsch (FT) process. The catalysts consisted of Co nanoparticles (NPs) and redox-active metal oxides, such as MnO, allows to get unusual FT selectivity with favorable formation of olefins, long-chain alcohols and other chemically valuable products [1]. The catalysts of this type are usually prepared by rapid co-precipitation of metal oxalates mixture followed by its reduction, to give intimate nanocomposite of Co NPs with corresponding metal oxide. However, the oxalate method is hardly compatible with application of inert catalytic supports, ensuring good diffusion characteristics of the catalyst and efficient heat sink from Co NPs, which is necessary due to high exothermicity of the FT process.

Herein we report novel nanocomposites of Co and Co/Mn catalysts with SiC and TiC carrier nanoparticles, prepared by oxalate precipitation. The nanocomposites were characterized by SEM, powder XRD, N_2 adsorption and H_2/D_2 dynamic exchange to measure specific surface of Co NPs. According to SEM EDX data, the active catalyst phase is uniformly distributed on the support. The supported catalysts appeared superior to unsupported ones in terms of specific catalytic activity (per Co unit mass) and selectivity to C^{5+} hydrocarbons and alcohols. Besides that, the catalysts Co/SiC and Co/TiC demonstrate enhanced selectivity to olefin formation, caused probably by the electronic effects of semiconducting SiC and TiC.

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Synthesis, characterisation and catalytic activity of TiO_2-based materials

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During last decade layered double hydroxides, also known as hydrotalcite-like compounds, have been extensively studied as catalysts or catalyst precursors. Since calcination of these materials yields mixed oxides with basic properties, layered double hydroxides have found applications in many organic reactions considered to be catalyzed by bases. However, different TiO_2 containing materials were investigated as promising materials for different catalytic processes. These properties induced by acid and base centers on surface, which obtained by different ways such as modification of surface, ion-exchange, post-synthetic treatment or composite formation. The physico-chemical properties of catalysts materials depend on preparation methods and post-synthetic treatment procedures. Formation of the Ti-containing layered double hydroxides may induce the lattice distortion and as a result different active sites obtaining.

The aim of this work was to improve the production of Ti-containing layered hydroxide materials and to study their catalytic activity. The layered double hydroxides were obtained by hydrothermal sol-gel method and characterized by XRD, TGA, N_2 ad/desorption, FTIR, SEM, TEM. The products of catalytic reactions were analysed by GC-MS.

It was shown that hydrothermal treatment of sol-gel reaction mixture with followed calcination of obtained powder induce double or ternary phase formation with small crystallite size with layer morphology. The phase composition depends on Ti-precursor nature, pH of reaction mixture and calcination temperature. These materials characterized by acidity that supported by Lewis acid sites that induce catalytic activity

As result, Ti-containing layered hydroxide materials were obtained by hydrothermal sol-gel method using different titanium precursors. It was shown, that phase composition strongly depends on reactiom mixture composition and postsynthesis theatment. This materials demonstrate catalytic activity.

Synthesis of substituted ((benzo[d]thiazol-2-yl) diazenyl) naphthalene-2-ols for holographic recording media application

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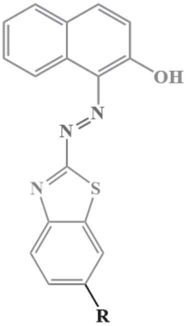
In recent decades, azo dyes based on various heterocyclic fragments have gained popularity among scientists. As they have a wide range of practical applications, for example, for dyeing fibers, photoelectronics, printing systems, optical data storage technologies [1], as textile dyes, they are also used in many biological reactions and in analytical chemistry [2].



R = $-CH_3$, -H, -Cl, -F, $-NO_2$

A series of substituted ((benzo[d]thiazol-2-yl) diazenyl)naphthalen-2-ols was synthesized with a good yield. The structure of the azo compounds was confirmed using 1H and 13C NMR spectroscopy, IR spectroscopy. The kinetics of photoinduced trans-cis-trans isomerization in ethanol solutions, as well as solvatochromic properties were studied using UV-Vis spectroscopy. It was shown that the rate of isomerization decreases upon passing from a donor substituent ($-CH_3$) to an acceptor one ($-NO_2$).

Thin polymeric films containing PMMA/Azo in 95/5 % ratio were formed from DCE solutions and the diffraction efficiency were studied. The diffraction efficiency values for the methyl-substituted compound at parallel polarization of the incident beam were 4 times higher than those for the nitro-substituted analogue, while the values of the diffraction efficiency at perpendicular polarization almost coincided.

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Prospects for the use of TiO_2/MOFs structures in photocatalysis

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Metal-organic frameworks (MOFs) are a class of porous materials with periodic lattice structures constructed by self-assembling organic ligands and metal nodes through bridging coordination bonds. Compared to conventional porous materials, MOFs have the following advantages: diverse structure, chemical functionality, ultra-high specific surface area, and tunable morphology and size [1].

Currently, MOFs are being actively studied due to the prospects of their use in the fields of gas adsorption, gas storage, gas separation, and sustained release of drugs [2]. In addition, due to their unique structural properties, MOFs have high photochemical properties. When nanomaterials are created with typical semiconductors, such as TiO_2 and ZnO, they enhance the photocatalytic activity of the latter by exciting the electrons of MOFs from the HOMO orbital to the LUMO orbital [3]. This can be explained by the photosensitivity of organic ligands and metal ions/clusters in MOF materials [4]. Therefore, the synthesis of nanomaterials is extremely promising for photocatalytic applications.

We have synthesized a series of TiO_2/MOFs samples for the photodegradation of pesticides.

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Selective nanoparticle layer for ceramic membranes

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Selective filtration plays a crucial role in various industrial and scientific applications such as water treatment, chemical and pharmaceutical industries, biomedical research, dairy production and more.

Ceramic membranes are highly regarded for their exceptional qualities, including resistance to high temperatures, chemical substances, and long-lasting durability [1]. These characteristics make ceramic membranes highly desirable for implementation in a wide range of industrial processes. Ceramic membranes can be enhanced by incorporating a layer of nanoparticles to further increase their selectivity and filtration efficiency.

This layer incorporates metal oxide nanoparticles like titanium oxide (TiO_2), zirconium oxide (ZrO_2), aluminium oxide (Al_2O_3), and others [2,3]. The presence of this layer can enhance the filtration properties of the membrane by enabling the selective permeation of specific substances while effectively retaining contaminants.

Using membranes with a selective nanoparticle layer allows for the efficient and selective removal of various hazardous contaminants from water.

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Effect of gold sputtered ceramic nanoparticles on the microstructure and shear strength of lead-free solder joints

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The miniaturization of soldered joints in electronic devices require the development of new lead-free solders (LFS) with improved thermophysical and mechanical properties. The Sn-Ag-Cu alloys of eutectic or near-eutectic compositions are considered the most promising and are widely used as solder materials. The reliability of solder joints is especially determined by the intermetallic compound formed at the joint interface. Unlike traditional Pb-Sn solders, SAC solders generally have a higher melting point and tin content. Therefore, formation and growth of the IMC layer occurs faster in the SAC solder joints, which leads to brittle fractures and a decrease in the service life of the joints due to thermal fatigue. To improve the properties and strengthen the base solder matrix, various nano-sized admixtures, in particular ceramic, are added. In contrast to metal nanoparticles, they are non-wettable by metal melts. To solve this problem, metallic coatings are applied to their surface to form core-shell structures and to improve adaptation to the solder matrices. As a result, the metal-coated layer forms a strong “bridge” that reacted with the LFS matrix to form an intermetallic layer during soldering. Another important requirement for the LFS application is their reliability in a wide range of operating temperatures, including sub-zero temperatures. In this work, the effect of ceramic Al_2O_3, TiO_2, SiO_2 and ZrO_2 admixtures coated with gold on the properties and microstructure of the solder joints based on Sn-Ag-Cu was studied both at elevated and sub-zero temperatures.

Quantum-chemical modeling of anthocyanin adsorption processes on the surface of inorganic sorbents

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To distinguish a most appropriate adsorbent (or its composites) for the release of Cyanidin 3,5-O-diglucoside via extraction methods, it is crucial to study the adsorption characteristics of each composite in respect to Cyanidin 3,5-O-diglucoside. Methods of quantum chemistry is convenient and prompt for theoretical calculation of such characteristics.

Therefore, the reaction enthalpy was calculated via computer simulation of intermolecular complex formation as means the consequent interaction of Cyanidin 3,5-O- diglucoside with silica, aluminosilicate and hydroxyapatite. Calculations were performed using the MOPAC 2016 software [1] using of the PM7 method [2]. The quantum chemical calculation results show that the smallest interaction enthalpy (ΔH 298 =-264.1 kJ/mol) among the three absorbents under investigation is belong to the silica. A much larger value is characteristic for aluminosilicate (ΔH 298 =-522.8 kJ/mol). And the largest enthalpy with the absolute value (ΔH 298 =-595.3 kJ/mol) was obtained for the interaction Cyanidin 3,5- O-diglucoside with a hydroxyapatite surface. Since the reverse the process to adsorption is desorption, therefore a release of Cyanidin 3,5-O-diglucoside molecules from the surface hydroxyapatite is thermodynamically the least likely among the three adsorbents tested.

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Peculiarities of iron titanate thin films synthesis and their physicochemical properties

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In terms of ecological photocatalysis, semiconductive materials have to satisfy the certain conditions as visible light absorption, non-toxicity, strong resistance to aggressive media and inexpensiveness. Titania is a commonly used photocatalyst in green chemistry application. Incorporation of Fe^{3+} cation in titania lattice depending on the synthesis conditions (heat treatment, iron content) can lead to crystallization of naturally formed phases such as hematite, pseudobrookite, pseudorutile, landauite.

The iron titanate thin films (Fe:Ti=1:1, 1:3 and 3:1) modified by urea have been synthesized via sol-gel method. Titanium isopropoxide, iron (III) chloride, 5 mol.% urea, ethanol and perchloric acid were mixed at 40°C. Three-layered films were obtained by dip-coating method on glass substrate with heat treatment (the 1st and the 2nd layers at 300°C; the 3d layer at 450 °C or 475 °C for all Fe:Ti=1:1 samples and 500°C for the rest).

The red shifted onset (~ 500 nm) of the optical band in the absorption spectra of all Fe:Ti=1:1 (450, 475, 500°C) samples is noted. The Fe:Ti=1:3 and 3:1 films show spectral shift to the shorter (~ 450 nm) and longer (~ 550 nm) wavelength, respectively. It was calculated the optical band gap energy values for indirect transitions from Tauc plots. Two Eg values, 2.2 eV and 2.7 eV, are obtained for all Fe:Ti=1:1 samples related to Fe_2TiO_5 and $Fe_2Ti_2O_7$ crystalline phases, respectively, as detected by XRD. The films with Fe:Ti=1:3 (Eg at 3.0 eV) and Fe:Ti=3:1 (Eg at 1.9 eV) are crystallized to anatase and the mixture pseudobrookite and diiron(III) titanium oxide phases, respectively.

The photocatalytic activity was tested in tetracycline hydrochloride destruction as well-known consumed antibiotic in cattle, poultry farming. The highest conversion percentage (46%) as well as the adsorption ability was detected under visible light ($\lambda \geq 400$ nm) using Fe:Ti=1:1 sample annealed at 450°C. Photoactivity of the 1 to 1 ratio films was decreased with calcination temperature increase. The Fe:Ti=1:3 film showed similar activity to Fe:Ti=1:1 (475°C and 500°C) samples. However, the last films were more active compare to the Fe:Ti=3:1 under both solar simulated ($\lambda \geq 330$ nm) and visible light irradiation.

Thus, the Ti and Fe ratios as well as the calcination temperature influence on the crystalline composition of the films that, in turns, determines the adsorption capability and photocatalytic activity in the process of tetracycline degradation.

Co-Ni-Fe heterometallic nanocomposites with different component ratios in the catalytic CO_2 hydrogenation

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The method of co-precipitation was applied for the synthesis of the nanosized heterometallic composites using appropriate metals' salts as precursors. The consequence procedures of drying-calcination-reduction provide the formation of Co-Ni-Fe nanosized materials that were tested in the catalytic conversion of CO_2 to methane. The catalytic behaviour of Co-Ni-Fe nanoparticles in the reaction of CO_2 hydrogenation was evaluated at the atmospheric pressure within the temperature range of 100-450 °C with GC registration of outlet gases. The structure of the tested catalyst was investigated before and after exposure to the catalytic process by the XRD, SEM and nitrogen adsorption methods. The thermodesorption procedure with MS analysis of desorbed particles from the surface of catalysts was applied for the reaction mechanism estimation. Evaluated results of catalytic activity are presented in the figure.

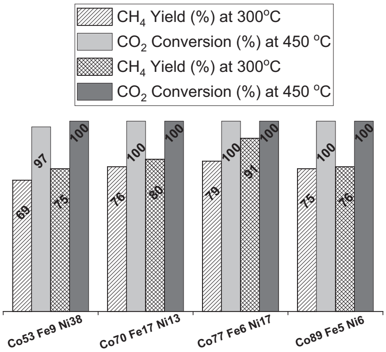

Fig. CH_4 yield and CO_2 conversion over Co-Ni-Fe catalysts estimated from the GC data

TPDMS spectra offered the species desorbed from the surface of catalysts with m/z=44 (CO_2), 28 (CO), 43 (C_3H_7*), 58 (C_4H_{10}). This indicates the formation of butane as the reaction co-product in addition to methane.

Atomic mechanisms and regularities of the temperature effect on strength of carbyne-graphene nanoelements

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Transition to the practical use of nanoelements requires the development of physical concept of the atomic mechanisms that govern the strength of these objects within a wide temperature range. This problem is of key importance for straintronics elements, since governing of their functional properties is realised by deformation during mechanical loading. Carbyne-graphene nanoelements (CGNs) are very attractive for use as straintronics elements, since their deformation significantly changes the band gap. In particular, this makes them promising for creating nanolasers and other optoelectronic devices with tunable wavelengths.

The atomistic model of the contact bonds breaking in CGN under the thermomechanical loading is proposed. It is shown that nature of the temperature dependence of the CGN strength is governed by two main factors, namely, *(i)* by thermally induced change in the contact bonds length (i.e. in the bonds between carbyne chain and graphene sheet) and *(ii)* by release of the elastic deformations energy, which accumulates during the nanoelement deformation. The effect of the second factor is decisive for carbyne-graphene nanoelements and other nanoobjects, which consist of a combination of one- and two-dimensional nanostructures; it makes it impossible to apply the Arrhenius reaction theory to predict the temperature dependence of the strength of such nanoelements.

A statistical criterion for failure of a carbyne-graphene nanoelement at a constant strain rate was developed. Dependences of the strength variance on temperature were obtained. It is shown that this statistical distribution differs from the one obtained earlier [1] under the condition of constant load.

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Hong-Ou-Mandel quantum effect on "rubber - carbon nanotubes" composites

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We investigated influence of multiwalled carbon nanotubes (CNT) on spectral characteristics of composites “rubber - carbon nanotubes” on the base of butadiene-nitrile rubber at 0–10% of CNTs. IR reflectance maxima of composites were measured in the spectral area of the rubber CH deformation and valence vibrations. IR absorption spectra of composites “rubber - carbon nanotubes” after vulcanization includes some giant two-polar oscillations. IR absorption spectrum of composites “rubber - carbon nanotubes” at 1% of CNTs without vulcanization includes the alone two-polar oscillation. Two-photon interference is a result of quantum entanglement of dipole-active vibrations and photon splitting according to Hong-Ou-Mandel (HOM) quantum effect. Two-photon maximal entanglement saturation is called as Bell states. HOM quantum effect is perspective for high-coherent optical quantum computers on composites “rubber-carbon nanotubes”.

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Measurement of thermal conductivity of carbon nanomaterials

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The method of carbon nanotubes (CNTs) synthesis by chemical vapor deposition (CVD) is widely used nowadays [1]. The advantages of CVD method are its simplicity and sufficient reproducibility, an available carbon precursor – hydrocarbon gases, and a CNTs yield of up to 95%. The possibility of sustainable growth of CNTs on surfaces of various shapes and sizes with low energy consumption is essential. The study of the peculiarities of the processes of interaction of electromagnetic radiation (EMR) with carbon nanosystems is practically important and relevant. The characteristic of a substance called "thermal conductivity", which is described by the coefficient of thermal conductivity, is one of the physical quantities. It characterizes the rate of change or equalization of the temperature of the material in non-equilibrium processes that are related to thermal energy. Thermophysical properties of carbon nanomaterials of various origins, including CNTs obtained by the CVD method, were studied using the impulse method of measuring thermal conductivity. Table shows the solution to the problem of thermal conductivity calculation.

# sample	τ, air [10^{-3} s]	τ, sample [10^{-3} s]	Sample thickness, [10^{-6}. m]. L, m	χ, [m^2/s] $\cdot 10^{-6}$ Thermal conductivity
CNTs-1	329	897	1400	2,2
CNTs-2	329	608	1025	3,76
CNTs-3	329	694	980	2,63
CNTs-4	329	746	950	2,16
CNTs-5	329	985	950	1,4
Thermally expanded graphite	329	709	1060	2,97
Intercalated graphite	329	653	1005	3,12

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Effect of temperature on the adsorption process of methylene blue by a copper-containing composite

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One of the simplest and most effective ways to solve the problem of industrial wastewater treatment from organic pollutants is the process of adsorption of organic compounds by porous materials, which can then be removed from the reactor. The purpose of this work was to investigate the effect of temperature on the adsorption efficiency of methyl blue (MB) dye from an aqueous solution by our obtained nanostructured magnetically sensitive composite of the «core-shell» type $SiO_2/CoFe_2O_4/SiO_2$(RL)/CuO and to determine the activation energy of the process. The core of the composite is cobalt ferrite deposited on amorphous SiO_2, which has magnetic properties and allows the composite to be easily separated from the reaction medium by magnetic separation for reuse. For stabilization, the core is covered with a layer of porous SiO_2 with the addition of surfactant (rhamnolipid (RL) *(Pseudomonas sp.)*), on which CuO clusters are deposited. The investigation of the kinetic regularities of adsorption by a composite as a sorbent (5 mg) was carried out by the spectrophotometric method at a wavelength of 620 nm on a MB model solution with a volume of 5 ml and a concentration of $5 \cdot 10^{-5}$ mol/L in a static reactor with stirring in the temperature range of 293-333 K.

The calculation of the main kinetic parameters of the adsorption process of methylene blue was carried out according to the equation derived earlier [1]. The high values of the reliability coefficient of the approximation of the obtained straight lines indicate that the kinetic parameters are well described by the previously considered pseudo-first-order model.

The calculated value of the activation energy for the temperatures of 293K and 333K (E_a=5375,8 J) indicates precisely the self-fluidity and the physical nature of the MB adsorption on the surface of the $SiO_2/CoFe_2O_4/SiO_2$(RL)/CuO composite, the rate of which is practically independent of the process temperature.

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Synthesis and characterization of 1D ZnO NPs modified with gold

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ZnO NPs with controlled morphology due to their non-toxicity, high photosensitivity, high surface-to-volume ratio, efficient charge transport, and chemical stability can find application in different scientific fields. Among different morphologies, the one-dimensional nanostructures provide a direct and stable pathway for rapid electron transport. The attachment of Au NPs to semiconductor ZnO nanorods or nanowires is a powerful approach for producing new chemically functionalized materials with improved photoelectrochemical activity. Au NPs are relatively stable, catalytically active, water-soluble, optically sensitive, and biocompatible.

In this work, we provided facile methods to synthesize ZnO-Au nanohybrids Several types of ZnO nanowires (NWs) and nanorods (NRs) were used. ZnO NRs were obtained by the sol-gel method as reported in [1]. The Au NPs were deposited from $HAuCl_4$ solutions directly onto ZnO NWs and ZnO NRs without adding any linking molecules. Two types of synthesis were compared: simple deposition from aqueous solutions and photo-deposition at room temperature. The Au NPs density and size of on ZnO NRs and NWs can be controlled by adjusting the concentration of $HAuCl_4$. The structure, crystallinity, and morphology of ZnO and ZnO/Au nanomaterials have been investigated with XRD, SEM, TEM, RAMAN, and FTIR spectroscopy.

Obtained results will allow to use ZnO 1D nanostructures as a potential platform for creation of electrochemical biosensors and photocatalysts.

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Nanodimension and magnetic state of copper-based Heusler alloys

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Cu-based shape memory (SM) alloys can exhibit unusual magnetic properties depending on their heat treatment, additionly to their functional properties. In this system, ferromagnetic nanosized particles of Heusler compound Cu_2MnAl are precipitated due to aging, which contributes to an increase in SM effect and superelastisity SE [1]. Depending on the size and distribution of nanoparticles, the alloys of this system can exhibit superparamagnetic, ferromagnetic and antiferromagnetic ordering [2].

The structural and magnetic analysis of Cu-Al-Mn and Cu-Al-Mn-Fe alloys depending on their heat treatment was performed in this work. The influence of aging on induced martensitic transformation was established. The magnetic behavior of Cu-Al-Mn and Cu-Al-Mn-Fe alloys is significantly different from each other, which is a consequence of the formation of Heusler ferromagnetic phases Cu_2AlMn, or Fe_3Al and $(Fe,Mn)_2Al$ during isothermal aging of ternary alloys and the transformation to a superparamagnetic state. In the quaternary composition doped with iron, antiferromagnetic ordering is dominated. Such precipitates create a significant cumulative effect on thermoelastic MT, as well as on both mechanical and magnetic behavior. The doping with Fe contributes to non-monotonic changes in MT temperatures.

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Study of Metal Doped Nanoporous Silicon to Enhance Glucose Sensing

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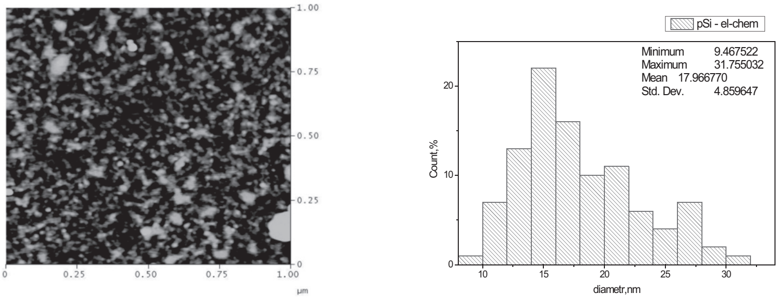
Our research has been focused on the preparation (1-3,6) and characterization of layered semiconductor (MIS metal-isolator-semiconductor) structures (5,6) based on porous silicon (Sipor) with embedded clusters of catalytic (Ni, W) metals by means of I-V characteristics and PL spectra under the influence of organic molecules (glucose) adsorption (7). The morphology of silicon composite was characterized by atomic force microscopy (AFM) (Fig.1)



(a) *(b)*

***Fig.1**. Morphology of porous silicon with a W clusters, AFM (a); size distribution of crystallites on the Sipor surface (~ 80% crystallites is in range 15 – 20 nm) (b)*

The porous silicon layer was prepared by electrochemical etching in HF-C_2H_5OH solution. Then a thin Ni and\or W film (5-10 nm) was deposited on surface of Sipor by dc magnetron method. The subsequent thermal treatment in range of 250-550 °C in Ar leads to incorporation of metal clusters into a porous silicon matrix. It was found (1) adsorption of glucose molecules reduces the intensity of photoluminescence spectra; (2) filling pores with W leads to increased sensitivity of the sensor structure based on porous silicon to adsorbed molecules of glucose; (3) the structures based on porous silicon with metal clusters are

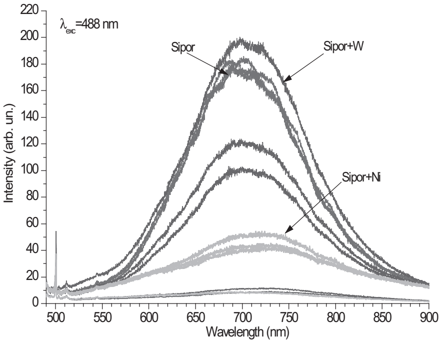


Fig.2. Pl spectra for Sipor and Sipor with W and/or Ni clusters; the highest intensity Pl in the case of Sipor+W

sensitive to adsorption of glucose (Fig. 2) and can be used to create sensors on glucose

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New approach to obtain the geopolymers based on the metakaolin for heavy metal ions removal from water

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Geopolymers are the promising materials for the removal of toxic substances from industrial and drinking water. The most popular and simplest method of its preparation is based on the reaction between an alkali such as $NaOH/Na_2SiO_3$ and metakaolin (gelation stage), mixture obtained is placed in an oven to cure for 24 h at 60 °C (polycondensation reaction) [1]. This method is used in work presented for obtaining the *pyramids* (last stage has been carried out in the special forms).

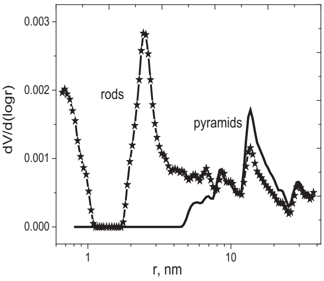

***Fig. 1**. Pore size distributions obtained in term of DFT method for the geopolymers synthesized by two methods.*

Another new approach is applicated for producing the spherical rods that is included the extruding of solution of reagents heated up to 60 °C to NH_4Cl solution for neutralization of NaOH. This process significant diminishes the time of washing the final material up to neutral pH. Morphology of kaolinite, metakaolin, and the geopolymers are analyzed via XRD, XRF and SEM techniques. It is found that porous structure of materials depends from the technology used for its production. Surface area of geopolymers increase from 25 (pyramids) up to 88 m^2/g (rods). As seen from pore size distributions obtained from nitrogen adsorption/desorption curves in term of DFT method rods have a great number of micro- and mesopores (Fig. 1) those are absent in the structure of pyramids.

The adsorption capacity of the geopolymeric samples for heavy metal ions decreases in the order $Co^{2+} > Cu^{2+} > Pb^{2+} > Cd^{2+} > Zn^{2+}$ and in the case of rods these values are greater than for pyramids. Capacities accounted by Langmuir model reach to 50-100 mg/g that could be compared with values for powder materials [2].

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Photoluminescence properties of carbon nanodots synthesized in highly dispersed SiO_2 matrix using diphenylsilanediol as a carbon precursor

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Luminescent carbon nanodots (CNDs) is a relatively new class of light-emitting nanomaterials. The broadband spectrum of luminescence in the visible region makes them promising objects for optoelectronics as phosphors for artificial light sources. For practical application as upconversion phosphor it is important to disperse CNDs in transparent solid state matrix. It has been demonstrated previously that treatment of the highly dispersed fumed silica powder by phenyltrimethoxysilane ($C_9H_{14}O_3Si$, PhTMS) in combination with subsequent annealing in a pure nitrogen at temperatures of 500 - 600 °C leads to the formation on the surface of SiO_2 particles nano-sized carbon precipitates (CNDs) which emit in the ultraviolet (UV) and visible regions. To study the effect of the amount of phenyl groups in the carbon precursor on the processes of formation of CNDs, their structural and photoluminescence (PL) properties, CNDs were synthesized by similar procedure using diphenylsilanediol ($C1_2H1_2O_2Si$, DPSD), the molecules of which contain two phenyl groups in contrast to PhTMS, that contains one phenyl group. It is shown that the treatment of the surface of SiO_2 particles with DPSD leads to the appearance of bright, broadband UV PL and thermal treatment leads to a decrease in intensity and a red shift of the PL maximum. Formation of the CNDs in the surface of SiO_2 particles and light emission mechanisms in terms of polycyclic carbon fluorophors are discussed.

Diagnostic of the Role of SnO_2 and PbI_2 in Enhancing the Stability of Perovskite Thin Films

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Over the last 15 years, perovskites have become popular materials among scientists working with photovoltaic effects, but also with non-linear optical effects [1,2]. Particularly groundbreaking was the use of thin layers of perovskites in solar cells, thanks to which efficiency of the solar cells exceeded 30% [3]. Moreover, non-linear optical effects (NLO) occur in thin layers of perovskites, which allows for new applications, for example, the generation and modulation of light or high-resolution imaging.

Apart from the many advantages that perovskites have, there is a problem related to their stability. Currently, this is the main reason for stopping

the commercialization of devices containing perovskites. The oral communication propose solution to extend the lifetime of perovskite thin films as $CH_3NH_3CdI_3$ and $CH_3NH_3PbCl_3$ by covering them with a thin layer of tin (IV) oxide or lead (II) iodide, which have no a significant effect on the optoelectronics properties.

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Approaches to fabrication and characterizing of ceramic-based thick-film nanostructures for sensor applications

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The utilization of thick-film ceramics based on the mixed transition metal manganite system, particularly in combination with humidity-sensitive nanostructured $MgAl_2O_4$ ceramics, offers significant advantages in the field of functional electroceramics. This study aims to fabricate and characterize the structural properties of thick-film nanostructures that are sensitive to both temperature and humidity.

The investigation focused on temperature-sensitive elements and multilayered structures composed of $Cu_{0,1}Ni_{0,8}Co_{0,2}Mn_{1,9}O_4$ *(p-type conductivity),* $Cu_{0,1}Ni_{0,1}Co_{1,6}Mn_{1,2}O_4$ *(p+-type conductivity)*, and dielectric $MgAl_2O_4$ *(i-type)*. The humidity-sensitive thick-film layer was applied onto a pre-formed temperature-sensitive layer. Importantly, the formation of various thick-film structures, including p-p$^+$, p-p$^+$-p, and integrated temperature-humidity-sensitive p-i-p$^+$ structures, was achieved within a single technological cycle. The structure of the humidity-sensitive thick films demonstrated a distinct contrast when compared to the Al_2O_3 substrate with a conductive Ag layer. The material exhibited shallow pores, serving as pathways for water absorption into the nanopores, where capillary condensation occurred. Macropores facilitated effective water absorption into the inner structure of the material from the environment. In contrast to the microstructure of humidity-sensitive $MgAl_2O_4$ thick films, $Cu_{0,1}Ni_{0,8}Co_{0,2}Mn_{1,9}O_4$ thick films exhibited a higher presence of macropores clustered together. This structure was also observed in the bulk material of the same composition. Hence, the structural characteristics of ceramics can be successfully transformed into similar compositions of thick films. The use of ceramic materials with a spinel structure as the primary component in thick film preparation ensured the density and interlayer contact within the multilayered structure.

Study of features of structure formation in high-temperature materials using carbon-containing additives during consolidation

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Any material containing a transition metal such as Zr, Hf, Ta, Mo, W or Nb together with B, C or N can be classified as ultra-high temperature. Our research on Ultra High Temperature Ceramics (UHTCs) focuses on ceramics and composites based on ZrB_2, ZrC, HfB_2, TaB_2 and HfC. We have developed new composite materials based on refractory borides, carbides and their solid solutions with an increased set of properties compared to existing materials. A high level of mechanical and damping characteristics is achieved due to high connectivity between the grains of the existing phases and a high concentration of defects (twins, dislocations, packing defects) due to the use of starting nanopowders and sintering under high and moderate pressure. Ceramic composites are promising for use as construction and wear-resistant materials at high operating temperatures.

However, despite high mechanical properties, an excellent level of resistance to high temperatures and oxidation, in general, such ceramics are quite brittle. One of the strategies for reducing fragility and improving the operational qualities of the composite is the creation of ceramic laminate structures [1]. One of the ways to improve the mechanical characteristics of layered structures is the development of laminates with weak interfaces to deflect cracks [2]. Since it is known that the addition of carbon can be used [3] to create a weak interface in the layered structure to deflect cracks, as well as to improve the physical and mechanical properties, we used carbon-containing additives (SiC, ZrC, HfC, NbC, TaC, and nanocarbon) at sintering of our UHTM materials. To compact the materials to a non-porous state, sintering methods were used under conditions of high pressure and temperature (1100-1900 °C, up to 4.1 GPa) - on anvil-type presses with a notch, as well as by the hot pressing method. (1600-2000 °C, up to 30 MPa). Such synthesis methods are effective and economical for obtaining material samples of the required dimensions. Also, their use can prevent the evaporation of early d-metals of the IV-V group of transition metals, which make up the basis of our ceramic composites.

Among the groups of studied materials, the samples based on the ZrB_2-SiC, HfB_2-SiC and TaB_2-SiC systems, sintered both under hot pressing conditions and under high pressures, performed best. Thus, the composites prepared under high pressures-high temperatures from HfB_2-30 wt.% SiC mixture had density ρ=6.21 g/cm^3 and high mechanical properties: microhardness HV(9.8 N)=38.1±1.4 GPa, HV(49 N)=27.7±0.2 GPa, HV(98 N)=26.3±2; fracture toughness K_{1C}(9.8 N)=8.2±0.2, MH•m0.5, K_{1C}(49 H)=6.8±0.6 MH•m0.5, Young's modulus E=817 GPa. The composites sintered at high pressure from ZrB_2-20 wt.% SiC mixture had density of 5.04 g/cm^3, HV(9.8 N)=24.2±1.0 GPa, HV(49 N)=16.7±1.1 GPa, K_{1C} (49 H)=7.1±1.55 MH•m0.5 elasticity modulus E=386 GPa. From the TaB_2-SiC based material, it is possible to consolidate very dense samples with porosity close to 0 by both methods of consolidation. Thus, HP samples TaB_2- 20 wt.% and 30 wt.% SiC were characterized by hardness up to 29.7 GPa and 34.4 GPa respectively, and compressive strength 876 MPa and 1090 MPa respectively.

The main idea of the research was to use an integrated approach to the creation of new materials: (1) obtain materials with excellent operational characteristics in a wide range of pressures and temperatures with the help of advanced technologies (2) and the use of nanopowders as precursors. with known consequences arising therefrom. The improvement of mechanical characteristics compared to pure materials can be explained by the formation of solid solutions in the structure of the materials.

Acknowledgments. Authors are grateful for the financial support, project NATO SPS G5773 “Advanced Material Engineering to Address Emerging Security Challenges”, and grant of the National Academy of Sciences of Ukraine “III-5-23 (0786) “Study of regularities and optimization of sintering parameters of composite materials based on refractory borides and carbides, their physical and mechanical properties in order to obtain products of complex shape for high-temperature equipment with an operating temperature of up to 2000 °C” (2023-2025).

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Modelling of ionic implantation in a nanoscale layer of a steel surface

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Currently there is an active search and development of methods to improve the surface properties of materials, create materials with specific characteristics, etc. One of such method is ionic implantation, a technology for surface nanoscale modification of materials by means of ion fluxes [1]. Among its advantages this technology has low consumption of active element, absence of thermal effect on the base material and the formation of nanosized modified layers with enhanced material characteristics.

However, ionic implantation is a technology that requires complex, expensive equipment and consumables. Obviously, one of the main problems of using ion processing is the need for accurate prediction of results for a wide range of base-ion combinations.

Therefore, the purpose of this work is to simulate the process of implantation of metal ions into steel.

Titanium, aluminum, molybdenum and chromium were chosen as the target materials. Stainless foil was taken as the base material.

The simulation was carried out by means of the author's computer application.

As a result of modelling, ion penetration indicators (runs, concentrations, layer thickness, etc.) were determined. It was found that these indicators directly depend on the target material, which indicates the prospects for continuing research in this direction.

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Studies on photocatalytic performance applications of undoped and Al-doped ZnO nanoparticles

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In the present study, transition metal Al-doped ZnO nanoparticles (TM-ZN NPs) were synthesized via the chemical co-precipitation method. The structural, morphological, electronic, optical, vibrational as well as the photocatalytic properties of the elaborated TMZO-NPs, are then investigated. Hexagonal wurtzite crystallinity of all elaborated NPs is confirmed by the phase analysis and particle size is found to be affected by TM doping. XRD peak shows that all samples prefer orientation along (002) axis and TM (Al) may substitute ZnO structure as the peaks shift toward higher angles. The surface morphology of all samples exhibits mixture of spheroid-like and hexagon-like shaped structures. FTIR analyses are carried out to identify the important bands attributed to TM-O and Zn-O stretching vibration modes. The absorption intensity and edge are found affected by adding TM dopant. Degradation by pure ZnO and TMZO NPs of the methylene blue is investigated after 90 min UV light exposure. TM dopant affects the degradation of MB dye, where a high percentage (97.14%) being achieved after reasonable time of exposure (90 min) under UV light for Aluminum doped ZnO nanoparticles (AlZO NPs).

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New mixed rare earth orthophosphates with monazite and zircon types of structure

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Crystal structure engineering is a very powerful tool for purposed tuning of functional properties of the materials. Application of chemical pressure caused by rare earth (RE) cation substitution in the orthophosphate lattice allows impact in prognoses way on structural parameters of monoclinic and tetragonal phases and energy band gap and hence on the important physical properties of the materials. In this respect over 35 new mixed RE orthophosphates from 25 different RPO$_4$–R'PO$_4$ pseudo-binary systems have been synthesized and their structural parameters were analyzed.

Single phase nanocrystalline powders of $R_{1-x}R'_xPO_4$ with average grain size of 21–31 nm were obtained by solid state reactions in air by sequential calcination of appropriate mixtures of corresponding RE oxides and $(NH_4)_2HPO_4$ at 1473–1673 K. Additionally, two series of $La_{1-x}Dy_xPO_4$ and $Ce_{1-x}Tb_xPO_4$ samples with average grain size of 120–160 nm and microstrain values of 0.01–0.05 % were obtained by co-precipitation method. It was established that the monazite type of structure is inherent for the RPO$_4$–R'PO$_4$ systems with "light" RE, namely $La_{1\ x}R_xPO_4$ (R=Nd, Sm, Eu), $Ce_{1-x}R_xPO_4$ (R=Pr, Nd, Sm, Tb), $Pr_{1-x}R_xPO_4$ (R=Nd, Sm, Eu, Gd) and $Nd_{1-x}R_xPO_4$ (R=Sm, Eu). In contrast, mixed phosphates with tetragonal zircon type of structure are formed in the systems of "heavy" RE and yttrium, e.g., $Dy_{1-x}R_xPO_4$ (R=Ho, Yb), $Ho_{1-x}R_xPO_4$ (R=Er, Yb, Lu) and $Y_{1-x}R_xPO_4$ (R=Tb, Dy, Ho, Er, Tm, Lu). In the mixed systems of "light" and "heavy" RE phosphates, two kinds of solid solutions are formed, as it was confirmed for $La_{1\ x}Dy_xPO_4$ system, in which an immiscibility range between monoclinic and tetragonal phase was found at $0.6<x<0.97$.

Structural parameters over 25 new mixed phosphates with monazite and zircon types of structure are included by International Centre for Diffraction Data (ICDD) as standard reference data in PDF-4 database.

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PEDOT:PSS Carbon Nanotube Nanocomposites and Textured Interfaces for Enhanced Si Solar Cell Efficiency

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Poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT:PSS) thin polymer films exhibit high light transmission and electrical conductivity. They can be produced on large areas using vacuum-free techniques at room temperature. By utilizing this polymer, PEDOT:PSS/Si heterojunction solar cells can be created, which offer promise due to their easy fabrication and low cost. However, there is a need to improve the efficiency and stability of these photoconverters. One approach to enhance the photoelectrical heterostructure parameters is to increase the film conductivity through physical or chemical doping of the PEDOT:PSS polymer layer. The texturing of the silicon surface can reduce optical losses, increase light energy absorption, and improve the electrical parameters of the semiconductor surface in certain cases.

This paper investigates the effects of carbon nanotube admixtures in PEDOT:PSS-based composite films on their optical and electrical properties, as well as the parameters of Si-based photoconverting heterostructures. Film thicknesses and optical parameters were determined using spectroscopic ellipsometry in the range of 250-2100 nm, while electrical dc-conductivity was measured using the four-point probes method.

Our studies demonstrate that composite films with a small volume fraction of carbon nanotubes exhibit higher conductivity compared to pure PEDOT:PSS. Additionally, the corresponding PEDOT:PSS/Si solar cell heterostructures exhibit higher efficiency. Moreover, it is possible to obtain films with different electrical properties by varying the morphology of the composite, which is influenced by the method of nanotube deposition. Wet chemical etching for Si interface texturing significantly enhances the heterojunction efficiency, possibly due to reduced optical losses and semiconductor surface passivation. Investigation of the photoelectrical properties of such composite films enables the creation of silicon-organic solar cell heterostructures with competitive photovoltaic characteristics.

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Analysis of structural characteristics in doped $BaTiO_3$ ceramics

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This study focused on investigating the inner-structure properties of undoped and Y-doped $BaTiO_3$ ceramics through a combination of methods. $BaTiO_3$ ceramics were doped with varying amounts of Y (0.2, 0.4, 0.6, and 0.8 mol%) and then sintered at a temperature of 1250 °C. The positron annihilation lifetime (PAL) measurements were conducted using an ORTEC spectrometer, with a 22Na source positioned between two ceramic samples.

The obtained data were analyzed using the LT computer program, and the most accurate results were obtained through a two-component fitting procedure [1]. Gwyddion open-source software were used for construction of SEM images and preprocessing (subtraction of planes, streak subtraction, elimination of scanning defects, etc.) and formation of a three-dimensional representation.

The short lifetime value of τ_1 (approximately 0.16 ns) observed in polycrystalline ceramic materials is typically associated with the free annihilation of positrons. This value was found to be consistent with the theoretically calculated free positron lifetime in $BaTiO_3$, indicating similarity to $BaTiO_3$ single crystals. Moreover, the observed values of τ_2 (approximately 0.37 ns) are believed to arise from the annihilation of positrons at vacancy complexes formed between oxygen vacancies and metal ion vacancies. It was observed that τ_2 decreases with increasing Y content in $BaTiO_3$ ceramics from 0.2 to 0.6 mol%, while in samples with 0.8 mol% of Y, the intensity I_2 decreased from 20% to 15%. These findings suggest that Y doping results in a reduction in the size and quantity of free-volume defects in ceramics, indicating a process known as "shrinking of defects" in $BaTiO_3$ ceramics doped with 0.4 and 0.6 mol% Y. However, increasing the Y content to 0.8 mol% led to a weakly expressed agglomeration of free-volume defects.

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Enhancing the thermo-physical characteristics of epoxy resin through single- and multi-walled carbon nanotube reinforcement

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Polymer nanocomposites are recognized for their exceptional thermo-physical properties. However, the widespread production of polymer composites reinforced with carbon nanotubes (CNTs) on a commercial scale heavily relies on stringent technological process standards. Therefore, it necessitates experimental approaches to regulate the impact of manufacturing conditions, with a key focus on achieving uniform dispersion of nanofillers. Our research concentrates on empirically investigating the thermal conductivity of engineered polymer nanocomposites by incorporating varying amounts of single-walled and multiwalled carbon nanotubes (CNTs) into the epoxy matrix structure.

In this particular study, we emphasize the examination of how increased loading levels and/or dispersion quality influence the overall thermosetting characteristics of the composite material. To gather relevant data and gain insights into the peculiarities of nanofiller incorporation into the host polymer matrix, visual thermographic analysis and direct thermal response measurements were employed. The experimental setup involved a NI USB-6009 DAQ unit that controlled a 5V/1A electrical furnace with a flat heated surface on which the cylindrical samples were placed. The temperature at the opposite edge of the samples was measured using a thermocouple. The thermocouple signal was acquired through one of the analog channels of the DAQ module, which provided a 14-Bit resolution and 48 kS/s sample rate, ensuring the collection of reliable temperature versus time plots during both heating and cooling phases. The entire experiment was managed through custom-developed NI LabVIEW software.

Visual insights into the heat flow processes within the samples were obtained using a FLIR TG series thermal camera. The recorded thermal response data were utilized to discuss the mechanisms underlying the differences in thermo-physical behavior observed in epoxy composites reinforced with single-walled and multi-walled carbon nanotubes.

Exploring the dynamics and consequences of ageing phenomena in thick-film nanostructures

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This study focuses on investigating the ageing processes in thick-film elements consisting of spinel temperature-sensitive ceramics. The ageing test was conducted through long-term isothermal treatment at 170°C to assess the thermal stability of the thick films. The duration of the ageing test was 250 hours, during which electrical resistance measurements (R) were performed at 25°.

It was observed that all the temperature-sensitive materials exhibited a characteristic linear dependence of electrical resistance within the temperature range of 298 K to 368 K. In the single-layered thick films, the change in electrical resistance after 250 hours was approximately -7.5% and -8.7%. This behavior an be attributed to two independent processes: initially, a rapid diffusion process of molecules in the surface layer dominates, followed by the burning of organic components, resulting in a decrease in relative electrical resistance.

The kinetic dependencies of the single-layered thick-film elements demonstrated a typical suppressed-exponential relationship with time, in accordance with a known relaxation function. This behavior is associated with the burnout of organic compounds, which is characteristic of structurally heterogeneous media like thick-film ceramic structures. In two-layered thick-film structures, an increasing trend in the thermally-induced ageing curve with relative saturation was observed within the first 50-150 hours. The maximum drift in electrical resistance was approximately 6%. The ageing kinetics in these structures were described by an extended exponential relaxation function. It is worth noting that the thermally-induced mechanism in these samples was complex and involved not only cation redistribution but also mass transfer processes.

Unfortunately, the two- and three-layered thick-film structures exhibited relatively high stability, with a drift in electrical resistivity of 1.5%. Achieving such high stability required modifications in paste compositions (to achieve the required viscosity) and the preparation of thick-film layers based on different ceramic compositions.

Analysis of evolution of free volumes in the $BaGa_2O_4$ ceramics doped with Eu^{3+} ions

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$BaGa_2O_4$ ceramics have garnered attention as a promising material for various applications such as insulators in optoelectronic devices and secondary coatings for plasma panels. The objective of this study is to investigate the development of inner free volumes, including extended defects and nanopores, in $BaGa_2O_4$ ceramics doped with varying amounts of Eu^{3+} ions, utilizing positron annihilation lifetime spectroscopy (PAL) as the analytical method.

The examination focused on the evolution of free-volume defects in $BaGa_2O_4$ ceramics produced through solid-phase synthesis, employing initial components of $BaCO_3$ and Ga_2O_3, along with different concentrations of Eu_2O_3 content (1, 3, and 4 mol%). PAL measurements were carried out using the ORTEC system, with a positron source of 22Na isotope. The investigation was conducted at 22 °C and a relative humidity of 35%, utilizing two identical ceramic samples placed in a sandwich configuration. The obtained PAL spectra were analyzed using LT software through a four-component fitting procedure, which is suitable for spinel ceramics with a branched porous structure.

In the $BaGa_2O_4$ ceramics, two PAL channels can be observed: the capture of positrons by bulk defects and the decay channel of ortho-positronium atoms. The short-term component of the PAL spectra reflects the microstructural characteristics of the main phase, while the middle component is associated with defect-related voids near grain boundaries. The lifetimes of the third and fourth long-term components are indicative of the transformation of nanopores.

Upon analyzing the second component of the PAL spectra for both undoped and Eu^{3+}-doped $BaGa_2O_4$ ceramics, it was observed that an increase in Eu^{3+} content from 1 to 3 mol% results in the agglomeration of free-volume defects near the grain boundaries of the ceramics. Simultaneously, the nanopores within the ceramics expand in size, and their quantity increases. However, further increments in the Eu^{3+} ion content lead to the fragmentation of both the free-volume defects and nanopores.

Exploring nanovoids in ceramic solids using positron-positronium trapping models

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Positron annihilation lifetime spectroscopy (PALS) is a highly sensitive method used to investigate the presence of internal nanovoids in solids. This research aims to study the presence of free nanovolumes in humidity-sensitive ceramics by employing multicomponent positron-positronium trapping models.

The findings reveal that humidity-sensitive ceramics exhibit two distinct components in the PALS measurements. The first component, characterized by specific parameters (τ_1, I_1), reflects the microstructural properties of the material. The second component, with parameters (τ_2, I_2), corresponds to volume defects near the intergranular boundaries, which are formed by additional phases. Another channel in the measurements contains only one component, characterized by parameters (τ_3, I_3), and represents the annihilation of ortho-positronium (o-Ps) through the "pick-off" process in nanopores.

By conducting PALS investigations on modified $MgAl_2O_4$ ceramics under dry and wet conditions, and employing high-statistical measurements, it was possible to observe and analyze the behavior of the four identified components. The second channel exhibited two components, with parameters (τ_3, I_3) and (τ_4, I_4), indicating the decay of o-Ps atoms within nanopores. The first component in this channel reflects the annihilation of o-Ps through the “pick-off” process in nanopores of approximately 0.2-0.3 nm in size and in the presence of water, resulting in an increase in intensity (I_3). The second component in this channel, characterized by parameters (τ_4, I_4), describes the annihilation of o-Ps through the “pick-off” process within an empty pore volume with a radius of 1.8-2 nm, where water molecules are formed as a layer on the pore walls.

In conclusion, the application of the multicomponent positron-positronium model proves to be more suitable for describing the transformation of free volumes in materials with well-developed porous structures. Additionally, it facilitates the study of adsorption-desorption processes in ceramics such as $MgAl_2O_3$ spinels.

Analysis of Structural and Optical Features of Nanosized ZnO Films by Modulation Polarimetry Methods

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The method of modulation polarimetry was used to study nanoscale films of zinc oxide. Samples of ZnO films were obtained by deposition from a solution of zinc acetate followed by annealing.

The studies performed have shown that the obtained ZnO thin films can be effectively used as optical plasmonic sensors. The use of the modulation polarimetry technique in the version of internal reflection, in particular, the Kretschmann geometry, made it possible to obtain detailed information on the optical properties and structural features of the films under study. An analysis of the spectral and angular dependences of the Stokes vector components confirms the presence of a cluster structure in ZnO films and resonant dipole interaction with an electromagnetic wave. As it turned out, in isolated dielectric clusters, the field is oriented along the normal to the cluster surface. The cluster structure of ZnO films detected by modulation polarimetry is confirmed by the results of atomic force microscopy (AFM).

Particular attention should be paid to the fact that the studied films exhibit a dipole resonant interaction independent on the light incidence angle, which indicates the versatility of the method and its potential for use in various areas of electronics and photonics.

The results obtained indicate the possibilities of using the studied nanosized ZnO films in various practical applications, in particular, in optical sensors. The use of polarization modulation can make it possible to create sensitive elements with high resolution and sensitivity to properties' changes.

Simulating the formation of conductive networks in composites containing nanotubes

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Nanocomposites achieve enhanced mechanical and electrical properties compared to the host material by incorporating nanotubes (such as carbon) into an insulating matrix. In the simulations presented, we introduce the concept of tunneling range. If the shortest distance between two nanotubes is within the tunneling range, they are considered to establish a tunneling contact.

Mathematically, the system is represented as a graph, and the percolation search involves identifying the connected component of the graph that includes elements touching opposite edges of the simulated box, acting as "electrodes". These "electrodes" are simulated as pseudo-tubes with zero dimensions. To determine the conducting cluster, we employed a weighted quick union algorithm with path compression. Around 20 simulations were conducted for each system using the same parameters, and the percolation threshold value was obtained as the average from these results.

Consequently, we developed a viable three-dimensional model that describes the percolation phenomenon in the nanocomposite system of "conductive nanotubes/insulating medium". The mathematical description captures the process of nanotube network formation, and the numerical calculations incorporate the tunneling mechanism of electrical conductivity. The resulting percolation threshold values exhibit satisfactory agreement with existing experimental data.

Moreover, it was observed that increasing the size of the simulated and/or conducting a greater number of computer experiments yield more accurate results, which better correlate with experimental observations. Additionally, our findings demonstrate that a "soft-core" model without tunneling capability cannot produce reliable results. Furthermore, our research reveals that increasing the alignment angle generally decreases the percolation threshold, with the alignment's influence being more pronounced within the angle range of 30 to 50 degrees.

Influence of magnetron deposition parameters on the formation of a multicomponent coating structure

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Currently, medium-entropy alloys (MEA) and high-entropy alloys (HEA) are actively being developed and investigated [1]. They represent a type of multicomponent alloy and are considered promising materials for industrial applications. Contents and ratio of each component is taken into account in the case of multicomponent alloys. By reducing or increasing the proportion of additional elements, one may generate a variety of metallographic structures which have a significant effect on the properties of alloys [2,3]. Here we present the results of the synthesis MEA coatings using magnetron sputtering in an argon plasma. The selection of the composition of the multicomponent composition is determined by the required level of performance properties. The mosaic target had a titanium base with inserts made of zirconium, niobium, and molybdenum. The TiZrNbMo coatings were synthesized under various plasma generation conditions. The influence of frequency modulation (10 Hz and 1000 Hz) and power (300 W and 1000 W) on the structure and properties of the TiZrNbMo coating was studied. Additionally, coatings were deposited by magnetron sputtering at various substrate biases (ranging from 0 to -150 V). Scanning electron microscopy with microanalysis was employed to determine the thickness, surface morphology and chemical compositions of the coatings. The mechanical properties of the TiZrNbMo coatings were determined by nanoindentation.

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Towards production of 3D printed concrete radiation shielding materials containing Bi_2O_3-Gd_2O_3-SiO_2 structures

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Heavy-weight micro- and nano-sized powders are widely used as additives to cementitious systems in construction and dental applications. Due to their high atomic number replacement of Portland cement with additives enable to produce composites with radiopacifying and radiation (gamma-ray and neutron) attenuation properties. In the recent years there is a growing concern to produce lead-free materials, thus various additives are used including Bi_2O_3, Ti_2O_3, WO_3, Gd_2O_3 or Fe_3O_4. Special interest is put on application of Bi_2O_3 due to its high atomic number (Z=83), low price, non-toxicity and biocompatibility. However, presence of Bi2O3 powder delays the hydration process of cement substantially resulting in increased setting time of cement pastes and low early strength. Therefore, incorporation of such material in additive manufacturing of concrete is limited.

One of the popular inexpensive methods is production of thin silica coatings on the nanoparticles surfaces' in order to increase their reactivity and improve their bonding withing the matrix. Therefore, new type of admixture composed of Bi_2O_3 and Gd_2O_3 particles coated with thin silica coatings has been proposed. Two types of sol-gel silica coatings towards production of core-shell structures were synthesized (varied with coating method and specific surface area) and their effect on the fresh properties of 3D printable concrete mix was evaluated. Static yield stress, dynamic yield stress and recovery rate were evaluated using rotational rheometer. Study showed that depending on the coating type incorporation of proper nanostructure can substantially improve the early age properties of 3DPC, resulting in higher thixotropy of the mix. Moreover, inclusion of silica coating minimalize the negative effect of delayed hydration, thus mixtures containing newly developed structure are suitable for 3D printing applications without threat of low early strength and potential failure of structure in plastic state.

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Interactions in organic-inorganic composites: an influence on structural and luminescent properties of materials

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Nanocellulose (NC)-based polymer composites with inorganic luminescent particles have attracted attention as materials for LEDs, document protection, interior decoration, smart ceilings, night indicators, luminescent logos and labels, transformers of mechanical energy to visible light, etc.

Despite the different nature of the matrix (nanocellulose) and the filler (inorganic micro/nano-sized particles of a complex oxide), the interaction between them can be a mechanism that allows to control and manage the properties of the composite material to some extent.

In this work, the features of the PL characteristics and the mechanisms of its excitation were investigated for NCs filled with oxide phosphors of three types ($K_3Tb(PO_4)$:Eu, (green-orange emission), $K_2Eu(PO_4)(WO_4)$ (orange-red), or $ScAl_2O_4$:Dy,Eu (green-yellow)) in comparison with the PL characteristics of the specified phosphors in their "free" powder state.

Correlations of the PL properties with morphology, spatial, electronic and vibrational structure of composites were identified and analyzed.

The ways of possible application of the studied composites were discussed, too. Particularly, the studied composites in “liquid” forms can be used as luminescent inks in 3D printing devices.

Inductive-resonance energy transfer in hybrid carbon nanostructures

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In recent years, many different materials based on hybridized carbon in its low dimensional forms (such as functionalized graphene, carbon nanotubes, graphene, graphene quantum dots, graphene nanoribbons, etc.) and these systems are widely used in optoelectronics, especially when interfaces with molecules are created [1,2]. Here, we present a microscopic view of the substrate-molecule interface interaction in an archetypal hybrid material consisting of graphene functionalized with dye molecules. The non-radiative energy transfer at a 0D/2D interface can be explained by two main mechanisms: Forster and Dexter couplings. The Forster process describes the direct transfer of energy from an optically excited molecule to the substrate (in our case graphene or its derivatives). The Dexter coupling is based on simultaneous transfer of charges between the molecule and graphene states after the photoexcitation process. The Förster and Dexter energy transfer rates can be calculated analytically via Fermi's golden rule with the momentum-dependent initial and final states of the graphene substrate and the HOMO and LUMO states of the molecule. Having characterized the hybrid material within the limits of DFT calculations, including the fully geometrical relaxation of the structure, its electronic band structure, optical properties and charge rearrangement, we will focus on energy transfer, which was measured recently experimentally. The obtained results will be applied to other carbon hybrid nanostructures and, in general, to the description of energy transfer processes when the molecular transition dipole moment and the substrate–molecule separation are known.

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Structural peculiarities of PVA-AgNPs hydrogel nanocomposites irradiated by high-energy electron beam

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As a result of the aggression of the Russian Federation on Ukraine, the demands for treatment of burns has increased significantly. For this purpose silver-containing hydrogel dressings cross-linked by high-energy electron irradiation are effectively used. Depending on the dose and the content of silver, the structure of hydrogel nanocomposite, the size and distribution of the Ag nanoparticles, reduced from silver nitrate, may change and that effects on the properties of the dressings.

Some structural peculiarities of PVA-AgNPs nanocomposite were studied by XRD analysis, SEM and TEM methods. XRD analysis of the unirradiated sample revealed a peak characteristic of silver nitrate. When the sample is irradiated by high-energy electrons this peak disappears and the $(111)_{FCC}$ Ag and $(200)_{FCC}$ Ag peak appear. With a further dose increase, the intensities of both peaks increase confirming the reducing of Ag from silver nitrate.

SEM analysis has shown that the nanocomposite has a porous structure with the small porous size 10-30 μm able to absorb water effectively and bubbles size 0.1-1 mm, which seems appear due to cross-linking, radiolysis and reduction reactions. The pore surfaces are smooth and uniform. Silver nanoparticles with the size of 40-90 nm and their agglomerates with the size of 160-470 nm were found.

TEM analysis revealed that in addition to Ag nanoparticles the Ag_2O oxide presents in the irradiated samples in a form of oxide shell on the silver nanoparticles or as standalone faceted nanoparticles with the size of 30-70 nm. Probably, this oxide is formed from reduced Ag, which interacts with the products of the radiolysis of water in hydrogel irradiated by high-energy electrons.

Application of nanostructured luminescent coatings for photodetection optimization

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The digitization of data has sparked a global trend, leading to the widespread use of digital photodetection tools. This shift has been accompanied by a drive for smaller, more affordable electronic devices, as well as advancements in digital data transmission, analysis, and storage systems. These developments have paved the way for new applications of digital photodetection tools across various domains, including industry, infrastructure design, logistics, medicine, social interactions, academic research, and the military-industrial complex [1]. With the rise of "Big Data," the transmission and storage of large volumes of digital information have become increasingly important. This concept aligns with the utilization of machine analysis methods, including sophisticated neural network algorithms capable of extracting high-level features through deep learning. These tools not only expand the researcher's capabilities but also facilitate machine-to-machine interaction analysis. By relying less on human intervention, this approach reduces the burden on personnel and helps mitigate issues associated with human error.

After conducting thorough research, a comprehensive approach has been devised to improve the effectiveness of digital photodetection systems. This is accomplished by utilizing nanostructured photoluminescent coatings, which facilitate the synchronization of the photoelectric converter's absorption spectrum with the transmission spectra of the light filters, aligned with specific color schemes [2]. Key factors influencing the system's performance include the photosensitivity of the photoelements and color balance. These factors are evaluated based on the photomatrix's color scheme, the optical characteristics of the photoluminescent coating, and the silicon substrate of the photoelectric converters. Through the implementation of this methodology, the efficiency of the digital photodetection system can be significantly enhanced. The model compounds used for calculations were pyrazoline photoluminescent dyes [3]. The advantage of this set of luminophores is their high quantum yield of photoluminescence (QY = 75-80%), absorption in the near ultraviolet and visible ranges, and a sufficiently wide Stokes shift (115 nm to 280 nm). Control over the luminophores' characteristics (absorption spectrum and Stokes shift width) is achieved through the selection of the base dye and additives during the synthesis stage. Nanostructuring of the synthesized luminophor involves the incorporation of dye molecules into submicron and nanoscale pores of a white zeolite, followed by laser thermal annealing. This process, characterized by the amount of white zeolite relative to the total mass and the duration of the thermal annealing procedure, allows for an increase in the main photoluminescence peak by 5-11%. However, depending on the sample's irradiation time, it also leads to a decrease in luminophor transmittance and partial bleaching, which affects the target parameters.

Thus, a methodology for synthesizing coating luminophores has been developed, which is based on the utilization of organic pyrazoline dyes and the introduction of additives such as polymethyl methacrylate and polystyrene. This approach enables controlled modification of the absorption and photoluminescence spectra, as well as nanostructuring of the luminophor through the incorporation of dye molecules into submicron pores of zeolite. Finally, a methodology for determining the optimal parameters of the photoluminescent coating layer on the elements of the photomatrix (with a silicon substrate for the photoelectric converters of the constituent elements) has been developed based on the target indicators of photosensitivity and color balance.

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Inductive-resonance energy transfer in hybrid carbon nanostructures

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In recent years, many different materials based on hybridized carbon in its low dimensional forms (such as functionalized graphene, carbon nanotubes, graphene, graphene quantum dots, graphene nanoribbons, etc.) and these systems are widely used in optoelectronics, especially when interfaces with molecules are created [1,2]. Here, we present a microscopic view of the substrate-molecule interface interaction in an archetypal hybrid material consisting of graphene functionalized with dye molecules. The non-radiative energy transfer at a 0D/2D interface can be explained by two main mechanisms: Forster and Dexter couplings. The Forster process describes the direct transfer of energy from an optically excited molecule to the substrate (in our case graphene or its derivatives). The Dexter coupling is based on simultaneous transfer of charges between the molecule and graphene states after the photoexcitation process. The Förster and Dexter energy transfer rates can be calculated analytically via Fermi's golden rule with the momentum-dependent initial and final states of the graphene substrate and the HOMO and LUMO states of the molecule. Having characterized the hybrid material within the limits of DFT calculations, including the fully geometrical relaxation of the structure, its electronic band structure, optical properties and charge rearrangement, we will focus on energy transfer, which was measured recently experimentally. The obtained results will be applied to other carbon hybrid nanostructures and, in general, to the description of energy transfer processes when the molecular transition dipole moment and the substrate–molecule separation are known.

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Crystallization of low-temperature gallium arsenide for device structures in the terahertz range

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The aim of this work was to grow epitaxial layers of low-temperature gallium arsenide by low temperature liquid phase epitaxy for optoelectronic devices in the terahertz range.

That was investigated that generation of additional defects in GaAs epitaxial layers and short carrier lifetime [1] makes GaAs an excellent candidate to realize fast THz modulation.

Generation of additional defects was achieved by complex doping rare-earth elements [2].

The Electrochemical Capacitance-Voltage (ECV) profiling technique was applied to investigate electrophysical properties of epitaxial layers. To investigate structural characteristics X-ray diffraction analysis (XRD) was used.

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Synthesis, characterization and antibacterial properties of modified calcium phosphates

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Apatite ($Ca_{10}(PO_4)_6(OH)_2$) and whitlockite (β-$Ca_3(PO_4)_2$) related calcium phosphates due to their biocompatibility and bioactivity are widely used in orthopedics and dentistry for bone restoration [1]. At the same time, the biphasic calcium phosphates (mixture of apatite and whitlockite-type phases) have also significant interest due to the possibility of regulation of material bioresorption by varying the weight ratios of their components [2]. The main way for influence on functional properties of synthetic calcium phosphates is their chemical modification with cationic and anionic substitutions (mainly carbonate (CO_3^{2-}) and trace metals (Na^+, K^+, Zn^{2+})). The foreign ions change chemical and thermal stability, mechanical and biological properties of such synthetic materials.

The aim of the study focuses on the synthesis of nanoparticles of calcium phosphates which contain of sodium or potassium cations as well as their combination with addition of Zn^{2+} and fixed amount of carbonate-anions, characterization of prepared phosphates using powder X-ray diffraction and FTIR spectroscopy methods and investigation of their antibacterial activity.

Chemically modified calcium phosphates were prepared from an aqueous solution. According to powder X-ray diffraction results the biphasic calcium phosphates which contain different amount of dopants were obtained. The antibacterial activity of obtained phosphate again Staphylococcus aureus have been evaluated.

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Electrophysical properties of InGaN/GaN LEDs with quantum wells

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Traditional lamp-based lighting systems,such as filament bulbs and fluorescent tubes, have been progressively replaced by LED-based solid-state lighting (SSL). LED emits lights when forward current is applied to its p-n junction. Small and energy efficient LEDs have quickly conquered the field of microelectronics and optoelectronics. Commercial LEDs aremade of III–V group compounds, which are GaAlAs (red-emitting), AlInGaP (yellow-orange), InGaN (blue, green), AlInGaN (ultra violet). Among them InGaN/GaN heterostructures with quantum wells (QW) as the core light-emitting region define an important standard for SSL [1].

The purpose of the study was to investigate the temperature dependence of electroluminescence and current-voltage characteristics (CVCs) of the InGaN/GaN heterojunction assembly in comparison to the homojunction ones (GaP, GaAsP).

The InGaN/GaN heterostructure with QWs was grown on sapphire (Al_2O_3) and demonstrated the maximum emission of electroluminescence at 505 nm [2]. It was found that at 290 K the single band splits into two peaking at 500 and 506 nm, the latter is of lower intensity. The separation of ~30 meV between them is close to the energy of acoustic phonone in GaN. The rise of injection current leads to a blue-shift by 0.043 eVdue to the band filling effect. It is a distinct feature of the heterojunction. The quantum yielddrops twice in a linear interval from 1 to 20 mA.

CVCs were acquired in the current generator mode for the 77-290 K temperature range. They demonstrate a power-law dependency. The negative differential resistance region most evidently appears at 77 K.Some decrement in the dI/dU slope before the S-shaped region is indicative of increment in the diode's differential resistance. The S-type regions are immanent to the systems with positive feedback [3]. The presence of instability within $dI/dU<0$ implies a variation in the current flow mechanism. The phenomenon might occur due to the resonant tunneling of carriers along the quantization levels, enhanced by the effect of their quasi-ballistic transfer through QWs.

We believe that both the appearance of a negative differential resistance and a decrease in quantum yield are manifestations of discrete levels in QWs.

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Differences in emission spectra of pristine and irradiated with 2 MeV electron beam InGaN/GaNLEDs with quantum wells

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The InN-GaN solid solutionsare used for the production of efficient InGaN LEDs emitting in the UV and Vis ranges thanks to their direct and wide band gap. They are typically fabricated on a sapphire substrate resulting in a lattice mismatch of ~12% between GaN and Al_2O_3. The development of mismatch dislocations especially in the quantum wells (QW) region introduces piezo-fields through the mechanical stress and additionally strengthens the natural polarization in the (0001) direction of growth [1]. The quantum-confined Stark effect is becoming more pronounced resulting in larger space separation of charges due to distortion of the energy zones and lower probability of their radiative recombination [2].

The permeable radiation is known to affect the electrophysical properties of materials by introducing structural defects and reducing the lifetime of minority charge carriers. The impact manifests in reduction of the emission intensity and of the current as it has been demonstrated for both the homo- and heterojunction LEDs [3]. The degraded characteristics might be partially restored by the thermal annealing [4].

In the present study we will focus on changes in electroluminescence spectra of InGaN/GaN LEDs with QWs caused by the 2 MeV electron beam irradiation with the flux up to $2.25 \cdot 10^{15}$cm^{-2}. The blue color (λ_{max} = 470 nm) emitting $InxGa_{1-x}N$/GaN (x = 0.2) LEDs were grown on sapphire substrates. Thetemperature-dependent emission study was performed in the temperature range of 77–300 K for both the pristine and the irradiated LEDs and results are presented in Fig. 1.

As can be seen from Fig. 1, the emission spectral line has the Gaussian type profile perturbed by a phonon repetition peak (the phonon energy is

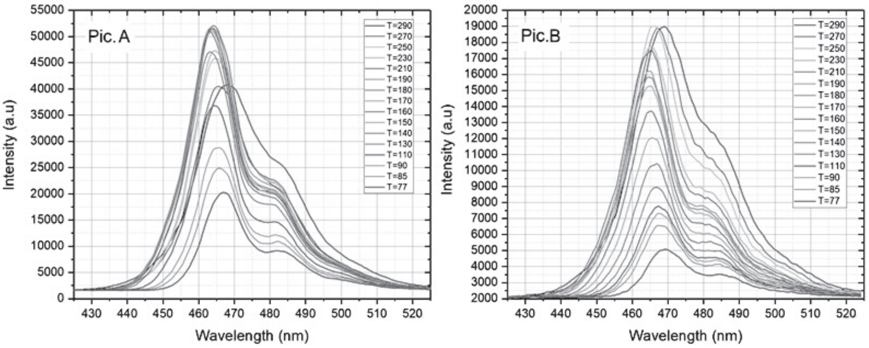

Fig.1. *Temperature-dependent (77–290 K) emission spectra of pristine (A) and irradiated with 2 MeV electron flux (B) InGaN/GaN LEDs with QWs.*

$\hbar\omega\Phi = 65$ meV) in the low-energy side. It was also observed that the intensity of the LED glow can be amplified by increasing the injection current. Although, this can be done within a certain interval only, because for the current value exceeding 20 mA, there is a tendency to saturation caused by the filling of QWs and rising ballistic transfer of carriers through them. These effects are even more prominent for the irradiated LED, where the characteristic maximum appears at currents much smaller than the nominal one (≈5 mA), and followed by a steady decrease in quantum yield.The luminescence intensity diminishesdue to the introduction of deep non-radiative levels in the QW.

The observed performance decrement of the heterojunction LEDs under study after being irradiated with the 2 MeV has been found less pronounced in respect to what was observed for the correspondent homojunction LEDs according to the literature [5], thus, suggesting a better radiation resistance.

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Dispersion of the Vibrational and Electronic Excitations in the Bulk Crystals of MoS_2 and Their 2D-Monolayers

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3D crystals of transition metal dihalcogenides (TMD materials) and their 2D structures belong to the class of materials, technologically promising for creation a variety of optoelectronic devices, photonics, light and display photodetectors, solar panels, quantum sensors, etc. They possess a unique electronic band structure, high charge carrier mobility (around 500 $cm^2V^{-1}s^{-1}$), and belong to the class of two-dimensional (2D) materials. The electronic and vibrational processes in these materials, especially double electron-photon resonances, require further investigation. Interestingly, a monolayer of a TMD such as molybdenum disulfide (1L-MoS_2) is a direct semiconductor with a bandgap ~1.8 eV, while the bulk crystal of 2H-MoS_2 is an indirect bandgap semiconductor with a bandgap ~1.2 eV.

We have investigated a correlation of vibrational modes, electronic excitations without taking into account an electron spin and with taking it into account and their dispersion for 3D crystals of the MoS_2 and their 2D-monolayers 1L-MoS_2 at high symmetry points of the corresponding Brillouin zones.

The influence of the lone electronic pairs, formed in the MoS_2 structures by the sulfur ions S^+, on the energy spectra and on the structure of electronic π-zones, and the nature of spin-dependent splitting of π-states of spinor excitations in K and H points of the Brillouin zone in 3D crystals of MoS_2 have been explained.

Influence of $BiFeO_3$ concentration in PLA on dielectric and piezoelectric properties of thin film nanocomposites

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Recently, the demand for harvesting different types of alternative green energy sources (solar, mechanical, thermal, etc.) increases due to the waste generated during the production of energy devices which cause significant problems related to environmental factors and human health. The one of common energy source available is mechanical energy, and the piezoelectric effect is frequently used to convert appropriate energy types (for example, human body motion and vibrations) into electrical energy [1,2]. Piezoelectric nanogenerators are dependent on a piezoelectric material for the conversion of mechanical stress into useful electrical energy.

The aim of this study was to investigate the effect of $BiFeO_3$ nanoparticles' weight amount (1-20%) on the properties of polylactide/$BiFeO_3$ thin films. BFO nanoparticles were fabricated using the facile reverse co-precipitation method, followed by annealing and ultrasonic dispersion in chloroform, which was used as a solvent for polylactide granules. Obtained mixtures were solution-casted on glass plates, cut into proper shape and gold electrodes were sputtered on both sides. Prepared thin films were characterized by means of filler dispersion (SEM), structure (XRD, DSC), dielectric properties and piezoelectric response of polylactide/ bismuth ferrite thin films to different air stream pressure.

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Development of polycarbonate composite films with antibacterial activity

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Recently, as the bacterial infection situation has been prolonged due to Corona 19, the popularity and consumption of various antibacterial products such as the packaging material, medical devices and implants are gradually increasing. The inorganic bacteriostatic agents such as ZnO, CuO and Ag nanoparticles have attracted a great deal of attention over the past years. The work is devoted to the study of effective polymeric composite films based on polycarbonate [1] and zinc oxide or silica carriers with immobilized nanoparticles of silver and copper oxides.

A standardized disk-diffusion approach was used to evaluate the antibacterial activity of composite film with a diameter of 5 mm relative to the gram-positive bacteria *(Staphylococcus aureus, Bacillus subtilis)*, gram-negative bacteria *(Escherichia coli)* and yeast *(Candida albicans)*. The antibacterial activity was determined by measuring the diameter of the inhibition zones were measured in millimetre (mm) around samples [2]. Materials containing silica carriers with immobilized silver and copper oxide nanoparticles demonstrated the antimicrobial properties and inhibit their growth of a wide range of microorganisms.

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Electronic and optical properties of of $AgXBr_3$ (X = Ca and Sr) Perovskites: An ab initio study with the Tran–Blaha-modified Becke–Johnson density functional

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In this study, we conducted an ab initio investigation of the structural, electronic and optical properties of $AgCaBr_3$ and $AgSrBr_3$ Calcium-based halide perovskites. using the full-potential linearized augmented plane-wave (FP-LAPW+lo) method [1] basis set as implemented in the WIEN2k code [2].Calculated structural parameters, including the lattice constants *(a)*, bulk modulus *(B)* and its pressure derivative *(B')*, for the considered compounds using both the local density (LDA) [3] and generalized gradient approximations (GGA–PBEsol) [4] are consistent with the available data in the scientific literature. To calculate the electronic properties, the exchange-correlation potential is treated with various functionals, and we find that the newly developed Tran–Blaha-modified Becke–Johnson (TB-mBJ) [5–7] functional significantly improves the band gap. Band structure, total and site-

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projected *l*-decomposed densities of states, charge-carrier effective masses, charge transfers and charge density distribution maps were obtained; analyzed and compared with the available theoretical data. The frequency-dependent complex dielectric function, absorption coefficient, refractive index, extinction coefficient, reflectivity and electron energy loss function spectra were calculated. The origins of the peaks and structures in the optical spectra are determined in terms of the calculated energy band structures.

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DNA-to-berberine excitation energy transfer in “silver nanoparticles / DNA/ berberine” nanosystem for X-ray induced photodynamic therapy

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X-ray photodynamic therapy (X-ray PDT) of cancer is based on generation of reactive oxygen species in tumor upon its irradiation by deep-penetrating X-ray irradiation. For this, nanosystems accumulated in the tumor should be developed, which absorb X-ray quanta and transform their energy into that of reactive oxygen species. Here we have studied formation of model nanosystem for X-ray PDT “silver nanoparticles / DNA / berberine” and electronic excitation energy transfer process in it. In this nanosystem, silver nanoparticles are suggested to absorb X-rays and produce secondary electrons used to excite DNA; electronic excitation energy of DNA bases is supposed to be further transferred to berberine which would enerate reactive oxygen species to destruct cancer cells.

Thus, we have synthesized silver nanoparticles on low molecular weight DNA and then added berberine to the obtained suspension. Absorption and fluorescence spectra of berberine in the presence of DNA-silver nanoparticles system proves the binding of berberine molecules to DNA-silver nanoparticles and thus the formation of “silver nanoparticles / DNA / berberine” nanosystem. Besides, fluorescence excitation spectra demonstrate that electron excitation energy transfer takes place from DNA bases to berberine in the formed nanosystem. This energy transfer is a necessary stage in the suggested process of energy transformation from X-ray quantum to reactive oxygen species.

In addition, interaction of “silver nanoparticles / DNA / berberine” nanosystem with the model phospholipid membrane was studied by differential scanning calorimetry. It was shown that this nanosystem leads to the increase in cooperativity of the membrane phase transition.

The work was supported by the National Research Foundation of Ukraine (project 2020.02/0367)

Structure and mechanical properties of PVA-PEG-TiO_2 hydrogel composites cross-linked by electron irradiation

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Hydrogels are highly sought after for their exceptional properties, including high water content, softness, flexibility, and biocompatibility. Ionizing radiation is favored for crosslinking hydrogels, improving their mechanical characteristics and resistance to high temperatures. Incorporating titanium oxide (TiO_2) particles is promising for enhancing hydrogel properties, particularly antibacterial activity.

In this work the structure of PVA-PEG-TiO_2 hydrogel composites was investigated and an influence of TiO_2 concentration on mechanical properties composites was evaluated. At the same time, studies of the antimicrobial activity of these composite systems were conducted.

The synthesis process of hydrogel samples incorporating titanium dioxide particles was described in detail [1,2]. Dynamic light scattering method determined the hydrodynamic diameter of the TiO_2 particles to be approximately 320 nm. Scanning electron microscopy was employed to visualize the distribution of TiO_2 particles within the polymer matrix. Analysis of the sample structure using wide-angle X-ray diffraction indicated a slight shift in the diffraction maxima responsible for the TiO_2 crystalline phase, suggesting an interaction between titanium dioxide and the PVA-PEG polymer matrix.

Mechanical testing conducted on a tensile testing machine revealed a decrease in both the tensile strength and elongation at break as the concentration of TiO_2 particles increased. This decrease in mechanical properties was attributed to the disruption of the polymer network's integrity and connectivity caused by the presence of TiO_2 particles.

Furthermore, antimicrobial activity was investigated by evaluating the hydrogel samples against Staphylococcus aureus and Escherichia coli. A hydrogel with a TiO_2 concentration of 1 wt.% showed no bactericidal effect, hypothesized to be due to the large size of the TiO_2 particles.

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Study of the surface relief of the Co-W(WOx)-TiO_2 composite systems

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The results of studies of the surface relief of the Co-W(WO_x)-TiO_2 composite systems influence by an atomic force microscopy are discusses.

The research was carried out on samples coated with Co-W(WO_x)-TiO_2 composition, at. %: 89.1 Co, 5.4 W and 5.5 Ti (in terms of metal), deposited from a citrate complex electrolyte containing 5 g/dm^3 of titanium dioxide, at a current density i_k = 3.5 A/dm^2, T = 323 K and the electrolyte mixing speed is 100 rpm [1].

The results of AFM analysis of the surface of the studied samples indicate the formation of a fine-grained, more ordered and uniform structure, compared to the base material. Areas of different morphology are observed on the surface: the main surface layer has a fine-grained structure, and cone-shaped agglomerates with a base diameter of up to 5 microns, similar to the structure of metallic cobalt, are located in certain areas. Separately located protrusions are also visualized on the surface of the coating, which differ significantly in height from the main surface. The surface roughness for the scanning area of 48 × 48 μm is R_a = 0.3 μm and R_q = 0.3, which indicates a significant surface (90° → 270°) indicates anisotropy of the properties of the obtained material.

The fractal dimension D for the Co-W-TiO_2 coating is 2.70, which reflects three-dimensional nucleation during coating formation. The fractal dimension decreases to 2.44 as the scan area decreases to 10 × 10 μm, and in the nanoscale relief (2.5 × 2.5 μm) it is 2.24, indicating local surface alignment when transitioning to nanoscale relief.

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Oxygen-deficient HfO_2 nanoparticles for nanoelectronics and sensorics

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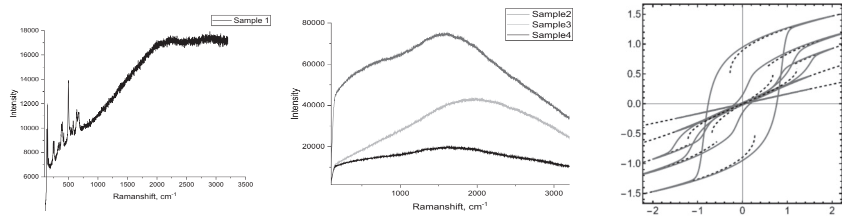
We revealed the formation of the ferroelectric orthorhombic phase in oxygen-deficient HfO_2 nanoparticles prepared at different annealing conditions for the controlled formation of oxygen vacancies. X-ray diffraction was used to determine the phase composition of the nanoparticles. Micro-Raman spectroscopy was used to explore the correlation of lattice dynamics and structural changes appearing in dependence on the average size of the nanoparticles and vacancies concentration. Landau-Ginzburg-Devonshire (LGD) phenomenological approach and phase-field modelling were used to calculate the phase diagrams, ground and metastable states, polar and structural properties of oxygen-deficient HfO_2 nanoparticles of various shape, which properties are strongly affected by surface and size effects. Special attention has been devoted to the comparison of modelling and experimental results. The combination of the Raman spectroscopy with X-ray diffraction, ferroelectric measurements, LGD, and phase-field theoretical approaches allows to establish the role of oxygen vacancies and to reveal the physical origin of possible correlations between the lattice dynamics, microstructure, phase composition and ferroelectric properties of the HfO_2 nanoparticles prepared in different conditions.



a *b* *c*

Raman spectra of stoichiometric (a) and oxygen-deficient (b) HfO_2 nanoparticles of sizes (9 - 14) nm. (c) Calculated polarization behavior in electric field (normalized units) changes from the dielectric curve for stoichiometric HfO_2 nanoparticles to the pronounced double and single hysteresis loops for the oxygen-deficient HfO_2 nanoparticles.

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Revealing of two relaxed forms in excited state in polymethines polymers by soliton theory

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Linear conjugated systems are called molecular compounds where the alternation of simple and multiple bonds. In general, the linear conjugated systems, which will be discussed here can be represented by the formula: $[R_1 - (CH)_m - R_2]$, where R_1 and R_2 - terminal group connected to the polymethine chain. These systems can be either electric neutral and charged positively or negatively - depending on what they injected - electron or hole. Methine carbon atom of (CH) in the chain is in sp2-hybridized state. To explain the properties of some organic compounds such as quasi-metallic conductivity, a significant change in the spectral properties of ionic dyes that absorb and emit light in the near infrared region of the spectrum managed, including through the use of the concept of solitons. Established that injection of electrons / holes in the conduction band leads to soliton level appearance inside the restricted area and this is accompanied by marked shift of the valence band top and the conduction band bottom, when electron injected - downward energy, in the case of holes injection - in the direction of energy increasing. In this work we use the charge transfer model based on the concept of solitons, according to Davidov A.D. which complements and develops other models. The joint spectral and quantum-chemical investigations of relaxation paths of symmetrical polymetine dyes are performed. They have shown existence of three relaxation paths: one symmetrical path with a conservation of the symmetry for the electronic structure and two unsymmetrical paths with various symmetry breaking mechanisms. All three components are experimentally detected by time-resolved fluorescent spectroscopy at low temperatures in polar medium. The fluorescent paths differ by their lifetime and spectral shape (band maxima) as well as strongly depend on rigidity and polarity. Reported studies give a significantly increased fundamental understanding of molecular electronic relaxations in excited state of symmetrical polymethine dyes.

Luminescent properties of amorphous glass-like compounds based on alkaline earth metal oxides

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In recent years, there has been scientific and practical interest in studying the luminescent properties of oxides based on alkaline earth metals. This interest is driven by their potential for creating high-performance phosphors and solid-state lasers with lamp pumping [1]. Calcium oxide (CaO), barium oxide (BaO), and potassium oxide (K_2O) are widely used in optical devices and light-emitting devices operating in the visible spectrum and exhibiting luminescent properties. To obtain samples of $(CaO)_x(P_2O_5)_y$, $(BaO)_x(P_2O_5)_y$, and $(K_2O)_x(P_2O_5)_y$, the method of vacuum melting of high-purity substances was used. Manganese was added step by step during the melting process to achieve better homogeneity of the melt with parallel stirring. Optimal melting conditions and melt stirring were chosen based on existing experimental data.The samples were polished plates measuring 50x15x15 mm. Manganese was added for doping in various percentage ratios. In this work, the influence of manganese concentration (Mn) on the luminescence intensity of these glass-like compounds was investigated.

For excitation of luminescence, a nitrogen laser LGN-10 with a wavelength of 337 nm was used. Luminescent characteristic studies were carried out at room temperature (20°C) under constant voltage and with the signal amplification coefficient from the photomultiplier tube (PMT). Luminescence spectra were examined using the spectral complex KSVU-12 in automatic mode. The photocurrent signal from the PMT was amplified by an original design instrumental amplifier [2] and recorded using a high-speed analog-to-digital converter (ADC). The measurement results were simultaneously displayed in real-time on a computer screen and recorded in a data file on a hard disk. Figure 1 shows the photoluminescence spectra of the investigated samples activated with manganese (a-b-c) with manganese content ranging from 1% to 10%. The dependence of luminescence intensity on the amount of activating impurity is also shown (g).

From the graphs, it can be observed that the introduction of manganese doping leads to the emergence of a single emission band (with a wavelength of

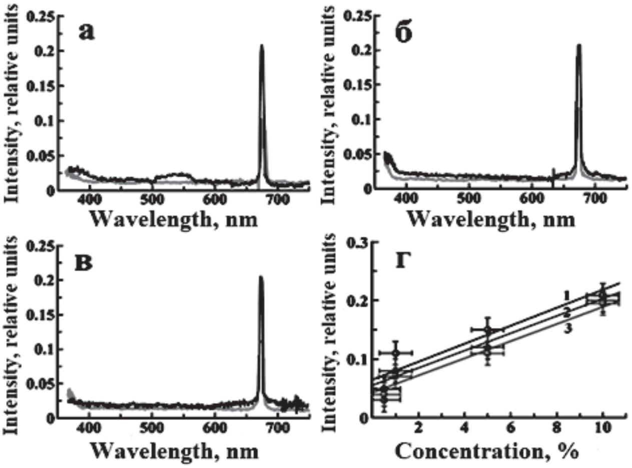

Fig 1. *Photoluminescence spectra of oxide compounds based on: (a) $(BaO)_x(P_2O_5)_y$, (b) $(K_2O)_x(P_2O_5)_y$, (c) $(CaO)_x(P_2O_5)_y$, doped with manganese (1-10%) and the dependence of emission intensity on the concentration of the doping impurity (g). 1 - $(BaO)_x(P_2O_5)_y$, 2 - $(K_2O)_x(P_2O_5)_y$, 3 - $(CaO)x(P_2O_5)_y$.*

approximately 672 nm), indicating the activating property of manganese. The spectral peaks are relatively narrow, indicating the elemental nature of the emitting centers. This suggests that the observed emission band is caused by centers of the same type. It can be hypothesized that the main luminescence band is due to the formation of paired and triple associates of Mn^{2+} ions in the investigated compounds.A comparative analysis of the position of the spectral peaks and the emission intensity showed that the percentage ratio of manganese practically does not affect the emission wavelength, while the luminescence intensity varies proportionally to the percentage content of manganese in the sample.

The Effect of Mechanical Surface Treatment on the Optical Properties of Nanoporous Al_2O_3 Matrices with Incorporated ADP, KB5, and KDP Crystals

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In works [1,2], it was established that nanoporous Al_2O_3 matrices with ADP crystals in the pores have a low reflection coefficient (~0.5%) in the spectral range of 1.0-10.0 µm. However, the mechanism of this phenomenon was not established in these works.

This work investigates the effect of mechanical surface treatment on the optical properties of nanoporous Al_2O_3 matrices with the inclusion of ADP, KB5, and KDP crystals in the pores. In addition, profilograms of the surfaces of the studied samples were taken before and after mechanical processing. The conducted studies make it possible to assess the presence of diffuse scattering by the surfaces of these studied nanomaterials and to evaluate its impact.

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Inductive-resonance energy transfer in hybrid carbon nanostructures

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In recent years, many different materials based on hybridized carbon in its low dimensional forms (such as functionalized graphene, carbon nanotubes, graphene, graphene quantum dots, graphene nanoribbons, etc.) and these systems are widely used in optoelectronics, especially when interfaces with molecules are created [1,2]. Here, we present a microscopic view of the substrate-molecule interface interaction in an archetypal hybrid material consisting of graphene functionalized with dye molecules. The non-radiative energy transfer at a 0D/2D interface can be explained by two main mechanisms: Forster and Dexter couplings. The Forster process describes the direct transfer of energy from an optically excited molecule to the substrate (in our case graphene or its derivatives). The Dexter coupling is based on simultaneous transfer of charges between the molecule and graphene states after the photoexcitation process. The Förster and Dexter energy transfer rates can be calculated analytically via Fermi's golden rule with the momentum-dependent initial and final states of the graphene substrate and the HOMO and LUMO states of the molecule. Having characterized the hybrid material within the limits of DFT calculations, including the fully geometrical relaxation of the structure, its electronic band structure, optical properties and charge rearrangement, we will focus on energy transfer, which was measured recently experimentally. The obtained results will be applied to other carbon hybrid nanostructures and, in general, to the description of energy transfer processes when the molecular transition dipole moment and the substrate–molecule separation are known.

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Abstract Title: Applications of Carbon Dots as Advanced Nanomaterials

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Carbon dots (CDs) with an average diameter less than 10 nm have garnered increasing attention in the research of material science and biomedical engineering due to their unique properties such as small size, photoluminescence (PL), high water-dispersity, biocompatibility, low toxicity, and tunable surface functionality. In this presentation, I will begin with the introduction of the methodologies used to synthesize a wide array of CDs. Specifically, three unique CD species that represent both top-down and bottom-up approaches will be scrutinized through extensive structural characterizations to optimize their properties and applications.

Then, I will shift focus to the wide scope of exceptional biomedical applications of CDs recently developed in our lab: (1), surface modification nanoarchiteconics of carbon nitride dots (CNDs) for enhanced drug loading and higher cancer selectivity; (2), a drug delivery system of CDs conjugated with memantine for targeting tau aggregation associated with Alzheimer's Disease; (3), the structure-activity relationship of CNDs in inhibiting tau aggregation (4), difluoromethylomithine (DMFO) derived CDs for the treatment of Neuroblastoma and imaging; (5) metformin-derived CDs showed a unique nucleus targeting property, which suggests a huge potential for future nucleus-targeting drug delivery.

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Applying of Direct Current Arc Discharge over the Crucible for Obtaining Ceramic Films in Electronic Production

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In the modern production of electronic devices, mechanical instrument, as well as details of engines in automotive, aviation and space vessels, the ceramic coatings of different applying are widely used. For example, in electronic industry dielectric coatings for the high-quality capacitors with low level of conductivity, are effectively applied today. Another way of application of dielectric ceramics films in the electronic industry is production of reactive elements for transmitters and receivers' antennas of communication devices [1 – 4]. In instrument-making industry the ceramic coatings are effectively applied as hardness protective means for defense at cutting instruments [5 – 7]. As for reinforcing coatings, their use allows you to significantly extend the period of trouble-free operation for important parts of mechanisms that rotate at high speed and are subject to significant friction [5 – 7]. Main industrial applications of new type of high voltage glow discharge electron guns (HVGDEG) in the technology of obtaining the ceramic films with the stable stichometry are considered in the papers [8, 9]. In the paper [9] the basic principles of High Voltage Glow Discharge (HVGD) self-aligned electron and ion optics are considered. Therefore, the main subject of this report is considering of self-consistent arc discharge over crucible for deposition of ceramics films with including the active gas components, such as oxygen or nitrogen [5 – 7]. The basic construction of technological device for lighting the arc over the crucible is presented at Fig. 1. The main geometrical parameters of this devices, as well as the electric circuit to switching it, are also noted at Fig. 1.

The mathematical model of such an electrode system for the physical conditions of non-self-sustained arc discharge combustion can be built on the basis of the following assumptions and theoretical propositions, which were proposed in the in the papers of gas discharge and discharge plasma physics [10, 11].

1. The distribution of the electric field between the ring electrode and the surface of the metal being evaporated is determined by analytically solving the Poisson equation in cylindrical coordinates [12]. The corresponding coordinate system *(r, z)* is shown in Fig. 2.

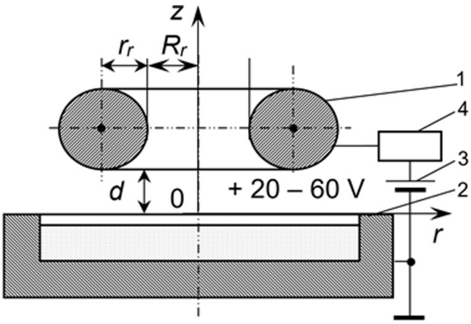

***Fig 1**. Structural scheme of the device for maintaining an arc discharge in metal pairs and the method of connecting this device to the electrical circuit. 1 – ring electrode, 2 – crucible, 3 – power source, 4 – electronic system for arc discharge current control*

2. The magnitude of the space charge is determined by the continuity equation for electron and ion currents [13, 14].
3. The energy of metal atoms above the surface of the crucible is determined by Boltzmann's law as kT_{ev}, where k is the Boltzmann constant, and T_{ev} is the evaporation temperature [15].
4. Metal vapors above the crucible are saturated. According to this physical assumption, the concentration of metal atoms nm is determined.
5. The level of metal vapor ionization is determined by the ionization coefficient βm.
6. The concentration of residual gas atoms is determined by the residual gas pressure in the technological chamber pg.
7. The level of residual gas ionization is determined by the ionization coefficient β_g.
8. The values βm and β_g for the mathematical model under consideration are considered constant and do not depend on the arc discharge burning voltage U_d.
9. According to the physical model of singly charged ions, the numbers of ions and electrons in the volume, where the arc discharge maintained, are considered the same.

The basic set of equations algebraic equation is follows:

$$j_d = en_{im}\left(\sqrt{\frac{2kT_{ev}}{m_{im}}}+\sqrt{\frac{2e\varphi(r)}{m_{im}}}\right)+en_{ig}\left(\sqrt{\frac{2kT_0}{m_{ig}}}+\sqrt{\frac{2e\varphi(r)}{m_{ig}}}\right)+en_e\sqrt{\frac{2e\varphi(r)}{m_e}},$$

$$\rho_\Sigma(r)=K\sqrt{\frac{1}{\varphi(r)}},\quad K=\sqrt{\frac{e}{k}}\left(\beta_m\sqrt{p_aN_AR}+\frac{\beta_g p_g}{\sqrt{T_0}}\right),$$

where jd is the current density of the arc discharge, m_{im} is the mass of metal ions, m_{ig} is the mass of gas ions, n_{im} is the concentration of metal ions, n_{ig} is the concentration of gas ions, T_0 is the temperature of the external environment in the technological chamber, ne is the concentration of electrons, m_e is the mass of an electron, K is the semiempirical coefficient of proposed model. The set of equation (2) is transformed into cubic equation relatively to the value of potential $\varphi(r)$ and it was solved with using Cordano formula [16].

Corresponded graphics solution for titanium vapors in nitrogen media with the different operation pressure in electron gun are presented at Fig. 2 [17].

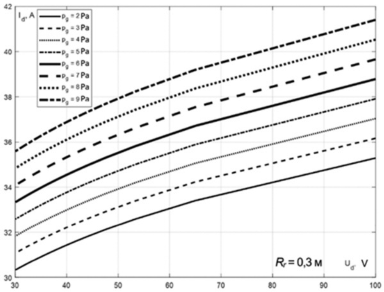

Fig 2. *The current-voltage characteristics of non-self-sustained arc discharge for the electrode system of the technological device, the structural scheme of which is presented in Fig. 2. Calculations with using formulas (1) were provided for residual pressure values in technological chamber* p_g *from 2 Pa to 9 Pa and for different values of the inner radius of the ring electrode* R_r

The proposed mathematical model of the arc discharge in metal vapors, based on set of equations (1), have been developed for the practical aspect of depositing high-quality ceramic coatings with including the components of active gases. Obtained and presented in the paper graphical dependences for the current-voltage characteristic of the arc discharge are also very important scientific results in a practical point of view for analyzing the electrical regimes of lighting the arc in the metal vapors and its dependence on operation pressure and geometry of ring electrode.

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ZnO nanoparticles: a key player in nonlinear optical phenomena

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Nanoparticles have attracted significant attention due to their unique properties and versatile applications in various fields, particularly in optoelectronics. Among these nanoparticles, zinc oxide (ZnO) has been extensively investigated for its exceptional optical and electronic characteristics, including its potential to enhance nonlinear optical phenomena such as third harmonic generation (THG)[1-2]. THG is a nonlinear optical process where three incident photons combine to produce a photon with triple the frequency (one-third the wavelength) of the incident photons[3]. In this study, we aim to investigate the influence of ZnO nanoparticles with sizes below 100 nm on the nonlinear optical properties of a pyrazoline compound incorporated into poly(methyl methacrylate) thin films. By incorporating ZnO nanoparticles into the polymer matrix, we explore the potential enhancement of THG in these composite thin films. The characterization of the THG was carried out using the Fringe Maker technique. The results obtained from this study will be presented and discussed in detail during this communication.

Acknowledgements: The presented results are part of IMAGE project that has received funding from the EU Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 778156.

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Ionic conduction in glassy and partially crystallized lithium-sodium tetragermanate

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Lithium-sodium tetragermanate $LiNaGe_4O_9$ (LNG) crystal demonstrates strong anisotropy of electrical conductivity σ contributed by interstitial Li ions moving through the channels within structural framework [1]. It is known, that under certain conditions preparation of the structures inhomogeneous in nanometer scale allows to enhance significantly ionic conduction of solid electrolytes. Earlier this assertion had been confirmed by studying single crystals, glasses and nanometer structured glass-ceramics of lithium heptagermanate $Li_2Ge_7O_{15}$. In particular, it was shown that ionic conductance of amorhous and nanocrystalline states in about three-five orders exceeded typical ---- values of the same single crystalline compound [2]. In this work we report the data on preparation of LNG glass and partially crystalized glass-ceramics. The structural content of the prepared compounds was characterized by XRD phase analysis. Electrical conductivity σ was measured in the temperature interval 300÷1000 K and in AC field frequency range $10^2 \div 10^6$Hz.

By using the fast quenching the melt [2], we have prepared LNG samples of the two kinds. The samples of the 1-st type were prepared by melting LNG single crystals and subsequent quenching the melt. The samples of the 2-nd type were prepared by grinding of the initial reagents in stoichiometric ratio in an agate ball mill and their melting without preliminary synthesis. The samples of the both types represent optically transparent and colorless plates with the widths of about 0.5÷1.0 mm.

XRD phase analysis showed that the samples of the 1-st type consist of 90÷92 % of LNG glass and contain near 8 % of the ordered regions with mean size of the crystallites of about 20 nm. Theses samples were devitrified on heating under the control of DSC. It was shown that the glass started to soften at T_g=780 K whereas final crystallization happened at T_c=820 K [3]. In the range included the temperatures T_g and T_c of DSC anomalies, electrical conductivity was measured on heating. It was shown, that conductivity of the glassy samples of the 1-st type exceeded in one-three orders σ values measured along the main axes of LNG single crystal [4]. Approaching Tg from below led to softening the glass and a more sharp increase of conductivity on heating. The final crystallisation of the glass at T_c was accompanied by the irreversible decrease of conductivity in about three orders of magnitude. An isothermal heat treatment of the samples of the 1-st type at the temperatures 10÷15 K below T_c allowed to increase the volume of the crystallized regions. Partial crystallisation of these samples was accompanied by decrease of electrical conductivity in about one order of magnitude.

XRD phase analysis evidenced that the samples of the 2-nd type practically did not contain amorphous phase and represented polycrystals with average crystallites sizes of about 40÷50 nm. Thermal treatment of these samples at 800÷815 K during a few hours resulted in σ increase in about one order of magnitude. Presumably growth of electrical conductivity of these samples can be attributed ot the appearance and increase in volume of nanocrystallites of highly conductive phase in $Li(Na)O_2 – GeO_2$ family.

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Exploring time-resolved luminescence spectroscopy in thin films of the DCM aryl analogue and its application in an OLED device

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In this study, thin films of 4-dicyanomethylene-2-aryl-6-[(4-dimethylamino)-styryl]-4H-pyran were successfully synthesized. The photoluminescence properties of the thin film were analyzed at room temperature, revealing the presence of two overlapping bands with maxima at 635 nm and 665 nm. Further investigation into the decay kinetics of the photoluminescence indicated the existence of two distinct components: a fast decay component (~3 ns) and a slow decay component (~7 ns). This observation provides valuable insights into the luminescence behavior of the thin film and contributes to a better understanding of the excited-state dynamics of the synthesized samples.

Additionally, this research marks the first successful fabrication and characterization of an organic light-emitting diode (OLED) based on the 4-dicyanomethylene-2-aryl-6-[(4-dimethylamino)-styryl]-4H-pyran compound. By exploring the performance characteristics of the OLED, such as current efficiency, luminance, and color purity, the study demonstrates its potential for the development of highly efficient OLED devices.

The findings from this investigation hold significant implications for the optimization and design of OLEDs. The understanding of the decay kinetics and the successful realization of an OLED using the abovementioned material pave the way for further advancements in the field of organic electronics. By leveraging this knowledge, researchers can work towards improving the efficiency, stability, and overall performance of OLEDs, leading to the development of more advanced and energy-efficient lighting and display technologies.

Acknowledgement. This research work was supported by National Research Foundation of Ukraine, 2020.02/0217 “Light-generation low-dimensional structures with polarized luminescence based on organic and inorganic materials”.

Yellow-green high-efficiency TADF OLED with phenoxazine and quinoxaline as emitter

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Skhirtladze L. **[2],** ***Bezvikonnyi O.*** **[2],** ***Volyniuk D.*** **[2],** ***Grazulevicius J.V.*** **[2]**

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The compound 2,3-bis(4-(10H-phenoxazin-10-yl)phenyl)benzo[5,6][1,4] dioxino[2,3-g]quinoxaline was synthesized and characterized as an emitter material for undoped OLEDs. This compound exhibits delayed thermally activated fluorescence (TADF) in the long wavelength region. The highest emission intensity of the synthesized compound film was observed at 556 nm. The electroluminescence of undoped organic light-emitting diodes demonstrated a similar emission maximum value when the compound was used as an emitter. It was found that the value of the photoluminescence decay time of 2,3-bis(4-(10H-phenoxazin-10-yl)phenyl)benzo [5,6][1,4] dioxino[2,3-g] quinoxaline in the Zeonex film (1 wt.%)) in vacuum are in the range of 30 μs at room temperature. Accordingly, there are 8.43 ns in air, which is associated with oxygen quenching of triplet states. The newly synthesized material demonstrates a bipolar charge transfer mechanism with drift mobility in the vicinity of 10^{-3} $cm^2/V×s$. The undoped OLED based on this TADF emitter showed a maximum external luminescent quantum efficiency of up to 10.0% and a maximum brightness of up to 28,000 cd/m^2.

Luminescent optical centers in $La_{1-x-y}Y_xNd_yF_3$ prospective for qubit states modelling

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Despite the fact that quantum computers running on superconducting qubits have already been created, as it was said by Prof. Srinjoy Ganguly "we are in the nisq (noisy intermediate-scale quantum) era and still very far from achieving the maturity level to have a fully fault-tolerant quantum computer". This leads to the proposal of other non-superconducting realizations of qubit states, such as: laser-controlled phonon vibrations of ions in laser-cooled traps; spin-spin transitions of nuclei in hydrocarbon molecules controlled by nuclear magnetic resonance; light-induced transitions of rare-earth ions in laser crystals.

A new look at the well-studied coherent states of rare-earth ions in laser materials as model of qubit states seems to be promising and prospective. The inhomogeneous broadening (Fig. 1) of the Nd^{3+} ions luminescence spectra in $La_{1\text{-}x\text{-}y}Y_xNd_yF_3$ nanopowder observed at liquid helium temperatures can be useful in view of greater variety of Nd^{3+} optical centers and their energy states as potential candidates (it looks that OC1 type centers are the most promising) for modelling of qubit states.

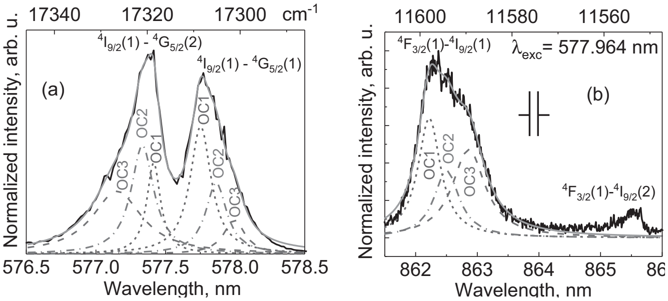

Fig. 1. $La_{0.89}Y_{0.1}Nd_{0.01}F_3$, $T = 4.2$ K: (a) luminescence excitation spectrum at the $^4I_{9/2}(1) \rightarrow {}^4G_{5/2}(1,2)$ transition of Nd^{3+} ion detected at the $^4F_{3/2}(1)$ $^4I_{9/2}(1, 2)$ transitions; (b) luminescence spectrum in the range of $^4F_{3/2}(1) \rightarrow {}^4I_{9/2}(1,2)$ transitions for $\lambda_{exc} = 577.964$ nm. Dashed lines show decomposition of spectral bands on Lorentzian components of groups OC1-OC3 of optical centers.

The work was supported by Estonian Research Council grant PRG347.

Al-based surface plasmon resonance for enhancement solar cells parameters

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Al nanoparticles and thin films are very attractive for light trapping in solar cells due to realization of surface plasmon resonance (SPR). Aluminum is promising alternative to noble metals because it has low cost, high prevalence in nature and ease of processing using a wide range of methods. In addition, the intrinsic property of broad plasmon resonances of Al, manifested in the ultraviolet–visible–near-infrared wavelength range, can be used in solar energy.

The purpose of this work was to obtain and study the structural and optical properties of the Al thin layer of on the surface of silicon for its further use to improve the parameters of solar cells due to the capture of light as a result of the SPR phenomenon. The structures of c-Si/Al, c-Si/Al/ SiO_x were studied before and after temperature treatment at T = 460°C, 600°C in an argon atmosphere for 30 min. The Al layer with a thickness of 13.5 nm was deposited by the thermal evaporation method. The SiO_x film with a thickness of d =191 nm was obtained by ion-plasma sputtering of the silicon target in the vacuum on the p-Si substrate in an atmosphere of argon and oxygen. The stoichiometry index of the original SiO_x film was determined by IR spectroscopy and was x=0.86, the refractive index was measured on an ellipsometer and was n=2.17.

The distribution of Al nanoparticles on the Si surface after thermal annealing obtained by AFM and Reflectance spectra are presented in Fig.1 and Fig.2 respectively. Based on analysis of obtained results it is possible to conclude that thermal annealing at T ≥ 460°C of ultrathin Al film as on the surface of Si substrate and in the c-Si/Al/ SiO_x structure transforms it into Al nanoparticles.

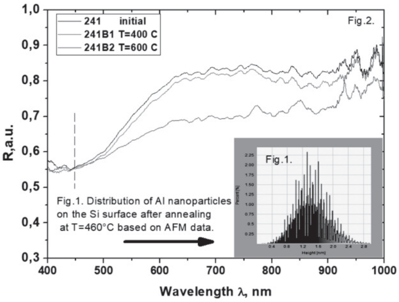

Fig.1. Distribution of Al nanoparticles on the Si surface after annealing at T=460°C based on AFM data.

Fig. 2. *Reflectance spectra of p-Si/Al/SiO_x structure before and after annealing.*

Evolution of Vibrational Spectra of $MoS_{2(1-x)}Se_{2x}$ few-layers nanoparticles

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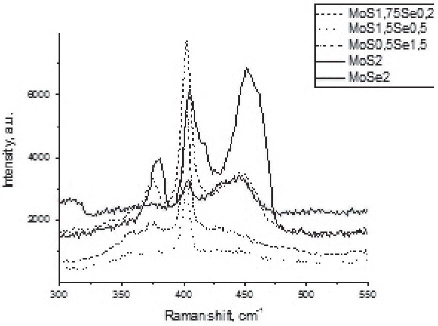
Transition Metal Dichalcogenides (TMD) solid solutions have gained significant attention due to their unique properties and potential applications in such fields as optoelectronics (photodetectors, solar cells, and light-emitting diodes) and energy storage, particularly in batteries and supercapacitors. By combining different TMD compounds, it is possible to create materials with improved sensitivity, selectivity, and response time for detecting various analytes, including gases, chemicals, and biomolecules.

By creating solid solutions of TMD compounds, it is possible to tune and modify the properties of the resulting material that are not present in the individual TMD compounds.

Here, we reported the synthesis of $MoS_{2(1-x)}Se_{2x}$ few-layers nanoparticles and their characterization by FTIR and Raman spectroscopy methods.

Figure below demonstrates the fragment of Raman spectrum (λ_{ex}=633 nm) in the region of two typical peaks of MoS_2 (E_{2g1} A_{1g} modes), which are attributed to in-plane vibration of S atoms and out-of-plane vibration of S and Mo atoms, respectively. These MoS_2-like modes shifted to low frequency by increasing the Se content in $MoS_{2(1-x)}Se_{2x}$. It is also seen, that spectra consist of the first order bands and those due to harmonics and combination modes.



Nanomilling-driven volumetric changes in arsenoselenide alloys at the border of glass-forming region

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The methods of positron annihilation lifetime spectroscopy (PALS) and X-ray powder diffraction analysis (XRPD) are employed to study volumetric changes in As-Se compounds at the border of glass-forming region exemplified by $As_{70}Se_{30}$ alloys subjected to high-energy ball milling *(nanomilling)* in dry and combined dry-wet modes. The glassy-crystalline nature of $As_{70}Se_{30}$ probes is confirmed by character halos in the XRPD patterns, showing domination of amorphous As-Se phase modified by inclusions of cubic arsenolite (As_2O_3) and rhombohedral arsenic (As) polymorphs. The formalism of modified *Positronics* approach based on the x3-x2-CDA (coupling decomposition algorithm) describing conversion of bound positron-electron (positronium, Ps) states in positron traps is applied to identify changes in wet-milled probes (stabilized by Polyvinylpyrrolidone, PVP) in respect to dry-milled ones. Under transition from wet-milled to dry-milled probes, the positron traps typical for nanostructured As-Se compounds with defect-specific lifetime of 0.376 ns (corresponding to multi-atomic vacancies in As-Se matrix) appear instead of Ps-hosting holes preferred in the PVP environment with Ps-related lifetime of 1.730 ns, these changes being accommodated in oxidized As-Se matrix with character defect-free bulk positron lifetime close to 0.264 ns.

Fabrication of composite macroporous polymer granules with ferrocyanide nanoparticles for selective adsorption of cesium ions

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The development of sorption technologies for the removal, separation, and concentration of radionuclides is an actual problem. In this respect the development of efficient adsorbents become especially relevant nowadays. Nanocomposite adsorbents with a sorption-active inorganic phase are of particular interest for the selective removal of radionuclides.

^{137}Cs radionuclides are the main component of liquid radioactive waste formed owing to the operation of nuclear facilities. Due to their long half-life (~ 30 years), and high chemical activity, and radioactivity as a gamma-ray emitter, cesium radionuclides pose a considerable threat to human health. Therefore, the treatment of liquid radioactive waste to a safe level is a crucial key to the sustainable development of nuclear energy.

Double transition metal ferrocyanide nanoparticles (FC NPs) possess high selective to cesium ions; however, due to the low hydromechanical stability they have not found wide practical applications. In the last decades, a variety of approaches have been developed for the synthesis of composite adsorbents by incorporating the FC NPs into the appropriate solid supporting matrix to improve their hydromechanical strength and adsorption characteristics.

Polymer granules with functional groups are a promising solid matrix for the fabrication of composite adsorbents with ferrocyanide phase. A novel composite adsorbent based on potassium copper ferrocyanide nanoparticles-loaded macroporous ion exchange resin was fabricated by in situ formation of ferrocyanide phase. Results of X-ray diffraction, Fourier transform infrared spectroscopy as well as scanning electron microscopy confirmed the formation of ferrocyanide phase, which consisted of crystalline cubic-shaped nanoparticles (70 to 100 nm). The FC NPs were revealed to form on the both surface and inner part of polymer granules.

The efficiency of the synthesized adsorbent for removal of cesium ions was evaluated under various experimental conditions. It has demonstrated a rapid adsorption process, high adsorption capacity over a wide pH range, and selectivity in Cs ion removal from model solutions with high salt content.

ZnO Nanoparticles: A Key Player in Nonlinear Optical Phenomena

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Nanoparticles have attracted significant attention due to their unique properties and versatile applications in various fields, particularly in optoelectronics. Among these nanoparticles, zinc oxide (ZnO) has been extensively investigated for its exceptional optical and electronic characteristics, including its potential to enhance nonlinear optical phenomena such as third harmonic generation (THG)[1-2]. THG is a nonlinear optical process where three incident photons combine to produce a photon with triple the frequency (one-third the wavelength) of the incident photons[3]. In this study, we aim to investigate the influence of ZnO nanoparticles with sizes below 100 nm on the nonlinear optical properties of a pyrazoline compound incorporated into poly(methyl methacrylate) thin films. By incorporating ZnO nanoparticles into the polymer matrix, we explore the potential enhancement of THG in these composite thin films. The characterization of the THG was carried out using the Fringe Maker technique. The results obtained from this study will be presented and discussed in detail during this communication.

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Magnetocapacitance effect in tunnel contact with perpendicular anisotropy of magnetic electrodes

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In this report, we want to consider the features of the magnetocapacitive effect in tunnel magnetic contacts with perpendicular magnetization of magnetic electrodes. Great interest in magnetic tunnel junctions is caused by the fact that not only a large value of tunnel magnetoresistance is obtained by the fact that in recent years in tunnel contacts with interfaces of the Fe/MgO type, a significant change in the capacitance in the magnetic field has been experimentally registered.This effect is called the magnetic tunneling capacity (MTC) effect, and it is considered one of the most promising effects that may have practical applications in memory cells and other spintronic devices. In contact tunnels with perpendicular anisotropy, the antiparallel orientation of magnetization radically changes the distribution of the magnetic field in the contact barrier layer and causes the appearance of a high-gradient magnetic field in the direction of magnetization of the contact magnetic electrodes. Under the action of such a high-gradient field, there is a spatial separation of spin-polarized major and minor electrons of electrons in the interface region, which creates an inhomogeneous distribution of electric charge in the contact barrier layer. As a result, an additional energy barrier for major spin-polarized electrons appears near each of the magnetic electrodes, and an additional effective capacitance, called spin capacitance, appears in the contact barrier layer. This additional spin capacitance can significantly reduce the total capacitance of the tunnel magnetic contact. The value of such additional spin capacity is proportional to the value of the spin polarization of electrons in the magnetic electrodes and the value of the magnetic field gradient with antiparallel orientation of their magnetizations. The mechanism of tunnel magnetic capacitance described by us is not only fundamentally different from the mechanism of tunnel magnetic capacitance in tunnel contacts with Fe/MgO interface boundaries, but also, in our opinion, has a better prospect for practical use. The large values of TMR and TMC in tunnel contacts with Fe/MgO interfaces are related to the features of the electronic structure of the Fe/MgO interface, where the effective spin-dependent tunneling effect is ensured by a good agreement between the crystal lattice parameters of the iron magnetic electrode and the crystal lattice parameters of the magnesium oxide nanolayer. In tunnel magnetic contacts with perpendicular magnetization of the electrodes, such matching of the grid of the magnetic electrode and the barrier nanolayer is not a strict necessity, which allows to simplify their manufacturing technologies. We conducted experimental studies of magnetoresistance and magnetocapacitive effect in tunnel magnetic contacts $Tb_{22}Co_5Fe_{73/}Pr_6O_{11}/Tb_{19}Co_5Fe_{76}$ with perpendicular magnetization of magnetic electrodes and a paramagnetic barrier layer. At room temperature, the value of tunnel magnetic resistance exceeds 110%, and the value of tunnel magnetic capacitance exceeds 115%.

Effect of heat treatment on sulfur-doped graphene oxide optical characteristics

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The sulfur-doped samples (S-GO) were grown by the Hammers method (heavily impregnated with strongly concentrated sulfuric acid), technology details in [1]. The multilayer S-GOs were thermally stable in an ambient environment.

In order to correlate spectral parameters with structural characteristics, the Raman spectra of graphene oxide for as prepared S-GO and heat-treated S-GO were examined. A heat treatment of S-GO samples was made inside a closed degassed graphite tube at temperatures 25 to 50°C for every 5°C interval over 15 min. Raman spectroscopy is a very powerful and widely used technique for identifying defects in graphite and graphene structures [2].

The synthesized S-GO samples were characterized by Scanning electron microscopy, Energy-dispersive X-ray spectroscopy, Raman and Photoluminescence spectroscopes (532 nm excitation laser).

The transformation of S-GO structure and PL spectra were estimated from the temperature-dependent shifts of Raman band peaks (components of deconvoluted spectra).

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Session 2

Nanobiotechnology for health-care

SKINOMITRONICS - a new challenge in research and development of sensors for medical diagnostics

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Over the past two decades, we have seen a tremendous growth in the bio/chemo-analytical sensing technologies of omics, approaches that comprehensively consider the entire genome, transcriptome, proteome, metabolome and microbiome. Combined with recent advances in material nanosciences, biotechnology, chemistry, electronics, and other disciplines, "omics on electrodes" is becoming the most powerful toolbox in biomedicine. Significant progress has been made in the field of "skinomics", a field of bioinformatics originally applied to the study of large-scale data in dermatology and skin biology [1]. In our opinion "skinomics" has been recently transformed into SKINOMITRONICS, which we defining here for the first time as an area of analytical chemistry dealing with the development of wearable devices for the detection of molecular targets on/under the skin. In this presentation, we would like to deliver an overview of recent advances and challenges in the research and development of omics based sensors for medical diagnostics.

This research was supported by the National Research Foundation of Ukraine (project №. 2022.01/0022 "Sensing platform based on graphene and textiles for analysis of metabolites in sweat").

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Effect of nano-complexes based on vanadium nanoparticles and cholesterol on immune system of tumor-bearing animals

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The interaction of cells of the immune system with the tumor is a delicate balance between the immune activation and immunosuppression processes. There are studies showing the role of vanadium compounds in the regulation of T-cell signaling, which allows them to be considered as promising antitumor drugs with an immune modulatory effect.

The purpose of this research was to evaluate the effect of nanocomplexes (NC) containing rare-earth orthovanadates $GdYVO_4:Eu^{3+}$ and cholesterol on the growth of Ehrlich ascites carcinoma (EAC) and changes in the immune system indices of tumor-bearing recipients.

The experiments were conducted in Balb/c mice, in the peritoneal cavity of which the EAC cells were grown for 7 days (group 1). The EAC cells were incubated for 3 hours with the NCs synthesized at the Institute for Scintillation Materials of the National Academy of Sciences of Ukraine. The EAC cells after incubation with NC were injected into mice ($3x10^6$/mouse) and *in vivo* cultivated (group 2). The intensity of tumor growth in animals of both experimental groups on the 4th and 7th days after inoculation was determined. The immune system of animals was examined by assessing the number of T-helper ($CD4^+$), T-suppressor ($CD8^+$), T-regulatory ($CD4^+CD25^+$), and natural killer ($CD16/32^+$) cells in the lymph nodes. The same indices were investigated in a control group.

It was established that on the 7th day of the EAC development, the number of all subpopulations of immunocompetent lymph node cells being under examination gradually decreased, with the exception of the subpopulation of T-regulatory ($CD4^+CD25^+$) cells, which was 1.5 times higher than in the control group. Induction of oncological pathology by tumor cells pre-treated with NC resulted in the inhibition of tumor growth by 74.70±4.38%. This was accompanied by an increased number of natural killer cells ($CD16/32^+$) and a decreased content of T-regulatory cells.

Peculiarities of silver nanoparticles synthesized using *Artemisia vulgaris* “hairy” root extracts

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"Green" synthesis of metal nanoparticles (NPs) is becoming increasingly popular due to its environmental friendliness and low toxicity. One of the advantages of “green” synthesis is a high degree of size and shape control of the resulting NPs. Silver nanoparticles (AgNPs), the most widely studied type of NPs, can be synthesized in different sizes and shapes using a variety of plant extracts. These NPs tend to be more stable than those synthesized using chemical methods due to the complex combinations of compounds, such as polyphenols and flavonoids. The extracts from the “hairy” roots of *Artemisia vulgaris* L. were used to obtain and study AgNPs. TEM was applied to evaluate the size and shape of obtained AgNPs.The results demonstrated the differences in size and shape of NPs when the extracts of different “hairy” root lines (independent transformational events) were used. In particular, the use of flavonoid-rich “hairy” root water extracts allowed us to obtain smaller (2.5-49 nm, Fig a) NPs than using the extracts of mother plants (18-235 nm, Fig b).

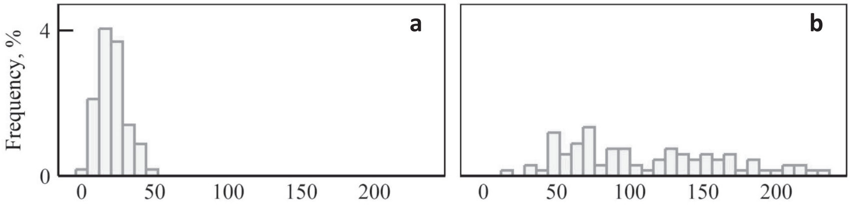

Fig.** - Size distribution of nanoparticles: NPs obtained using extract from Artemisia vulgaris "hairy" roots **(a)** and extract from control plants **(b)

AgNPs synthesized using A. vulgaris “hairy” root extract due to a narrow range of nanoparticle sizes have a potential source of biocompatible, antimicrobial nanoparticles with potential applications in medicine and other fields.

Eryptosis can be used in hemocompatibility studies of complex nanosystems

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Eryptosis, which is a Ca^{2+}-dependent regulated cell death modality of erythrocytes, has been suggested to be an alternative and more sensitive approach to test hemocompatibility of nanomaterials. In the current study, eryptotic parameters are used to detect erythrotoxicity of a nanocomplex consisting of dextran-graft-polyacrylamide (D-PAA) and ZnO nanoparticles synthesized from zinc sulphate (D-PAA/ZnO NPs (SO_4^{2-})). Experimental evidence shows that this nanocomplex demonstrates anti-cancer potential *in vitro.*

Aim. The aim of our study was to analyze the ability of D-PAA/ZnO NPs (SO_4^{2-}) nanocomplex to induce eryptosis *in vitro.*

Materials and methods. Blood (hematocrit 0.4%) was exposed to the D-PAA/ZnO NPs (SO_4^{2-}) nanocomplex during 24 h at concentrations from 0 to 800 mg / L. Following the incubation, the cells were stained with annexin V-FITC according to the standard protocol to detect the cell scrambling common for eryptosis. Furthermore, analysis of forward scatter (FSC) signaling was used to detect changes in the morphology of RBCs.

Results. Our flow cytometric data indicate that D-PAA/ZnO NPs (SO_4^{2-}) nanocomplex did not promote cell shrinkage, evidenced by no statistically significant changes in FSC signaling indices. Cell shrinkage is a typical sign of eryptosis. In addition, the nanocomplex at all the concentrations used increased neither the number of phosphatidylserine-displaying cells, nor the fluorescence of Annexin V-FITC indicating the lack of cell scrambling in erythrocytes exposed to D-PAA/ZnO NPs (SO_4^{2-}). Taken together, it can be assumed that the D-PAA/ZnO NPs (SO_4^{2-}) nanocomplex does not trigger eryptosis.

Conclusions. Our findings indicate that eryptosis can be used in hemocompatibility studies of complex nanosystems and confirm good hemocompatibility of D-PAA/ZnO NPs (SO_4^{2-}) nanocomplex.

Medium-dependent differences in osmotic fragility of erythrocytes exposed to dextran-graft-polyacrylamide/zinc oxide nanosystem

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Hemocompatibility is an important parameter in the complex evaluation of biocompatibility of various nanomaterials. Erythrocytes can undergo either hemolysis, a lytic cell death, or eryptosis, a non-lytic regulated cell death, in response to nanomaterials. The latter is generally considered to occur in order to prevent the former. Both parameters are suggested to be used in nanotoxicological hemocompatibility studies. Furthermore, the osmotic fragility test (OFT) is used to evaluate resistance of red blood cells (RBCs) to hemolysis.

Aim. The current study was designed to assess the impact of cell culture medium on osmotic fragility of erythrocytes incubated with a nanocomplex made up of dextran-graft-polyacrylamide (D-PAA) and ZnO nanoparticles produced using zinc sulphate (D-PAA/ZnO NPs (SO_4^{2-})), which is reported to have anti-cancer activity.

Materials and methods. The D-PAA/ZnO NPs (SO_4^{2-}) nanocomplex was incubated for 24 h with blood (hematocrit 0.4%) at different concentrations (0-800 mg / L) either in Ringer solution or RPMI-1640 supplemented with 10% fetal bovine serum (FBS). After incubation, the samples were centrifuged and the pellets were resuspended in 0.2% NaCl. After further centrifugation, the supernatant was analyzed spectrophotometrically at 541 nm.

Results. Our experimental data suggest that D-PAA/ZnO NPs (SO_4^{2-}) nanocomplex has the ability to induce hemolysis during OFT depending on the medium used for incubation. Incubation of RBCs in RPMI was found to trigger hemolysis to a higher degree compared with Ringer solution. This can be associated with interactions of nanocomplexes with proteins to form protein corona. However, further studies are required to figure out the interactions of D-PAA/ZnO NPs (SO_4^{2-}) nanocomplex with different molecules and their impact on biological effects.

Conclusions. *In vitro* toxicity studies are important for assessing the hemocompatibility of nanomaterials. Researchers should carefully choose a medium used for incubation of blood cells with nanomaterials in toxicological studies.

Drug delivery with thermosensitive star-like Dextran-graft-Poly-N-iso-Propilacrylamide copolymer

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Polymer nanoparticles represent one of the innovative non-invasive approaches for drug delivery applications in cancer therapy. In this study, the star-like Dextran-graft-Poly-N-iso-Propilacrylamide (D-g-PNIPAM: D6 and D70 modifications) was developed for the temperature-triggered targeted delivery of the common chemotherapeutic drugs – Doxorubicin (Dox) and Cisplatin (Cis-Pt). The size distribution of particles in aqueous solution was determined by dynamic light scattering technique at different temperatures. Model studies of the release rate of the drugs from the D-g-PNIPAM copolymer depending on the temperature were performed using a mass-spectrometric analysis. D-g-PNIPAM nanoparticles increased toxic potential of the drugs against human and mouse lung carcinoma cells (A549 and LLC (Figure)), but not against normal human lung cells (HEL299). The drug-loaded D-g-PNIPAM-nanoparticles promoted further oxidative stress and apoptosis induction in LLC cells by increasing intracellular ROS generation and activation of caspase 3/7. The data obtained indicate that the strategy of chemotherapeutic drugs encapsulation within the branched D-g-PNIPAM nanoparticle allows not only to realize temperature-triggered drug release but also to potentiate its cytotoxic, prooxidant and proapoptotic effects against lung carcinoma cells *in vitro*.

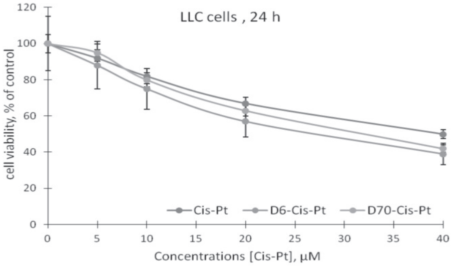

Fig. *LLC cells viability treated with free Cis-Pt or D-g-PNIPAM-Cis-Pt.*

Water-soluble C60 fullerenes protect muscle soleus functioning in the rat muscle trauma models

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Muscle trauma is one of the most common body injuries. The intensification of free radical processes takes place in almost most pathological conditions, including muscle trauma. Water-soluble C_{60} fullerenes (C_{60}) with powerful antioxidant properties are promising nanoagents for developing an effective therapy for skeletal muscle trauma. Here the selective biomechanical parameters of *muscle soleus* contraction (Fig. 1) and biochemical indicators of blood in rats were studied after intramuscular injection of C_{60} at various doses 1 h before the initiation of muscle injury and ischemia of varying severity using the tensometric and biochemical analysis. So, analysis of the force response of the skeletal muscle after C_{60} injection at a dose of 1 mg/kg has revealed its protective effect at the level of 30% for ischemia, and at the level of 17% for muscle injury. The analysis of biomechanical markers responsible for the correction of accurate positioning confirmed C_{60} effectiveness at a level of more than 50%. With the C_{60} administration, there is a clear tendency to a decrease in the biochemical parameters of blood in ischemia by about 33%, and in muscle injury - by 8%. These findings demonstrate the ability of C_{60} to correct the pathological state of the skeletal muscle that occurs when it is mechanically injured and most effectively affect the restoration of the system of precise control of motor reactions. This research was supported by the NRFU.

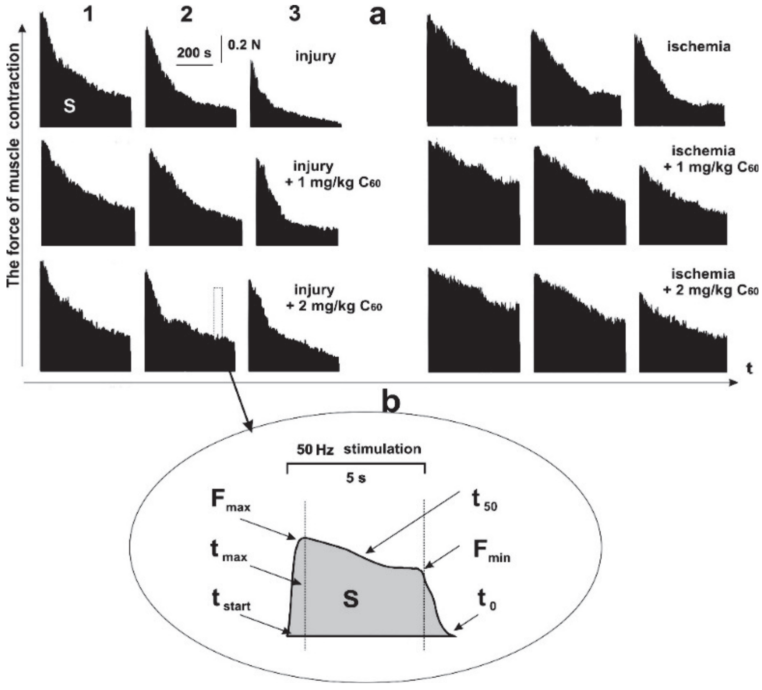

Fig.1. Rat muscle soleus contraction force when applying 50 Hz stimulation for 5 s with a total duration of 500 s without relaxation (a): injury/ischemia - muscle trauma; injury/ischemia+ 1/2 mg/kg C_{60} - corresponding pathology against the background of C_{60} injections at doses 1/2 mg/kg, respectively; 1,2,3 - the 1,2 and 3 degree of the pathological process in the muscle. The investigated biomechanical markers of muscle contraction (b):
S - integrated muscle power (calculated area under the force curve); F_{min}/F_{max} – minimum/maximum forces of a single contraction; tmax - time to reach maximum muscle contraction force; t_{50} - time to decrease muscle contraction force by 50% from the initial level; t_0 - time after stimulation cessation until muscle force returns to its initial value (characterizes muscle rigidity); t_{start} – the time between stimulation start and contractile process start (delay in the start of a muscle contraction).

C_{60} fullerene effect on the mechanokinetics of muscle gastrocnemius contraction in chronically alcoholized rats

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The biomechanical parameters of *muscle gastrocnemius* contraction, biochemical indicators of blood and muscle tissue as well as histological changes in rat muscle tissue after chronic alcoholization for 3, 6 and 9 months were studied. The oral administration of C_{60} fullerene aqueous solution (C_{60}FAS) at a dose of 1 mg/kg throughout the experiment was used as a therapeutic agent. C_{60}FAS was shown to reduce the pathological processes development in the muscle apparatus by an average of 35-40% (Fig. 1). In particular, it reduced the time occurrence of fatigue processes in muscle during long-term development of alcoholic myopathy and inhibited oxidative processes in muscle, thereby preventing its degradation (Fig. 2).

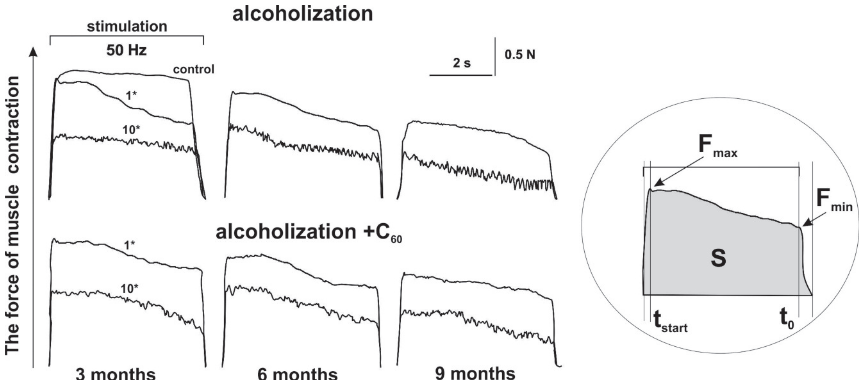

Fig.1. *The forces of the 1st (1*) and 10th (10*) contractions of the muscle gastrocnemius of alcoholised rats induced by 6 s non-relaxation stimulation pools at 50 Hz: alcoholization - rats treated with alcohol; alcoholization+C_{60} - rats treated with a mixture of alcohol and C_{60}FAS at a dose of 1 mg/kg during the whole period of alcoholization; 3, 6 and 9 months - alcoholization lasting 3, 6 and 9 months, respectively.*

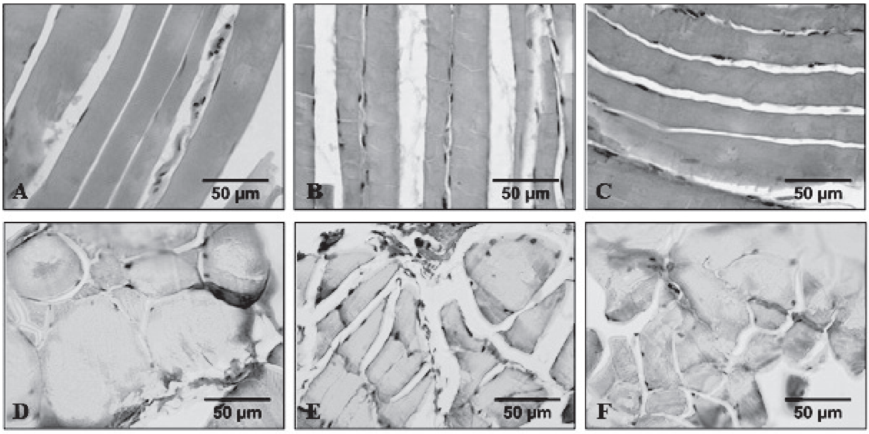

Fig.2. *Representative histological images of muscle gastrocnemius: A and D – control group; B and E – alcoholization group; C and F – alcoholization+*C_{60} *group. A, B, C – hematoxylin and eosin staining; D, E, F – hematoxylin and picrofuchsin staining by van Gieson. Scale bar – 50 μm.*

Thus, these findings indicate promising prospects for the usage of water-soluble C_{60} fullerenes as potent antioxidants for the corrections of the pathological conditions of the muscle system arising from alcohol intoxication.

Assessment of the C_{60} fullerene permeability through the lipid envelope of SARS-CoV-2 coronavirus using molecular dynamics method

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According to recent WHO data, the spread of SARS-CoV-2 is observed in all countries without exception. Therefore, research on possible ways to mitigate the impact of SARS-CoV-2 on the human body is a global challenge for modern biomedicine. Existing research data [Piotrovsky et al., 2005] indicate that the high lipophilicity of C_{60} fullerene determines its "membranotropic" mechanism of antiviral action.

Obtained results indicates that a single C_{60} fullerene is capable to penetrate the lipid envelope of the coronavirus and subsequently exit it (Fig. A), which correlates with [Zhang et al., 2013]. When investigating systems with 5 and 10 C_{60} molecules, the latter is able to form nanoclusters that, as it turned out, penetrate and exit the lipid envelope faster (Fig. B,C). Thus, the formation of an equilateral triangle (3 C_{60} molecules) or a tetrahedron (4 C_{60} molecules) occurs, which begin to immerse themselves in the envelope, and by the end of molecular dynamics (MD), they are on the other side. Therefore, the aggregation of C_{60} fullerenes occurs either before penetration into the lipid envelope of the coronavirus, or inside it. It can be assumed that C_{60} fullerenes as part of nanoclusters are capable of forming pores in the envelope of the SARS-CoV-2 coronavirus, thereby disrupting its structural integrity. This undoubtedly leads to a disruption of the corresponding stages of the replication cycle of the virus and the suppression of its functional activity in general.

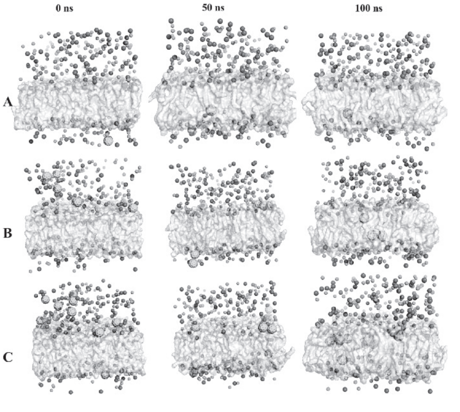

Fig. *The lateral view of the constructed systems with different numbers of C_{60} molecules at different time intervals of MD simulation is shown: the lipid envelope is depicted in gray, the C_{60} fullerene in yellow. Panels A, B, and C correspond to systems with 1, 5, and 10 C_{60} molecules, respectively.*

Cytotoxicity and divalent cation chelation by quinoline derivatives in aqueous solutions

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Derivatives of 8-hydroxyquinolines (STQ) are widely used in various fields, including agriculture, medicine, testing industry, etc [1]. They have strong chelating properties due to the proximity of the hydroxyl group and the heterocyclic nitrogen atom. 8-hydroxyquinolines form four- and six-valent complexes with Mg^{2+}, Cu^{2+}, Zn^{2+}, Bi^{2+}, Mn^{2+}, Cd^{2+}, Ni^{2+}, Fe^{3+}, and Al^{3+} [1]. One of the limitations of their practical use is a low solubility in water. Different polar groups are grafted to the main core to improve solubility. The chelating ability of 8-hydroxyquinoline derivatives STQ-H, STQ-Cl, STQ-CN and STQ-NO_2 was tested. Aqueous solutions of $Zn(CH_3COO)_2$, $CaCl_2$ and $MgCl_2$ were prepared on the basis of 0.9% NaCl. Solutions of each cation separately and a mixture of Ca^{2+}, Mg^{2+}, Zn^{2+} in a 1:1:1 molar ratio were used. The initial concentration of each cation was 0.5 mM, which was diluted twice up to 0.0078125 mM. One of STQ derivatives in DMSO was added to each cation. Final STQ concentration of 0.05 mM. Optical absorbance was measured after 5, 20, 40, 60 min in the wavelength range of 200-700 nm. Cytotoxycity was tested at breast cancer cell line MDA-MB-231. The STQ-Cl/cation complexes were the least stable in aqueous solutions. A decrease in the optical absorbance about 300 nm was detected after 20 min. STQ-CN/cation complexes were stable up to 60 min. A significant increase in the absorbance about 300 and 365 nm was found when Ca, Mg, Zn (each concentration was 0.0625 mM) were present in a solution. This effect was not detected during chelation of individual cations and other tested STQ derivatives. MDA-MB-231 EC50 was 1.3 μM for STQ-H, 1,2 μM for STQ-Cl. Maximal cytotoxicity for STQ-CN and STQ-NO_2 was about 70% at 0,125 mM after 48h incubation.

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Computationally designed sensing elements for BPA analysis using smartphone

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The novel, user-friendly, colourimetric biosensor for bisphenol A (BPA) was introduced. The BPA-sensitive molecularly imprinted polymers (MIP) films were designed and used as sensing elements of smartphone-based biosensor for BPA analysis. Using computational modelling method, we demonstrated the successful design of BPA-sensitive artificial binding sites, which were formed in the structure of the proposed MIP-based sensing elements. The MIP films were synthesized using the method of in situ polymerization with BPA as a template, ethylene glycol methacrylate phosphate (EGMP) as a functional monomer, the tri(ethylene glycol) dimethacrylate/oligourethaneacrylate (TGMA/OUA) mixture as the main component of the polymeric network. The colourimetric detection of BPA, selectively adsorbed by the artificial binding sites in the EGMP-based thin MIP films' structure, is based on the 4-aminoantipyrine method. The sensor responses associated with BPA binding to the MIP films surface were registered by the smartphone camera (Meizu 16, 20 MP, F/1,8) and the captured images were analyzed with the smartphone application Spotxel® Reader (Sicasys Software GmbH, Germany) within real-time. The pink-coloured intensity of MIP films was proportional to BPA concentration in the analyzed samples. Some parameters of analyzed samples including pH, buffer and salt concentration, affecting sensor performance were tested and optimized. A dynamic linear range of 10 μM to 1000 μM was obtained. The detection limit of the designed biosensor was calculated equal to 10 μM. The smartphone-based biosensor with computationally designed MIP film sensing elements can successfully identify and quantify BPA in samples of natural and waste waters contaminated with BPA.

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Chemiluminescent and Bioluminescent Imaging Technologies

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Imaging technologies are significant in bioinformatics and medicine. The great progress are in last decade for their utilization in biomedical implementations and discovering the molecular basis of life. In this work we discussed recent chemiluminescent (CL) and bioluminescent (BL) imaging approaches established for imaging of different significant analytes. [1] CL and BL detection imaging technology are characterized by their excellent signal-to-noise ratio, high sensitivity, wide linearity, fine rapidity and are techniques of choice in real-time noninvasive imaging. So, BL and CL phenomenon have been extremely perspective as detection approaches in many fields, including immunology, genetics, pharmaceutical analysis, cytology, forensic medicine, liquid chromatography. Their integration with other methods like ELISA and molecularly imprinted polymers has a great potential. Moreover, BL and CL imaging microscopy exhibit the merits of high detectability, selectivity, and easy estimation of the luminescent signal response for carrying out a simple and accurate quantitative assay of the labeled probes, which is considered to be a significant advantage over the traditional fluorescencebased imaging technology. As a result, it can be applied to characterization new material properties including nanostructures.

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Nanostructural and biochemical properties of natural isoprene hexaoligomer from amaranth oil

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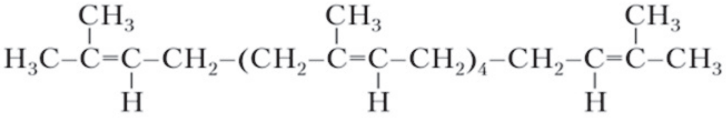
Hexaoligomeric isoprene (squalene) is an organic unsaturated compound with the formula $C_{30}H_{50}$. It is a liquid oligodienic hydrocarbon, an acyclic triterpene composed of six isoprene units with a freezing point of -55 °C and boiling point of +203 °C, predominantly found in the surface tissues of plants, animals, and human skin. It is a colorless hydrocarbon, and its hydrogenated derivative is called squalane ($C_{30}H_{62}$), with most commercial samples having a natural origin [1]. Unlike unsaturated squalene, due to the complete absence of double bonds, squalane is resistant to autoxidation. This, combined with its lower cost and desirable physical properties, has led to its wide use in cosmetics and perfumery [2].



$$H_3C-\overset{CH_3}{\overset{|}{C}}=\underset{H}{\underset{|}{C}}-CH_2-(CH_2-\overset{CH_3}{\overset{|}{C}}=\underset{H}{\underset{|}{C}}-CH_2)_4-CH_2-\underset{H}{\underset{|}{C}}=\overset{CH_3}{\overset{|}{C}}-CH_3$$

сквален

Squalene-2,6,10,15,19,23-hexamethyltetracosane-2,6,10,14,18,22-hexaene.[3].

Traditionally, squalene was obtained from shark liver. Approximately 3,000 sharks are needed to produce one ton of squalene. [4]. Due to environmental concerns, alternative sources such as amaranth and olive oil, rice, and sugarcane have been commercialized and as of 2021, they supply around 40% of the total industry volume [5]. One highly valuable property of squalene is its ability to react with water molecules and release oxygen, converting to squalane through the following reaction:

$$C_{30}H_{50} + 6\ H_2O = C_{30}H_{62} + 3O_2\uparrow \qquad (1)$$

Thus, it can serve as a source of oxygen, which is essential for the human body. Research conducted by many scientists has allowed for the identification of anticancer, antimicrobial, and fungicidal effects of amaranth oil. Therefore, the targeted components are widely used in medicine, perfumery, the production of baby food, the chemical-pharmaceutical industry, the bakery, confectionery, and other industries [6,7].

As squalene accumulates in the human body, it strangely activates the immune system, making a person more resistant to various illnesses. In addition, it effectively rejuvenates the skin, which is why it is considered a revolutionary product in cosmetology. After all, such a useful carbohydrate is produced in the human body to the maximum extent only up to the age of 25 (40%), and then its level decreases, with the average level of squalene in us being only 5% in middle age! Squalene is found not only in shark liver, especially since the product is expensive and very exotic. In small amounts, it can be found in olive oil, rice bran, and even yeast. Many studies, including the experiment of the Kansas Medical Center at the University of Kansas in the USA, have been conducted to confirm the benefits of squalene. Three groups of mice were selected for the experiment, one of which was given regular food, and the other two were fed food with a 2% squalene content of the total volume (one for two weeks, the other for a month). All laboratory mice were exposed to radiation, the dose of which was lethal for small rodents. However, the results showed that after a month, the mortality rate in the first group was 100%, and the mice from the third group, which received squalene throughout the entire experimental period, remained alive, despite the fact that they were supposed to die from a large dose of radiation [8]. Squalene has low acute toxicity and is not a significant irritant to human skin or sensitizer. [9]. The highest amount of squalene is found in amaranth oil, from 6 to 8%, depending on the extraction technology.

At the chemistry department of the Faculty of Natural Sciences of Vasyl Stefanyk Precarpathian National University in Ivano-Frankivsk, Ukraine, applied research was conducted on various technological methods for the extraction and deparaffinization of squalene and squalane from amaranth oil (amaranthus seed oil). The amaranth oil was extracted from the seeds of two species of the Amaranthus genus - A. cruentus and A. hypochondriacus, which grow in the botanical garden and dendropark of the Precarpathian University [10]. This is a transparent liquid ranging in color from light to dark yellow. In cosmetology, it is used as a softening, nourishing, and rejuvenating agent. Amaranth, or amaranthus (Latin: Amaránthus), is a widely distributed genus of mainly annual herbaceous plants with small flowers gathered in dense spike-like or corymbose inflorescences. There are over 100 known species that grow in warm and temperate regions.

As a result of experiments conducted by scientists, three methods for isolating squalene and squalane from amaranth oil were proposed. The first method involves neutralization and precipitation of salts of higher carbon acids, which make up up to 90% of amaranth oil, and isolation and rectification of squalene. However, large losses of squalene, exceeding 50%, were observed with this method. The second method, which we tested, is deparaffinization - precipitation of squalene and squalane using urea, which we previously used for deparaffinization and increasing the octane and cetane numbers of motor fuels [11]. With this method, only paraffinic and olefinic hydrocarbons with a chain length greater than C_{10} are separated from amaranth oil, making it suitable for squalene and squalane, which have a carbon content of up to $C_{30}H_{62}$. As a result, losses of squalanes decreased, and we were able to separate up to 90% of squalene and squalane from amaranth oil. However, the amount of squalene decreased to 1%, and the amount of squalane increased to 7%, according to the reaction (1) which we previously presented in our work. As a result of our work, we proposed a new, improved method for isolating saturated squalane from amaranth oil by converting unsaturated squalene through hydrogenation in an aqueous environment.

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Liposomal ciprofloxacin for the treatment of chlamydia

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Chlamydia avoids the effects of drugs by hiding in the fat droplets contained inside the cells.The presence of these parasites in the body can lead to inflammation in the genitourinary system, lungs, eyes, also can lead to arthritis. In our studies, we used the Bu L2 strain of lymphogranuloma venereum as an infectious agent and 6-7-day-old chicken embryos as a model. Infection with Chlamydia trachomatis was carried out inside the yolk sac. There were used the liposomes from the natural lecithin and from the original mixture of negatively charged polar lipids. The percentage of inclusion of the antibiotic ciprofloxacin in liposomes obtained from polar lipids with a negative charge was 91%, which is 3 times higher than the inclusion in liposomes from lecithin. That's why we continued to work only with negatively charged liposomes. 1% liposomes with ciprofloxacin were injected to the experimental groups of embryos after Chlamydia trachomatis infection. Commercial ciprofloxacin was introduced into the control groups of embryos after Chlamydia trachomatis infection. The death of chicken embryos infected with a suspension of venereal lymphogranuloma without any treatment was 100% on the 4th-5th-6th day after infection. The results of the experiment are visible in the table.

Table

Survival table of Chlamydia trachomatis -infected chick embryos

№	The amount of ciprofloxacin per 1 chick embryo in mg				
	0,24	0,12	0,08	0,022	0,012
% of surviving embryos with the introduction of a commercial solution of ciprofloxacin	100	67	60	56	5
% of surviving embryos with the introduction of loaded liposomes with ciprofloxacin	100	100	100	100	100

As much as possible a positive therapeutic effect has been reached: 100 % of chicken embryos with Chlamydia trachomatis were healthy after one injection of the liposomal ciprofloxacin. The use of liposomal ciprofloxacin makes it possible to reduce the therapeutic dose of this antibiotic in 20 times.

The "surface - particles" interaction can be evaluated by changes in the fractal dimension of this surface

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The formation of textured films on various surfaces is studied considering the wide range of applications. For example: gettering of materials for integrated circuits, coating of "biosolar panels" by modified *E. coli* cells with lycopene capable of converting sunlight into electric current, immobilization of biotechnological producers or diagnostic biosensors based on porous silicon. The formation of biofilms has a negative impact for implants in regenerative medicine.

The orderliness of yeast, microalgae and probiotic bacteria has been detected, which corresponds to the microscopic or grain-heterophase level of distribution of structural elements (5 nm - 100 μm). In order to carry out the detection a drop of a suspension of microorganisms was applied to a plate of degreased polished silicon or glass, left to dry completely spontaneously. Then the surface texture was photographed in reflected light at various magnifications. The same was conducted under the influence of a static magnetic field (MF) with an induction of 0.15 to 0.17 T, directed perpendicular to the surface of the sample.

Visually, there were found significant differences both in the preservation of the shape of dried cells (under the influence of MF, the structure of cells has not been collapsed within 2 years of observation) [1], and in the self-organization of cells during drying on the silicon surface. The trend for different types of microorganisms was an increase in fractal dimension D (formation of figures) and a decrease in lacunarity *L*. The authors attribute cell distribution to the interaction of the predominantly negative ζ-potential of microorganisms with positively charged silicon impurities that getter the surface under MF exposure.

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Gold nanosystems improve male reproductive function

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Polymers with a dextran core and grafted polyacrylamide chains dextran-polyacrylamide (D-PAA) in the anionic form of D-g-PAA(PE), as a polymer matrix carrier, in particular gold nanoparticles (AuNPs) - are being actively studied.

The aim is to evaluate the effect of five treatment of gold nanosystems (D-g-PAA(PE)/AuNPs) and Ouercetin on male reproductive function in mice under conditions of experimental chronic kidney disease (EChKD).

The study was performed on male and female mice with EChKD, a model of which was created by immunizing animals with kidney homogenate. AuNPs loaded (synthesized, retained) in D-g-PAA(PE) are spherical in shape, size 4-11 nm. D-g-PAA(PE) (2,0 and 10,0 mg/kg), D-g-PAA(PE)/AuNPs (1,96 and 9,78 mg/kg) was administered intravenously, five times. Quercetin (Sigma, USA) (50 mg/kg) was administered intraperitoneally, five times after the introduction of gold.

Our data suggest that under conditions of EChKD takes place disorder of male reproductive function. Under conditions of EChKD and exposure to 1.96 mg/kg of D-g-PAA (PE)/AuNPs decreased: the number of abnormal sperm, the number of necrotic cells of the testes, the number of necrotic cells of the epididymis, values of preimplantation mortality compared to such a value in conditions of EChKD. Under conditions of EChKD+D-g-PAA(PE)/AuNPs+Quercetin found: decrease in the number of abnormal sperm, increase in the number of spermatids, increase in the number of living cells and decrease in necrotic cells of the epididymis, reduction of preimplantation mortality of embryos, increase in the number of live newborns (pups) compared to such values under the conditions of EChKD. Under conditions of EChKD and exposure to 9,78 mg/kg D-g-PAA(PE)/AuNPs, male reproductive function is impaired and additional probable damage occurs, namely in the value of pre-implantation mortality compared to EChKD.

Conclusion: Treatment of 9,78 mg/kg D-g-PAA(PE)/AuNPs leads to disorder of the male reproductive system, but is not critically dangerous for therapeutic use. Whereas the treatment of 1,96 mg/kg D-g-PAA(PE)/AuNPs has possible therapeutic applications to improve male reproductive function. The effect of such gold nanosystems may reduce oxidative stress and improve sperm DNA repair, which requires further study.

The role of ions with changeable valency in the antioxidant activity of $GdVO_4:Eu^{3+}$ nanoparticles

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The imbalance between reactive oxygen species (ROS) production and scavenging in living cells is known to be one of the main sources of cell mutations and death, as well as the development of various diseases at the organismal level. Recently, NPs with ROS-regulating abilities have emerged as a novel nanotherapeutic approach [1].

The aim of this study is to evaluate the role of vanadium ions in the antioxidant activity of $GdVO_4:Eu^{3+}$ NPs.

Material and methods. In this study, $GdVO_4:Eu^{3+}$ NPs were synthesized as water colloids using previously described methods [2]. ROS-scavenging (antioxidant) ability of synthesized $GdVO_4:Eu^{3+}$ NPs was evaluated by optical spectroscopy methods using specific organic probes for hydrogen peroxide (H_2O_2), superoxide anion (O_2 -), and hydroxyl radicals (×OH).

Results. Synthesized $GdVO_4:Eu^{3+}$ NPs are in the form of ellipsoid of 12 x 6 nm size. About 60 % of vanadium ions in the nanoparticle's crystal lattice were found to be in lower valence states (V^{4+} and V^{3+}). Multiple switching between V^{5+}/V^{4+} and V^{4+}/V^{3+} states is responsible for the effective ROS scavenging activity with respect to H_2O_2, O_2, and OH.

Conclusion. $GdVO_4:Eu^{3+}$ NPs hold great potential as ROS-down regulation agent for biomedical applications.

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Mechanisms of redox activity of nanoceria revealed by spectroscopic studies

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Cerium oxide NPs (such as nanoceria) are well-known for their vast biological applications related to their antioxidant activity in living cells [1]. The most recent findings revealed that a wide class of inorganic nanoparticles (such as nanoceria) can take an active part in intercellular processes mimicking the action of large biomolecules, such as enzymes. Redox-active NPs potentially can revolutionize the nano-drug market in the next future, but the following applications of these materials should be preceded by careful studies of the mechanisms of their action in biologically relevant conditions.

Our experimental results show that Ce^{3+} -Vo-Ce^{3+} surface defect complexes on the surface of nanoceria acting similar to active sites in enzyme molecules actually provide nanoceria with enzyme-like activity. In accordance with this supposition, the processes of hydrogen peroxide (HP) decomposition by nanoceria can be well described using the Michaelis-Menten equations usually used in the description of enzyme-substrate interaction. The maximum rate of HP decomposition shows clear dependence on the size of nanoparticles i.e. on the number of available surface sites for binding of HP molecules. At HP concentrations, for which almost all Ce^{3+}-Vo-Ce^{3+} sites are involved into HP decomposition, the process of slow $Ce^{3+} \rightarrow Ce^{4+}$ oxidation turns into fast redox cycling and Ce^{3+}/Ce^{4+} oscillations are observed [2]. Both the change of C^{e3+}/Ce^{4+} ratio and change of pH play an equally important role in initiation and synchronization of Ce^{3+}/Ce^{4+} redox cycling in nanoceria colloidal solutions.

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Control of TiO_{2-x} antioxidant behavior by a $Ti^{3+}(Ti^{2+})/Ti^{4+}$ ratio

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Recent developments in TiO_2-related photocatalysis have been linked to highly defective TiO_{2-x} nanoparticles (NPs). It has been demonstrated that high levels of oxygen vacancies and diverse defects, such as Ti^{3+} ions, can significantly improve TiO_{2-x} photocatalytic performance [1]. At the same time, some researchers have reported on a crucial role of the Ti^{3+}/Ti^{4+} ratio in the TiO_{2-x} structure on antioxidant properties of TiO_{2-x} surfaces and NPs [2]. Based on these findings, we hypothesize that changing the $Ti^{3+}(Ti^{2+})/Ti^{4+}$ ratio in the TiO_{2-x} structure we can modify its antioxidant behavior.

In this study, two types of TiO_{2-x} NPs were synthesized using a modified method that involved varying the amount of nitric acid as a catalyst and peptizing agent. The TiO_{2-x} NPs were of uniform size (about 5 nm), but possessed different $Ti^{3+}(Ti^{2+})/Ti^{4+}$ ratios [3]. The structure of the synthesized TiO_{2-x} NPs was characterized using TEM, XRD and XPS. Additionally, the antioxidant properties of the synthesized TiO_{2-x} NPs were assessed using the Total Antioxidant Capacity (TAC) test and specific organic probes for various Reactive Oxygen Species (ROS). The results of this investigation demonstrated that TiO_{2-x} NPs with a higher $Ti^{3+}(Ti^{2+})/Ti^{4+}$ ratio exhibited greater antioxidant activity, specifically in the scavenging of ROS.

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Thiacalix[4]arene chalcone amides effects on myometrium mitochondria

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Calixarenes are supramolecular compounds with a unique three-dimensional structure, which have a biological activity determined by the chemical groups on the upper or lower rims. Thiacalix[4]arenes C-1191 and C-1192 each have 4 chalcone groups on the lower rim, which are attached to the thiacalix[4]arene ring. In such macrocycle the phenyl rings are connected not through methylene groups (CH_2), but through sulfur atoms (S). *Tert*-butyl groups are located on the upper rim of both compounds. The thiacalixarene cycle in C-1191 has a *cone* conformation and chalcone fragments are connected to it through one methylene group (CH_2). Therefore, all chalcone fragments are located close to each other and close to the sulfur atoms. The thiacalixarene ring in C-1192 exists in a *1,3-alternate* conformation and the chalcone fragments are connected to it through three methylene groups (CH_2-CH_2-CH_2). Therefore, the chalcone fragments are located quite far from each other and from the thiacalixarene cycle. The purpose of the work is to investigate the effects of thiacalyx[4]arenes C-1191 and C-1192 on the mitochondria of rat uterine smooth muscles and to compare them with the effects of calix[4]arene C-1011, which contains 4 chalcone amide groups in its structure but does not contain sulfur atoms. Experimental models - mitochondrial fraction and isolated myometrial cells.

The hydrodynamic diameter of mitochondria was investigated using the dynamic light scattering method. It was shown that short-term incubation of mitochondria with thiacalix[4]arenes was not accompanied by changes in mitochondrial size, with the exception of 10 μM C-1192, which increased mitochondrial hydrodynamic diameter by an average of 25% compared to control. We previously showed that calix[4]arene C-1011 significantly increased the hydrodynamic diameter of mitochondria. Using the Ca^{2+}-sensitive fluorescent probe (fluo 4AM) and a spectrofluorimeter, it was shown that 1 μM thiacalix[4]arenes C-1191 and C-1192 did not affect both the basal Ca^{2+} concentration ($[Ca^{2+}]_m$) and the accumulation of this cation in the mitochondria matrix. Previously, it was shown that the incubation of mitochondria in the presence of C-1011 was accompanied by an increase in the $[Ca^{2+}]_m$ values both in the absence and in the presence of exogenous Ca^{2+}. Using a myometrial cell suspension treated with digitonin, flow cytometry and a potential-sensitive probe (TMRM), it was shown that 1 μM thiacalix[4]arenes C-1191 and C-1192 increased the level of mitochondrial membrane polarization. Calix[4]arene C-1011 had a similar effect, as was established earlier.

Thus, compared to calix[4]arene chalcon amides, thiacalix[4]arene chalcon amides had a less powerful effect on the size of mitochondria, did not affect $[Ca^{2+}]_m$ during short-term incubation, but caused hyperpolarization of mitochondrial membranes.

Poly-2-oxazoline: from the synthesis to nanomedicine

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The using the biodegradable synthetic polymers for drug delivery systems attract considerable attention of researchers during last ten years [1]. A lot of polymers were studied as platform for drug delivery: polyethylene glycol (PEG), poly(N-vinyl-2-pyrrolidone) (PVP), poly(N-isopropylacrylamide) (PNIPAM), hyaluronic acid (HA), polyglutamic acid (PGA), polylactic and polyglutaric acid (PLGA), N-(2-hydroxypropyl) methacrylamide (HPMA), polyvinylpyrrolidone (PVP). Nanoscale drug delivery systems (DDS) often improves solubility and as results the better therapeutic activity observed and the side-effects reduced scientifically. NDDS can passively accumulate in cancerous tissue due to high vascularity and through lymphatic system.

Another class of polymers polyoxazolines (POx) was investigated as perspective materials for DDS. Ten types of POx were prepared by living cationic ring-opening polymerization of 2-oxazolines. The living nature of polymerization can lead to narrow molar mass distributions and allows for controlled introduction of chain-end (initiation/termination) and side-chain functionalities.

It was found that the living nature of the cationic ring opening polymerization, subsequently by postpolymerization modification using click chemistry, with highly defined structures with specific architectures and properties.

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Synthesis of thermoresponsive polymer pNIPAM for drug delivery system using gold nanostructures

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Due to their unique physicochemical properties, gold nanoparticles are used in various ways in the field of cancer treatment, including disease diagnosis, drug delivery, and photothermal and photodynamic therapies [1]. Drug delivery is a method of administering a drug to achieve a therapeutic effect in humans or animals [2]. For the desired controlled release of the drug, "smart" polymer carriers are used, which allows the delivery of the drug at the right time and concentration due to the release of the drug in response to an external stimulus [3].

In this work, the processes of synthesis of poly-N-isopropylacrylamide (pNIPAM) by RAFT polymerization on the surface of gold nanoshells and silver nanoparticle seeds were investigated. The studies were performed by means of absorption spectroscopy technique. The absorption spectra of the aqueous solutions were measured before and after the addition of monomer and iniferter, and also were compared depending on different concentrations of components and ultraviolet irradiation time. It was established that using an iniferter with citrate-coated gold nanoparticles leads to their aggregation. It was found that the creation of a thermoresponsive polymer layer simultaneously with the synthesis of silver nanoparticle seeds leads to the formation of nanoparticles with a polymer coating. Due to the performed studies, it is proposed to create a thermosensitive polymer layer simultaneously with the synthesis of nanoparticles, which showed a positive result on the example of the synthesis of silver nanoparticles.

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Investigation of the properties and microstructure of gelatin-alginate hydrogels for wound healing

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Hydrogels based on natural polymers (gelatin, alginate) are a popular material in biomedical research and applications, as they have multipurpose properties [1]. The microstructure of such hydrogels, which includes porosity, pore size and distribution, fiber orientation, granulation, and morphology, has a significant impact on their physical, mechanical, and biological properties [2].

Gelatin/alginate hydrogel materials structured with PEG diglycidyl ether were obtained. After fabrication, the hydrogels were characterized by IR-FTIR, SEM, DSC, swelling was also investigated, and then their stability was studied using degradation studies. To give the products a specialized medical purpose, they were filled with a number of painkillers (novocaine, lidocaine, diclofenac) and antiseptics (chlorhexidine). The drugs were introduced after studies of the compatibility between the active ingredients and their release was studied. Drug release studies have demonstrated rapid release of analgesic drugs and sustained release of antiseptics, so such hydrogel materials may be useful for patients who require immediate anesthetic and long-lasting antiseptic effects during wound healing therapy.

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A New Photoacoustic Method Diffusion study in Soft mater

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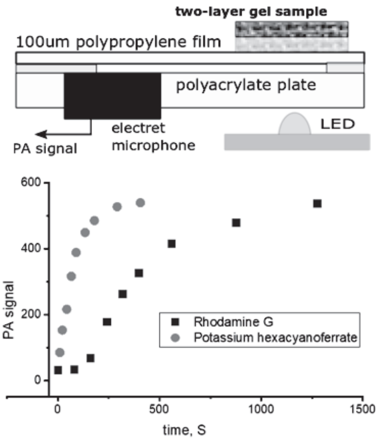
The processes of diffusion of nanoscale objects in living tissues are important for understanding the peculiarities of using a number of diagnostic and therapeutic methods [1]. However, the study of diffusion by known methods is usually costly and time-consuming. Among the promising methods for these tasks is the group of photoacoustic (PA) methods. The important thing here is that the parameters of the PA response depend on the spatial distribution of substances that absorb the excitation radiation.

In the present work, a new PA method suitable for studying diffusion processes was developed and tested on model objects. The method is based on the use of an effect similar to the one known in the PA literature known as the "drum effect" [2]. The method has been modified (see Fig.). The advantage is the use of samples in the form of thin (several hundred microns) plates. Agarose hydrogels were used as a model environment.



For the same medium and dyes, the method of studying diffusion using the kinetics of changes in the optical contrast of digital images and mathematical modelling was also used.

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The physical mechanism of the sensory effect in the structures "prism – gold nanolayer – protein receptor"

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Fragments of protein molecules are considered as sensitive elements of surface plasmon resonance (SPR) biosensors in the layered structure "prism - gold nanolayer - protein receptor".

On the basis of studies of proteins as channels of metabolic electron transfer, the specific conductivity of protein chains was found. This characteristic is important for modeling the sensory effect on SPR, as it directly determines the dielectric permittivity of proteins. The change in dielectric constant upon at the interaction of the protein receptor with the protein ligand determines the sensory effect. This effect is characterized by changes in resonance characteristics, such as wavelengths and angle of incidence of the SPR.

It was established that the basis for the sensory effect is the dependence of specific conductivity on the length of the primary structure of protein chains. The length was considered in the terms of the number of amino acid residues N. Unlike an all-nucleotide biosensor, in which N is the number of nucleotides, in an all-protein biosensor the specific conductance has a different dependence on N.

It is shown that the sensory effect appears only at certain lengths of the primary structure of protein chains. The lower limit of the number of amino acid residues above which a sensory effect occurs was estimated.

Thoughts are expressed about the mechanism of interaction between the protein receptor and the protein ligand and the influence of this interaction on the spectral and angular position of the SPR.

Nanoliposomes form of curcumin and miRNA for Alzheimer’s disease therapy

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A large body of scientific research points to inflammation as a mechanism most often present in the development of Alzheimer's disease (AD). Curcumin targeted delivery may be a viable alternative to classical treatment protocols. The delivery system can be liposomes - universal systems that can be loaded with both lipophilic and hydrophilic compounds. Mixture of sunflower phospholipids in the form of powder (defatted dry lecithin) was used as a raw material for the formation of liposomes.

Phospholipids and their fatty acid composition were identified by tandem mass spectrometry. Liposomes were prepared by "freezing-heating" methods; "sonication" and extrusion. The most effective method for liposomal form of curcumin creating was determined. It was the extrusion through membranes method. Curcumin liposomal form obtaining method included dissolving a mixture of sunflower phospholipids, cholesterol, and polyethylene glycol and curcumin solution adding; evaporating of mixture until a lipid film was formed; hydration, and sequential extrusion through membranes with pore diameters of 200, 100, and 50 nm. The size of "empty" liposomes and liposomes with curcumin and microRNA was determined using: a) dynamic light scattering using a laser photocorrelation spectrometer and b) atomic force microscopy (AFM). The efficiency of curcumin encapsulation was 95.34 ± 3.76%.

The effect of curcumin on the expression of APP and Aβ in response to treatment with curcumin at different concentrations and the effect of curcumin on the expression of APP and Aβ from miRNAs were evaluated. Curcumin was shown to decrease mRNA, APP, Aβ40 and Aβ42 levels compared to untreated cells.

The obtained data found the sunflower phospholipids using as raw material for the nano-sized containers creation – liposomes for pharmacologically active ingredients transport and strategy for the Alzheimer's disease treatment, taking into account the key role of the liposomal form of flavonoids and micro RNA.

Anti-cancer activity of zinc-tetraphenylporphyrin photosensitizer / dextran-graft-polyacrylamide copolymer/ Au(Ag) nanoparticles nanohybrids

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The comparative studies of the anticancer activity of triple nanohybrids of zinc-tetraphenylporphyrin (ZnTPP) photosensitizer / dextran-graft-polyacrylamide (D-g-PAA) copolymer / Au (Ag) nanoparticles depending of the presence of Au or Ag nanoparticles in the nanosystem were performed. The 420 nm light irradiation of low power (10 mJ/s) has a significant cytotoxic effect on LNCaP prostate cancer cells in vitro under adding of ZnTPP/D-g-PAA/AuNPs and ZnTPP/D-g-PAA/AgNPs hybrid nanohybrids into the incubation solution. ZnTPP/D-g-PAA/AgNPs nanohybrids has considerably higher anticancer activity (82%) comparing to ZnTPP/D-g-PAA/AgNPs one (45%). Most possibly, for ZnTPP/D-g-PAA/AgNPs nanohybrid it is due to resonance of light irradiation wavelength of 420 nm both with absorption Soret peak of the ZnTPP photosensitizer and localized surface plasmon resonance (LSPR) in AgNPs. Meanwhile, for ZnTPP/D-g-PAA/AuNPs nanohybrid the 420 nm light is out of resonance with LSPR in Au NPs. Therefore, the plasmon enhancement of reactive oxygen species (ROS) by ZnTPP molecules is considerably higher for the nanohybrid containing the Ag NPs comparing to one with Au NPs. Another possible cause of higher anticancer activity of silver containing nanohybrid is higher cytotoxicity of Ag NPs than Au NPs. In conclusion, due to the high cytotoxic activity of D-g-PAA/AgNPs and D-g-PAA/AuNPs hybrid nanohybrids in combination with 420 nm light irradiation of low power such nanohybrids have quite high potential in photodynamic treatment of prostate cancer.

Nanoparticles for efficient drug delivery to tumors

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Nanoparticles (NPs) are widely used in modern medicine in high-resolution imaging of tissues, antimicrobial coatings, nanofabrication of implants, gold NPs are used for bone tumor treatment with external magnetic fields [1]. Different types of magnetic NP, nanofibers and nanocapsules are used for targeted drug delivery to the cells and tissues [2]. In this study a review of different types of NPs used for the drug delivery to different types of tumors and their documented efficiency is given. External magnetic field, light or infrared radiation via an optic fiber or acoustic streaming are used for activation of the release and transportation of the drug-loaded NPs toward the tumor cells and adsorption of the drag [3].

A novel mathematical model of movement of the NPs in the capillaries, through the capillary wall and in the interstitial in the field of acoustic force accounting for the diffusion and temperature-induced coupled phenomena is presented. The tumor and healthy tissues are modeled as a set of capillaries surrounded by their ‘influence domains’ (Krogh model). Numerical solutions of the problem with different tumor types and volumes (V_t), number of NPs (N_{NP}) injected into the blood stream, drug load (m_j) on NP, blood velocity (V_b) and acoustic field mean force, frequency and temperature (F_{ac}, ω, T) have been found. Functional dependence of the minimal N_{NP} needed for efficient therapy (i.e. mean amount of drug Md for a given Vt was found as a relationship $\min\{N_{NP}\}=f(Fac, \omega, T, V_b, V_t, R,L)$, where R and L are radius and length of the Krogh cylinder.

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Magnetic resonance proton signal response noise reduction by deep neural networks

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Using the deep neural network REDNet capable is allow to structure automatically data clean restoring while accounting for their noisy nature. It is one of the possible approaches for medical images existing noise reducing [1]. REDNet has already been effectively used in several computer vision and image processing applications [2].

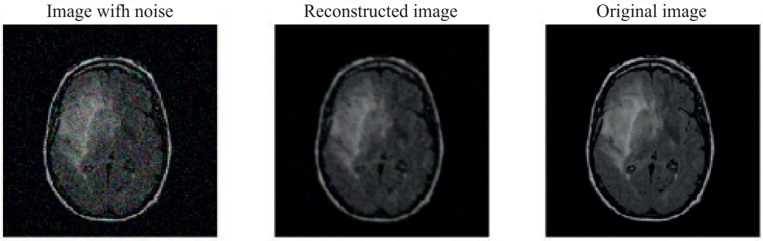

Fig. 1. MRI brain images: with noise, reconstructed and original.

The denoising results thanks to REDNet network using with artificially added 15% Gaussian noise are shown on Fig. 1. The received images quality was checked by PSNR and SSIM metrics. The medical images noise reduction with corresponding influence for more accurate diagnosis is shown by quantitative calculations.

The results for medical images REDNet denoising using confirmed its flexibility and ability for different noise levels and image types adjust.

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Composites of clay/silica/hydroxyapatite/herbals as components of therapeutic and preventive medicaments

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Previously [1,2] we showed that diverse combinations of inorganic substances coupled with appropriate herbal material via mechano-chemical activation facilitates formation of composite materials that causes the therapeutic and preventive medication properties in cosmetic products. Due to the specific adsorption capacity of composite components towards to biologically active substances (BAS), as well as the diversity in their dispersion, the simultaneous release of herbal active components and microelements of clays is feasible.

The main factors that allow successful application of such composites are the non-toxicity and sedimentation resistance in various systems achieved by particle size.

Via the method of mechanochemical activation, composite materials were obtained, which were used as activators of cosmetic products.

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2. V.V. Paientko, E. Skwarek, COMPOSITES WITH IMMOBILIZED Bioactive Compounds ON SOME INORGANIC MATRICES FOR COSMETICmPURPOSES// eritage of European science: Chemistry and pharmaceuticals,Medicine, Biology, Agriculture, Pedagogy, Psychology, Philology. Monographic series «European Science». Book 17. Part 4. 2023-p.22-27

Polymer hydrogels based on PAA as matrices for the controlled release of bioactive molecules

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Polymer hydrogels are natural or synthetic materials with high water content. They are excellent for treating wounds of various geneses due to their biocompatibility, softness, plasticity, and ability to transfer biologically active compounds and absorb wound exudate. Functionalization of hydrogels with drugs is essential. Hydrogel bandages for the treatment of wounds must release the active substance for a long time. Long-term maintenance of therapeutic concentrations of antimicrobial drugs significantly accelerates wound healing and reduces the risk of inflammatory processes [1].

Polymer chemical structure and cross-linking density are determining factors in drug adsorption and desorption. Drug penetration into human tissues and interaction with bacterial cells promote by functional groups, which often have a positive or negative charge. Cross-linked PAA hydrogels containing polymer fragments with ionizable cationic/anionic functional groups were synthesized as model matrices to study their ability to absorb and release ionic dyes.

Hydrogels were synthesized by graft copolymerization of acrylamide on chitosan, dextran, and dextran sodium sulfate with simultaneous cross-linking using N,N-methylene-bis-acrylamide.

Study of swelling kinetics and sorption–desorption of acid fuchsin, basic fuchsin and neutral red as drug models to assess the transport of bioactive molecules by synthesized gels was carried out.

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Sulfur-contained calix[4]arene C-1193 modulates the functional activity of mitochondria

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Today in molecular biological studies considerable attention is paid to macrocyclic nanoscale compounds calix[4]arenes (the size of the macrocycle cavity is more than 1 nm^3). The advantages of calix[4]arenes include their easy synthesis and low toxicity [1]. A research of effectors capable of modifying the intensity of redox reactions in the inner mitochondrial membrane and the activity of Ca^{2+} transport systems in it is an urgent issue of biochemical membranology and molecular biotechnology. The currently synthesized calix[4]arene C-1193 (5,17-bis(dihydroxyphosphonylmethylol)-25,27-dibutoxythiacalix[4]arene) contains four sulfur atoms, which cause nucleophilic properties and high reactivity.

The experiments were carried out on a suspension of isolated rat myometrial mitochondria. Using the Ca^{2+}-sensitive probe Fluo-4 AM, we demonstrated a time- and concentration-dependent (0.01-10 μM) inhibition of Ca^{2+} accumulation by mitochondria. It was established that C-1193 inhibits the oxidation of NADH and $FADH_2$ too. The investigated calix[4]arene, depending on the concentration, inhibited the formation of reactive oxygen species in mitochondria (DCF fluorescence). At the same time, according to the results of photon correlation spectroscopy C-1193 did not change hydrodynamic diameter of mitochondria, so it did not cause their swelling. The selected calix[4]arene inhibited the synthesis of nitric oxide, Ki is 5.5 ± 1.7 nM very effectively, which makes the studied compound a high-affinity blocker of endogenous NO generation in mitochondria.

These results are the basis of the possible application of the selected calix[4]arene as a tool in the research of biochemical processes associated with mitochondria and directed regulation of smooth muscle functioning.

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Noncovalent nanocomplexes between drugs and transmembrane transfer facilitating agents: formation, structure and application for drug delivery purposes

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Development and usage of nanostructures for drugs delivery is one of the most promising directions of nanoscience and nanobiotechnology application for health-care area. Among effective ways to enhance drug molecules transmembrane transfer there is a way when membrane penetration facilitating agent molecules form noncovalent nanocomplexes with the drug molecules to be delivered.

In the current combined mass spectrometry and quantum chemical study, we examined the formation of nanocomplexes between the molecules of selected anticancer mercapto-derivatives of nucleobases and drug delivery facilitating agents dimethyl sulfoxide (DMSO) or ascorbyl palmitate (AP). DMSO is known as a transmembrane drugs penetration enhancer, while AP is a fat soluble form of vitamin C, which can form nanosomes promising for the drug delivery. Formation of stable noncovalent complexes of DMSO or AP with 6-mercaptopurine and 2-mercaptoadenine in the polar solvent methanol was revealed by the electrospray ionization mass spectrometry (ESI MS) probing. The complexes are similar to the nanocomplexes of DMSO with the molecules of a number of antibiotics, formation of which was demonstrated in our previous study [1]. Structural and energetic parameters of the DMSO-drug complexes were calculated using the DFT method.

The results of the study on formation of noncovalent nanocomplexes between the anticancer drug molecules and the delivery facilitating molecules or molecular clusters can be considered as a basis for the development of nanostructures for facilitating of transmembrane transfer of the fat insoluble drugs.

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Silver nanoparticles in biomedical research of RBCs

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One of the promising areas of application of nanotechnology is diagnostic and clinical nanomedicine. It is known that silver nanoparticles (AgNPs) exhibit broad antimicrobial activity [1], but there is a high probability of adsorption/adhesion effects of Ag nanoparticles (average diameter 100 nm) on erythrocyte membranes [2]. The work investigated the activity of monodisperse silver nanoparticles of different sizes (18 nm, 30 nm, 50 nm, 85 nm, and 100 nm). AgNPs were synthesized according to the method [3]. Absorption spectroscopy and dynamic light scattering were used to estimate the size of AgNPs. Absorption spectra were recorded using a Hitachi spectrophotometer (Japan) in the range from 400 to 800 nm. Studies included Red Blood Cells (RBCs) morphology and viability, RBCs membrane integrity, oxidative stress, and cell cycle progression. Cytotoxic effects significantly increased from AgNPs-50 nm to AgNPs-100 nm. The obtained results can help in the development of modulators of AgNPs, and give an understanding of their toxicity.

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The spectral manifestations of heavy atom effect on π-electron system of tryptanthrin as a part of new effective drug

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Tryptanthrin is a naturally occurring yellow indoloquinazoline alkaloid, the well-known π-electron-containing compound. Tryptanthrin and its derivatives possess broad "spectrum" of health-care activities including anti-pathogenic, antibacterial, anticancer and anti-inflammatory [1,2] due to its unique feature of binding to telomeric G4 DNA and stabilizing it. In particular, complexes based on iodo-tryptanthrin and bromo-tryptanthrin possess the higher anticancer activity than other tryptanthrin derivatives. The feature of tryptanthrin binding to G4 DNA can be used in nanobiotechnology for the development of new antitumor drugs.

Comparative investigations of optical absorption (at room temperature), fluorescence (at room temperature and T=78 K) and phosphorescence (at T=78 K) of the molecular complexes based on tryptanthrin (Try-Pt) and iodo-tryptanthrin (ITry-Pt) with platinum chloride and DMSO were done. The positions of the first excited singlet (S1) and triplet (T1) energy levels of these complexes were obtained. The existence of two optical absorption centers in the Try-Pt molecule was confirmed. The short-wavelength shift of optical absorption spectrum of ITry-Pt in comparison with the corresponding spectrum of Try-Pt as well as the appearance of new bands, the significant decrease of fluorescence intensity of ITry-Pt in contrast to the corresponding fluorescence intensity of Try-Pt, the short-wavelength shift of fluorescence and phosphorescence spectra of ITry-Pt relative to the corresponding spectra of Try-Pt are, in our opinion, the spectral manifestations of the effect of the iodine atom on the pi-electron system of tryptanthrin.

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Novel sensitive materials based on poly(2-oxazoline)s for theranostics

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Nanotechnology is emerging as an efficient platform for theranostics, since nanoparticle-based contrast agents are powerful tools for enhancing in vivo imaging, while therapeutic nanoparticles may overcome several limitations of conventional drug delivery systems. Theranostic nanoparticles have drawn particular interest in cancer treatment, as they offer significant advantages over both common imaging contrast agents and chemotherapeutic drugs. However, the development of platforms for theranostic applications raises critical questions [1].

Poly(2-oxazoline)s are a perfectly suited class of polymers for the preparation of well-defined (co-)polymers, allowing the integration of a wide range of functionalities. Poly(2-oxazoline)s have the potential to find a variety of applications in biological systems due to their known biocompatibility. In particular, poly(2-oxazoline)-based block copolymers can be synthesized in an efficient way via a living cationic polymerization process represent attractive systems to be applied in diverse fields.

In this work we present synthesis of star–shaped polymers with three and four chains poly(2-ethyl-2-oxazoline)s (POxs) as thermo-sensitive building blocks. POxs were prepared via living cationic ring opening polymerization by using 1,1, 1-tris(hydro- xylmethyl)ethane tristriflate and pentaerythritol tetratriflate as initiators.

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Conjunction of alternative mechanisms of Gramicidin S embedding into model lipid membranes

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Gramicidin S (GS) is a prospective antimicrobial peptide which maintains its effectiveness over 80 years since its discovery [1]. It was established that antimicrobial action of GS is directly related to damages of lipid membranes of bacterial cells and related elevation in its non-specific permeability [2], though the detailed mechanism is still under consideration.

Literature data reveal two-modal GS embedding into lipid membranes due to the ability of GS to form associates inside the membrane bulk [2]. As a result, nano-emulsion is formed consisting of the lipid domains containing GS monomers or GS associates. It seems a sufficient reason for the permeability elevation underlying GS antimicrobial action. We supposed conjunction of the alternative mechanisms of GS embedding and showed that GS monomers concentration in membrane could follow the low $s = A_s c^\alpha + p_1 A_s c^\alpha A_d c^\beta$, where α and β are exponents in Freundlich equation of independent sorption, and $\gamma = \alpha + \beta > 1$ which is in line with our experiment. Our model also describes impact of GS monomers that restricts the growth of GS associates inside the membrane. Generally, nano-emulsification of lipid membrane with conjunction of two modes of GS embedding appeared to be a conceivable model which explains a lot of GS effects.

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The effect of low-intensity artificial light and colloidal solutions of nanometals on the growth and biosynthetic activity of a medicinal macromycete Fomitopsis

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The development and implementation of biotechnological processes with edible and medicinal macromycetes aimed on the effective and safe production of biological medicinal preparations and medicines is the important priority of the modern pharmaceutical industry. The study of the main growth and biosynthetic activity of medicinal macromycetes regulation and stimulation factors is a necessary component of the such biotechnological process [1].

The ecologically safe regulation and stimulation factors, as low-intensity artificial lighting, and new drugs based on the colloidal solutions of metal nanoparticles able, under certain conditions, to have the essential effects on the biophysical and biochemical processes in living organisms, including fungi [2].

We have used a pure culture of the valuable medicinal macromycete F. officinalis IBK-5004. The impacts of colloidal solutions of metal nanoparticles (FeNPs, MgNPs, AgNPs) in combination with low-intensity artificial lighting at wavelength of 470 nm on the growth and biosynthetic activity of F. officinalis IBK-5004 was studied.

It was established that both of these factors (adding the metal nanoparticles solution to the growth substrate and artificial lighting) revealed its effectiveness as a growth regulator, demonstrating the ability to both grows stimulation and inhibition.The obtained results showed that low-intensity blue light induce an growth in the synthesis of endopolysaccharides by 38.4% and reduce the exopolysaccharides by 12.4% on media without NPs. Addition of silver nanoparticles (AgNPs) to the inoculum significantly inhibited the synthesis of polysaccharides compared to the control. The addition of colloidal solutions of nanoparticles (FeNPs, MgNPs) to the seed mycelium of F. officinalis stimulate the synthesis of polysaccharides.

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Functionalization of gold nanoparticles with metal complexes of boron clusters

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Inorganic nanoparticles (NPs), including noble metal nanoparticles are one of the platforms employed for promoting selective cellular delivery and uptake of boron-rich compounds [1]. Besides known strategy for functionalization of metal nanoparticles surface with metallacarboranes through thiol bonding [2], herein we propose a method for their attachment to the gold nanoparticle (AuNPs) through a phosphorothioate function using as a model ligand thiophosphate derivative of bis(1,2-dicarbollido)-3-cobalt(1-)ate, [8,8'-μ-O_2P(O)SH-3,3'-Co(1,2-$C_2B_9H_{10}$)2]HDBU(1).

For this novel AuNPs functionalized with **1** (AuNPs/**1**) the position of the maximum of localized surface plasmon resonance band was shifted to the long-vawelength region for a several nanometers, from λ_{max} = 524 nm to λ_{max} = 526 nm, and the intensity of the band was increased compare to untreated AuNPs. The mass spectrum of the AuNPs/1 recorded in negative mode unambiguously showed a diagnostic signal corresponding to a singly and doubly ionized **1** at 434.2 m/z and 216.6 m/z and characteristic boron isotopes pattern. Based on theoretical calculations and UV-vis data the coverage of AuNPs surface was estimated as self-assembled two layers of modifier. The obtained AuNPs and novel AuNPs/**1** nanocomposite were characterized using DLS and ELS techniques, and the binding constant of AuNPs/**1** with BSA protein were calculated using the data on emission quenching.

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Effect of the surface charge, cholesterol content and medium composition on liposomal nanocontainers fusion with cell membranes

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Liposomes loaded with antitumor molecules are used for targeted drug delivery to the site of neoplastic growth, reducing the overall toxicity of drugs and controlling their spread within the biological niche, increasing their effectiveness in cancer therapy [1]. Variation of the lipid composition of liposomal membranes makes it possible to create delivery vehicles of the desired diameter, surface charge, stiffness, permeability, bioavailability etc. and paves the way for controlled action of encapsulated drugs [2]. Surface charge density on the membrane and the asymmetry of lipid distribution between leaflets can have a significant impact on the bioavailability of drugs.

We have studied the effect of surface charge density, cholesterol content and a composition of suspending medium on the effectiveness of liposomal incorporation into the cultured fibroblasts. It appeared that negatively charged DPPC–Cardiolipin liposomes are most aggregation prone in PBS solutions. This aggregation is reversible in both PBS and DMEM solutions. Confocal microscopy certifies the fastest fusion of DPPC–Cholesterol liposomes with cultured monolayers of murine fibroblasts. Cholesterol controls accumulation and release of antimicrobial peptides from liposomal nanocarriers. Our data suggests methodology for choosing optimal biophysical properties of liposomal vesicles for loading them with cationic antineoplastic medicines including redeployed antimicrobial peptides.

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Session 3.
Nanochemistry and biotechnology

Urease inhibition based biosensor for heavy metal ions determination to control wastewater treatment in textile industry

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Textile wastewater heavy metal pollution has become a severe environmental problem worldwide [1]. A lot of dyes that are used in the textile industry contain heavy metals [1]. The high concentrations of heavy metals in effluents from textile industry cause severe toxicological implications on the environment with a dramatic impact on human health [1]. Conventional heavy metal detection methods often require expensive equipment, highly skilled personnel, the application of complex operational procedures, long detection times, and they are not applicable for real-time detection [2].

As a result of this work new impediometric urease-inhibition based biosensor was developed for determination of heavy metal ions in water. A differential pair of gold interdigitated electrodes deposited on a ceramic substrate was used as impediometric transducer. As a bioselective element urease was chosen, which was immobilized by cross-linking with glutaraldehyde on the surface of electrodes. Sensitivity of urease biosensors toward different heavy metal ions was investigated. The possibility of biosensor reactivation with EDTA after inhibition was demonstrated. The biosensor was characterized by high reproducibility of responses and showed high storage stable during 6 months at -4 °C. In future the developed biosensors can be used for heavy metal ions detection to control wastewater treatment in textile industry.

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Characteristics of nanoparticles obtained via "green" synthesis using *Artemisia tilesii* Ledeb. "hairy" root extracts

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Obtaining of "green" synthesized nanoparticles is one of the directions of modern bionanotechnologies. This method involves the use of plant extracts that have reducing properties instead of various chemical compounds. It is worth noting that extracts from "hairy" roots obtained via Agrobacterium rhizogenes-mediated transformation demonstrated reducing activity due to the presence of polyphenols. That is why such extracts can be effectively used for the synthesis of metal nanoparticles, in particular, silver nanoparticles (AgNPs).

In our study, four Artemisia tilesii "hairy" root lines (No. 2-5) were chosen for the preparation of 70% ethanolic extracts. AgNPs were obtained using the extracts by standard method with 1mM $AgNO_3$. Size and morphology of AgNPs were examined by transmission electron microscopy (TEM 1230 JEOL, Tokyo, Japan) with an acceleration voltage of 80 kV. Dimensions of AgNPs were measured using ImageJ software and calculated as diameters.

Silver nanoparticles of all samples had rather non-uniform ellipsoid or barrel-like shapes. Therefore the areas of transections were measured, diameters were calculated and presented on the distribution histograms. The diameters of AgNPs for different samples were between 2.86…45.42 nm, and the range of distribution for all four samples was almost the same. However, the samples differed in the quantitative distribution of nanoparticles according to their sizes (diameters). In particular, in sample No.2, the largest number of nanoparticles had a size of 5-10 nm, although in general the size of most nanoparticles varied from 2.8 to 30 nm. Most of nanoparticles from sample No. 3 had sizes from 5 to 20 nm, and no significant dominance of nanoparticles of a certain size was observed. Sample No.5 differed from the others because 61.4% of all nanoparticles were 5-10 nm in size. Such broad dissimilarities among the samples may represent the diversity of chemical compositions of various extracts obtained from different "hairy" root lines.

Thus, it is probably worth studying the chemical compositions of "hairy" root extracts and properties of obtained NPs due to their possible use in bioengineering.

The effect of bentonite nanoparticles on the synthesis of vitamin B1 and PP by bacteria *Azotobacter vinelandii* IMV B-7076

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In recent decades, considerable attention has been paid to the use of microbial preparations in agroecosystems to improve the growth, development and productivity of plants by improving their nitrogen and phosphorus nutrition, the release of plant growth stimulators, and their protection from phytopathogens and phytophages. Particularly promising are complex microbial preparations, the effectiveness of which is due to their multifactorial

One of them is the complex bacterial preparation Azogran, developed at the Zabolotny Institute of Microbiology and Virology NAS of Ukraine. It is created on the basis of the interaction of nitrogen-fixing bacteria *Azotobacter vinelandii* IMV B-7076 and the phosphate-mobilizing strain *Bacillus subtilis* IMV B-7023 with particles of the clay mineral bentonite. The preparation improves the growth and development of a significant number of plant species, increases the yield of cereal, vegetable and technical crops by 18-37% [1].

It was established that Azotobacter vinelandii IMV B-7076 bacteria are able to improve nitrogen nutrition of plants, synthesize a number of biologically active substances, and inhibit the growth of phytopathogenic micromycetes [2]. However, the synthesis of vitamins by this strain by interaction with bentonite nanoparticles was not investigated, which became the purpose of this work.

It was shown that during the cultivation of *Azotobacter vinelandii* IMV B-7076 bacteria in a medium containing 0.1% bentonite nanoparticles, the content of vitamin B1 was 1.96 μg/ml, while in a medium that did not contain these nanoparticles, its concentration was significantly lower-1.40 μg/ml. At the same time, the cultivation of *Azotobacter* in a medium with bentonite nanoparticles had a slight effect on the accumulation of vitamin PP (niacin).

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Synthesis and investigation of spectroscopic properties of bodipy derivatives obtained from 2,4-Dimethylpyrrole by click reaction

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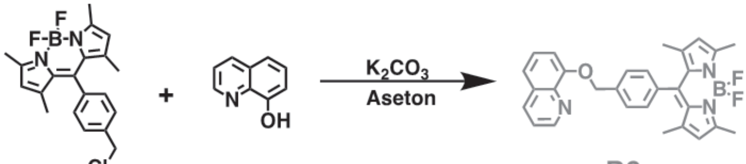
In this study, the synthesis of three Bodipy compounds was carried out using 2,4-dimethyl pyrrole as a precursor. To obtain both intermediate and final products in pure form, column chromatography was applied at each stage of the synthesis. The products were obtained in a pure form and characterized using various methods. First, melting point determination and FT-IR spectroscopy were performed, followed by functional group analysis using FT-IR spectroscopy, and then 1H-NMR and 13C-NMR spectra of these compounds were obtained. Deuterated chloroform was used as the solvent for NMR spectra.

The synthesized compounds were named as B-Cl, B_2, and B_3. After the initial characterization, the spectroscopic properties of these compounds were investigated using fluorescence spectroscopy and UV-vis spectroscopy. In addition, a study was conducted to investigate the effect of the solvent on the fluorescence properties of these compounds [1,2,3].

Bodipy, Fluorescence, 2-4 dimethyl pyrrole, Spectroscopic Properties



B2

Fig. 1 -Synthesis of 5,5-difloro-1,3,7,9-tetrametil-10-(4-((kinolin-8-iloksi)metil)fenil)-5H-4λ^4, 5λ^4-dipirolo[1,2-c:2',1'-f][1,3,2]diazaborinin (B2)

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Nanoparticles of $MnFe_2O_4$ spinel for the persulfates activation in the decolorization process of safranin T azine dye

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Nanocrystalline ferrites with a spinel structure are used in gas sensors, magnetic storage media, supercapacitors, magnetic hyperthermia, and controlled drug delivery systems. The use of nanosized spinels as activators of oxidizing agents in advanced oxidation processes of toxic organic water pollutants is also known [1]. The most common method of synthesis of spinel nanoparticles is the co-deposition method. The aim of the work was to study the structural and phase characteristics of $MnFe_2O_4$ spinel particles, synthesized by co-deposition in an ultrasonic (US) field, and their approbation as persulfates activators in the decolorization process of safranin T azine dye.

The regularities of the influence of the calcination temperature on the average size of $MnFe_2O_4$ spinel crystallites and the temperature of the reaction medium on the kinetics of safranin T decolorization were determined. According to the results of XRD analysis using the Debye-Scherrer equation, the average size of $MnFe_2O_4$ crystallites was calculated, and it was equal to ~7 nm at a calcination temperature of 400°C. It was found that using an advanced oxidation process of $US/MnFe_2O_4/S_2O_8^{2-}$ for 2 hrs at a safranin T concentration of 20 mg/L, a $K_2S_2O_8$ concentration of 5.7 mM, a catalyst dose ($MnFe_2O_4$) of 0.1 g/L, a pH of the reaction medium of 3.00, a temperature of 60 °C, and a specific US power of 68 W/L, the decolorization rate of safranin T was 98.3% and the decolorization rate constant was 1.529×10^{-3} s^{-1}.

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4,4’-stilbenedicarboxylic acid as building block for multidimensional coordination polymers construction

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Multidimensional coordination polymers that are based on stilbene derivatives are widely reported metal coordination compounds. Their structural and physicochemical properties are strongly determined by the type and conditions of the synthesis methods but also by the precursors of metal centers used. Coordination polymers have received extensive research attention due to their applicability in various fields including catalysis, sensing, storage and separation or transport of active substances [1-5].

The aim of the work was to optimize the synthesis conditions and characterization of multidimensional coordination polymers based on the 4,4'-stilbenedicarboxylate ligand as a bridging building block. Different inorganic compounds of s- and d- block metals were applied as sources of metal centers. The preparation of metal complexes has been conducted at different conditions (pH, solvent, temperature, and way of supplying energy). Physicochemical characterization of the obtained coordination polymers was performed using the following methods: single crystal X-ray diffraction, ATR-FTIR, TG-DSC, TG-FTIR, PXRD and SC-XRD.

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The binding of polysubstituted acridine-based telomerase inhibitors to quadruplex DNA: a FID assay

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Certain guanine-rich sequences of telomeric DNA form specific four-stranded assemblies – G-quadruplexes (G4). Their stabilization by small molecules results in the inhibition of telomerase, a tumor-associated enzyme responsible for telomere elongation. G4 structures were also found in the promoters of proto-oncogenes. So quadruplex DNA is a promising target for novel anticancer drugs [1].

We have previously designed new tri- and tetrasubstituted acridine derivatives as efficient telomerase inhibitors (IC_{50} 1.6–3.8 μM) with antiproliferative activity *in vitro* in the nanomolar range [2]. In the present research, we have studied the interaction of these inhibitors with their molecular target, DNA quadruplex.

G4 of antiparallel topology was obtained by folding the deoxyoligonucleotide d[AGGG$(TTAGGG)_3$] (Tel22, a fragment of telomeric DNA) in the presence of Na^+ cations stabilizing the nano-sized quadruplex structure.

The binding affinity of compounds was evaluated using a semi-automated FID (Fluorescent Intercalator Displacement) assay [3]. It is based on the competitive displacement of Thiazole Orange (TO) dye from its fluorescent complex with DNA by the tested ligand resulting in concentration-dependent emission decrease.

Using a microplate fluorescence reader, DC_{50} parameters (ligand concentration at which 50% of TO was displaced) and binding constants of the inhibitors were determined. These values correlate well with biological activity of compounds, and efficient inhibitors show high affinity to G4, with Kb in the range $(0.8–4)\times10^6$ M^{-1}. Thus, the studied bioactive compounds strongly bind to quadruplex DNA target.

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Validation of sensors based on nanostructured biomimetic polymers with tyrosinase activity for phenols detection in natural and waste waters.

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Nanostructured polymers with tyrosinase activity capable of selective cleavage of o-hydroxyphenols were synthesized using the method of molecular imprinting. The catalytic molecularly imprinted polymers (MIP) were obtained by co-polymerization of 4-imidazolacrylic acid, ethyleneglycoldimethacrylate, and Cu(II) in the presence of o-hydroxyphenol as a template molecule. The synthesized nanostructured polymers were used as a sensitive part of the biomimetic sensor based on a portable oxygen-meter for *o*-hydroxyphenol revealing in aqueous samples. The sensor provided detection of *o*-hydroxyphenols within the range 0.08–2.5 mM with the detection limit 0.08 mM. The selectivity of the developed sensors as for the detection of different phenols was investigated using *o*-hydroxyphenol, phenol, 2-nitrophenol, 4-nitrophenol, *o*-cresol, *p*-cresol, 2-methoxyphenol, *m*-hydroxyphenol, 2-(3,4)-dihydroxyphenyl)-ethylamine, and1,2,3-trihydroxybenzene as analytes. High selectivity of the synthesized nanostructured polymers with tyrosinase activity towards o-hydroxyphenols was confirmed. Methods of calibration of the laboratory prototypes of the sensor device based on biomimetic polymers for the determination of o-hydroxyphenols in natural and wastewaters were developed. The analysis of real samples of natural and wastewaters from Kyiv, Cherkasy, Odesa, and Sumy regions of Ukraine as for the content of *o*-hydroxyphenols was carried out using the developed sensor systems. A comparison of the biosensor analysis data with the results of traditional analytical methods was made and good correlation between the data obtained with different methods was demonstrated. The proposed method is superior to traditional analytical methods in terms of the simplicity of the analytical procedure, its cost, as well as the cost and compactness of the equipment.

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Development of AST-sensitive amperometric enzyme biosensor

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Aspartate aminotransferase (AST) is a specific enzyme found in the liver and heart. Its normal blood concentration blood should not exceed 40 unitsL-1. Thus, blood AST activity serves as a diagnostic marker of liver and myocardial diseases [1]. Therefore, the development of rapid, precise, and user-friendly devices for AST monitoring is an important task in biotechnology.

This paper describes the development of a highly selective amperometric biosensor based on glutamate oxidase for determining AST activity in multi-component biological fluids. The bioselective element was created by cross-linking BSA and glutamate oxidase using glutaraldehyde. The membrane thickness was approximately 120 nm. Optimal concentrations of reactants were determined, and the selectivity of the amperometric transducer to electroactive substances was enhanced by employing a semipermeable polyphenylenediamine membrane.

The biosensor's capability to measure AST activity was demonstrated, and a calibration curve depicting the relationship between the biosensor's response and AST concentration was obtained. The calibration curve was then utilized to determine the linear range, minimum limit of detection, noise, drift, sensitivity to the substrate, and other analytical characteristics of the biosensor. Additionally, various parameters of the biosensor were investigated, including signal reproducibility, stability of functioning, signal duration, and the total duration of one analysis, taking into account the preparation process.

After the completion of the development and optimization of this biosensor, it will be possible to proceed with testing the performance of the developed AST-sensitive biosensor in blood serum.

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Development of new approaches for improving the analytical characteristics of enzyme biosensors

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Enzyme biosensors are generally characterized by good selectivity towards potential interferents and the ability to maintain their working parameters over multiple applications, making them highly specific to certain analytes. However, there are also disadvantages of such systems. The main limitation lies in the narrow operational range of concentrations of the analyte that can be measured using these devices, as enzymes can become saturated at certain substrate concentrations and no longer respond to further increases in concentration[1].

There are various methods for improving the analytical characteristics of enzyme biosensors. For example, the use of microfluidic systems and nanomaterials can significantly enhance sensitivity and measurement accuracy. Additionally, by optimizing the immobilization conditions, the design of the bioselective element or by applying a multi-enzyme membrane approach[2-3]. Methods based on the usage of several enzymes in the composition of the bioselective element or the addition of nanoparticles were used in our researches and showed promising results for application in the field of biosensors.

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Biological activities of new complexes based on germanium and silver complexes

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Complexes of germanium with biologically active ligands, vitamins, medicinal forms of chemical compounds significantly expand the areas of their application, as well as sensitize the pharmacological effect and reduce the toxicity of pure organic molecules, which are precursors in the production of drugs. Thus, coordination compounds of germanium and preparations based on them are characterized by antitoxic, anti-inflammatory, antihypoxic, immunostimulating, reparative and nootropic properties, which not only expands the field of their practical application, but also solves an important task for synthetic chemistry: the synthesis of new compounds of a given composition with predicted properties. This effect was observed on complex compounds of germanium with amino acids, vitamins, nucleic acids and their components, carbohydrates, lipids, fatty acids, enzymes, hormones, steroids and others.

Therefore, the purpose of this research is the synthesis of new mono- and heterometallic coordination compounds of germanium and silver with ethylenediaminedisuccinate acid (edds), research of their composition, structure and properties. Silver was chosen as the second complexing metal to increase the antibacterial and antiviral properties of the synthesized compounds.

Complexes were synthesized in aqueous solutions at pH=6.5-7. White precipitates fell out of the solutions, but in the case of the heterometallic complex, upon drying, the colour of the solution became pink, which is due to the recovery of surface molecules. All synthesized coordination compounds were investigated by the methods of IR, ESP, chemical and thermal analysis, DLS, SEM microscopy. The method of IR spectroscopy made it possible to establish the method of coordination of ligands to t.i. metal. It is shown that MMC forms a core-shell structure, where the core is a germanate ion and the shell is formed by complex silver particles.

Geomechanics and Nanochemistry of Bottom Sediment Formation from Dispersed Polymineral Iron-Aluminosilicates in Seas and Oceans

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Experimental and model-theoretical studies were conducted to investigate the peculiarities of geomechanical, physical, colloid-chemical, and nanochemical factors influencing the nanoscale contact formation and rheological behavior of real and model iron-aluminosilicate (IAS) bottom sediments, considering their layered deep-seated occurrence. The study examined the features of rheological phenomena and physicochemical geomechanics during nanostructural layered transformations of iron-aluminosilicates. The findings demonstrate that the formation of different IASs under dynamic conditions depends on the physicochemical transformation of iron compounds, silicate and carbonate conversions, leading to the rapid preliminary acquisition of nanostructures. For the first time, it was shown that decreasing moisture content in IAS dispersions correlates with decreased flow, while the rate of micro- and macrostructure formation increases, particularly in the context of sliding marine sediments. These sediments further consolidate in deep-seated layered deposits. The obtained results are important for the development of modern concepts related to ecological equilibrium mechanisms in marine and oceanic environments [1, 2], as well as for the advancement of new technological solutions aimed at preventing catastrophic events on ocean slopes and maintaining ecological balance in underwater marine sediments using the methods of physicochemical geomechanics.

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Peculiarities of Microorganism Activity in Biocolloids on the Formation of Marine Bottom Sediments

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Specialized methods were employed to investigate the peculiarities of microorganism activity in biocolloids based on carbonates and iron-aluminosilicates (IASs) in relation to the formation of structures in marine bottom polymineral carbonate-iron-aluminosilicate turbidite-pelitic sediments, with a preliminary influence on such processes of geomechanical, nanochemical, colloid-chemical, and rheological factors. It was examined in detail the model conditions of the displacement of marine pelitic-turbidite dispersions accompanied by the reformation of geocenoses composition depending on their depth of occurrence on the shelf (up to 200 m), on underwater horizontal sections of continental plates (abyssal plains) both at depths of up to 2 km and 8 km, as well as their behavior in deep-water dips reaching 11 km. It was demonstrated that microbiological processes in polymineral IAS structures lead to the final formation of crystalline microgoethite or magnetite and iron-manganese concretions. Biocolloidal transformations are also accompanied by parallel inorganic reactions, resulting in the formation of various IASs in the deep oceanic regions and calcium and magnesium carbonates in the shelf zone. The obtained results are of significant importantance for the development of modern concepts regarding the impact of oceanic environments on the disruption of ecological equilibrium, which, according to preliminary data, exceeds the similar impact from terrestrial ecosystems by several orders of magnitude. However, their investigation remains insufficient, posing a threat to the future of life on Earth [1, 2].

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A challenging test for DFTB semiempirical quantum-chemical methods built with AI

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Semiempirical quantum-chemical methods compise an attractive compromise between accuracy and computational efficiency in modelling electronic structure and properties of nanoscale systems. However, their underlying physical models rely on highly parameterized interpolations and thus require thorough accuracy testing, even in case of such physically sound models as DFTB [1].

In this contribution, we present a methodology for selecting the molecules which tend to be as difficult as possible for a given semiempirical method (in our case, GFN$_{1\text{-}x}$TB). To this end, we create an ensemble of machine-learning models predicting the error of the given method on a specific molecule, given its structural formula. The created model can be used to rank large databases of molecular structures, based on their 'difficulty' the selected semiempirical method (see Fig. 1 for the selectde examples).

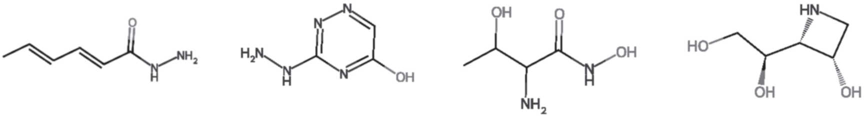

Fig. 1. *Examples of molecules selected from ChEMBL database using the proposed model*

The proposed approach can be helpful in revealing the weaknesses of the physical models underlying the existing semiempirical quantum-chemical methods and in this way can stimulate their further development.

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Antibacterial properties of various forms of clinoptilolite in the complex with 3-[5-(1H-indol-3-ylmethylene)-4-oxo-2-thioxothiazolidin-3-yl]-propionic acid

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Clinoptilolite is a naturally occurring zeolite mineral with unique structure and chemical composition. It has been studied for its various properties and applications, including its potential antibacterial qualities. The available literature suggests that certain forms of clinoptilolite exhibit antibacterial activity, however, the search for new forms and complexes with higher efficiency continues.

Our research is aimed at the antibacterial properties of various forms of clinoptilolite originating from the Transcarpathian region in Western Ukraine in the complex with 3-[5-(1*H*-indol-3-ylmethylene)-4-oxo-2-thioxothiazolidin-3-yl]-propionic acid (Les-6614). As previously described Les-6614 has slight antimicrobial activity, simultaneously possessing anti-inflammatory features [1]. Therefore, the complex of clinoptilolite with Les-6614 may prove a promising agent for antibacterial treatment.

The obtained results demonstrate that complexes, formed by clinoptilolite with Les-6614, exhibit significant antibacterial effect against *Pseudomonas aeruginosa* (gram-negative bacterium) but not against *Staphylococcus aureus* (gram-positive bacterium). Furthermore, the antibacterial properties of the complexes depend on both, the form of the clinoptilolite itself, and the conditions of chemical reactions during the sorption of Les-6614 onto clinoptilolite samples.

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The study of the biochemical markers of liver functioning under chronic action of ZnO nanoparticles

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A dominant pathway for xenobiotics to penetrate the systemic blood flow and spread further into tissues and organs is the portal system of the liver. Zinc oxide (ZnO) is one of the nanomaterials that are widely commercially available ZnO nanoparticles (NPs) are used in modern pharmacology as antimicrobial preservatives [1]. However, there is an open issue regarding the mechanisms of action of ZnO NPs, in the form of nanocolloids, on the hepatobiliary system.

Our study was to analyze the impact of nano-ZnO (average size 25 nm) water colloids on the functioning of rat liver cells *in vivo* under long-term oral application by Wistar rats. During the chronic intragastric introduction of the ZnO nanocolloids, there was a considerable increase in the activity indices for enzymes ALT and AST.

We also studied the bilirubin of blood, which is one of the main indices of pigment exchange and being a highly informative parameter of the functional state of the liver. A significant increase in the bilirubin concentration in the blood plasma of the animals in these conditions demonstrated considerable destruction of liver parenchyma, which allowed bilirubin to penetrate blood.

We performed the thymol test, and the analysis of its results demonstrated the increase in its indices. Thus, the results obtained demonstrate that the ZnO nanocolloids are hepatotoxic, and under the chronic effect of NPs cause the impairment of protein and pigment exchange in the liver.

Thus, the results of the research indicate that at the long-term oral input of the ZnO nanocolloids into the organism, there is considerable the cytotoxic damage, the impairment of protein degradation pathway, and the pigmentation disorders in liver tissues.

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Influence of hydrogen mixtures with natural gas on technical polyethylenes

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Existing ecological trends in replacing of the natural gas as main fuel both for industry and private consumers create new challenges for polymeric science as well as for the science in general. Considering the armed aggression of RF against Ukraine transition to alternative sources of fuel is more than actual both for Ukraine and for the rest of the world.

The paper presents the results of complex studies of the effect of gas mixtures of hydrogen with natural gas in the ratios of $10\%H_2/90\%CH_4$ and $20\%H_2/80\%CH_4$ on PE-80 and PE-100 polyethylene pipes and their material. The results of complex strength and thermophysical studies of the materials of PE-80 polyethylene pipes, which were previously operated in the existing gas distribution networks of Ukraine for 15 years and PE-100 polyethylene pipes which were not used before, are presented.

The influence of gas mixtures on the thermophysical properties of polyethylene pipes has been established, which is manifested in a decrease in the size of polyethylene crystallites and their orderliness in the volume of pipes under the influence of gas mixtures. During analysis of results of the strength tests, it was determined that all pipe samples, according to their strength characteristics, meet the requirements of regulatory documents issued for polyethylene pipes used for natural gas transportation [1, 2].

Submitted results are the basis for a further more wide-scale investigation aiming to study the possibility to transport pure hydrogen and hydrogen mixtures using the gas distribution networks operating in Ukraine and EU.

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Development and application of Clinoptilolite-Argentum based preparations for the healing of burn wounds

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Burn wounds are one of the major medical problem worldwide due complexity of the healing process. Development of new effective pharmaceutical compositions with active antimicrobial agents as argentum and supporting components as clinoptilolite sorbent for improving the wound healing is an important task for health care. This study aimed to develop preparations based on clinoptilolite-argentum and argentum nanoparticles and evaluate their effectiveness in treating burn wounds in rats.

Ethics Commission of the Institute of Animal Biology of the NAAS approved all experimental procedures on animals in accordance with the Ukrainian current legislation. Second-degree burns with size 6 cm^2 were created on the dorsal area of 32 male rats under general anesthesia. The animals were randomly divided for 4 experimental groups (8 rats in each): animals from a control group were treated by saline solution; group 1 - pure clinoptilolite; group 2 - clinoptilolite with metallic argentum; 3 - clinoptilolite with chitosan-argentum nanoparticles. On Days 0, 3, 7, 9 and 11 of treatment wound areas in all animals were measured. On Day 12, all rats were euthanized and burn samples for histological and biochemical examinations were collected.

The results showed that the wound areas of group 3 animals (3,14 ± 0,17 cm^2 on Day 11) reduced more rapidly compared to the control (4,38 ± 0,23 cm^2) andsm experimental groups 1 (4,13 ± 0,28 cm^2) and 2 (3,75 ± 0,19 cm^2). Best positive effect on burn healing of clinoptilolite-argentum based preparations (groups 2 and 3) was confirmed by histological analysis. Reduction of the inflammation level and acceleration of the tissue regeneration in the wounds of groups 2 and 3 were established. There were no significant changes in activity of superoxide dismutase, catalase, and concentration of malondialdehyde and proteins oxidative modifications between the control and experimental groups.

Therefore, the clinoptilolite-argentum based preparations are effective for treatment of burn wounds in rats.

The impact of nanotechnology on ensuring sustainable economic development

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Sustainable economic development is the development that takes into account the balance of interests between the present and future generations, and the foundation for shaping the goals of sustainable development is the concept of a balanced interaction between the economic, social, and environmental spheres of societal development. According to the FAO report, the world is moving in the wrong direction [1]. Nanotechnology can become the very tool for sustainable development that will contribute to combating hunger and malnutrition, poverty and destitution, preserving public health, promoting the use of affordable and clean energy, conserving marine ecosystems, fostering innovation, and driving economic growth. Thanks to nanotechnology, goods can be improved, becoming more affordable and compact, while acquiring new properties. It is important that nanotechnology to continue to be a critical component of the convergence of knowledge, technology and society (CKTS) as its offers the potential to expand the limits of sustainability and address all critical needs of human development on Earth including basic commodities (e.g., energy, water and food), finished goods (e.g., cell phones, cars and airplanes) and services (e.g., shelter, healthcare and employment) [2]. Almost everything that humans need for their livelihood can be created by molecular robots directly from atoms and molecules. This mode of production that is expected to be much more cost-effective and environmentally friendly than traditional agricultural and industrial methods. Humanity will be able to exist in an entirely different environment that is conducive to life, where disease, poverty and hunger will be almost eliminated, and the climate and ecological conditions will be greatly improved.

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Optimization of enzyme inhibition based biosensor for silver ions determination to control wastewater treatment in textile industry

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The use of silver nanoparticles and silver salts in various fields is increasing every year, that already has a negative impact on the environment and human health [1,2]. There was a problem of developing new methods for silver detection.

As a result of the work, an impediometric biosensor based on urease was optimized for the inhibitory determination of silver ions. The main analytical characteristics improved: sensitivity, linear range of detection, limit of detection, reproducibility, the ability to reactivation. The minimum detection limit of Ag^+ ions was improved to 1 nM. The biosensor is characterized by high signal reproducibility (RSD=2.28%) and high stability during long-term storage (at -4 °C) that allows these biosensors to be stored for up to 6 months without a significant decrease in their sensitivity. It was found that the biosensor can be reused by reactivation with EDTA. The developed biosensor can be used to determine silver ions to control the quality of wastewater purifiers in textile production.

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The properties of graphene complexes functionalized by a single transition metal atom: the coordination chemistry concepts

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The application of ideal graphene in electronic, optoelectronic and catalytic systems is impossible due to the zero band gap. The modification of graphene by various methods is provided to overcome this disadvantage. The most effective method is a single-atom functionalization (SAF) by a transition metal atom (ATM), which is considered in this report. Based on the characteristics of the coordination centers, if graphene is considered as a multifunctional ligand, the SAF ATM methods can be divided into five categories: (1) coordination on the π-electron system of graphene; (2) coordination on the heteroatoms, which are pre-doped into the graphene sheet; (3) coordination on graphene defects, such as vacancies and edge; (4) coordination on the functional groups of doped graphene; (5) coordination using a combination of several options.

The report presents the results obtained by DFT method (B3LYP, 6-31G(d,p), with the involvement of Grimme dispersion correction) at SAF ATM (iron atom) system formed by the replacement of four carbon atoms (surrounding the double vacancy in graphene) by four nitrogen atoms (Fe-N_4-graphene) using the concept of coordination chemistry. The *d*-metal complexes play an important role in inorganic chemistry, materials science and nanotechnology. The method used to describe the nature of the ligand-metal bond is based on ligand field theory and includes a useful and simple crystal field theory (based on the electrostatic model) as well as a more complex approach based on molecular orbital theory.

The Fe-N_4-graphene complex has a planar structure with local symmetry D_{4h}. For this case the diagram of the *d*-orbitals splitting of the Fe atom in the field of ligands (four nitrogen atoms) would be analogous to a square planar complex (fig. a). The dxz and d_{yz} orbitals are degenerate and have eq symmetry; the other orbitals are singly degenerate: the d_{z2} orbital has a_{1q} symmetry; the d_{x2}-y_2 orbital has b_{1q} symmetry; the dxy orbital has b_{2q} symmetry. The d-orbitals of the Fe atom with lobes on that axis have lower energy due to the lack of ligands on the *z*-axis of octahedral coordination. The *σ*-bonding orbitals of the Fe atom have lobes in the *x* and *y* directions. The d_{xy} orbital interacts with the px orbitals from the nitrogen atoms in the Fe-N_4-graphene complex, and the d_{xz} and d_{yz} (e_q) orbitals interacts with the p_z orbitals of nitrogen atom, as seen in fig. *b*.

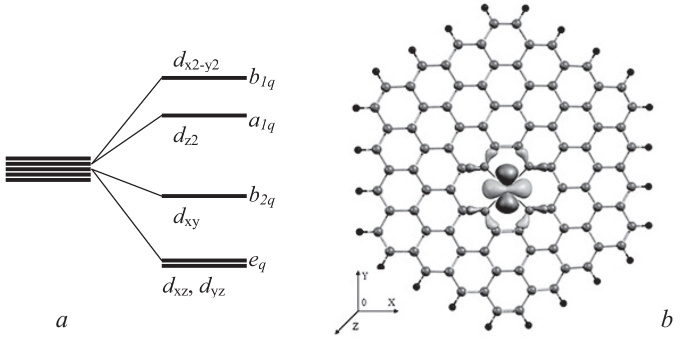

Fig. The d-orbital splitting of levels of the Fe atom in the field of tetragonal symmetry (a), the molecular orbital illustrating the interaction of the d_{xz} orbital of the iron atom with the p_z orbital of the nitrogen atom (b).

The coordination of transition metals on graphene can be understood in terms of the local symmetry of the coordination center and the molecular orbitals formed during the coordination of the TM atom. The d-orbitals of the TM atom can mix with graphene orbitals of the same symmetry, which leads to a redistribution of molecular orbitals in energy and, consequently, to a change in the splitting in the ligand field.

Nanomicelles of biosurfactant-rhamnolipid with ethyl thiosulfanilate

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Increasing the bioavailability of hydrophobic substances is possible via creating compositions with surfactants, in particular biogenic ones. Priority is given to biosurfactants of a glycolipid nature – rhamnolipids – products of bacteria of the genus Pseudomonas. This is due to their properties (emulsification, micelle formation, foaming, wetting of surfaces, solubilization of substances, that poorly soluble in water, low toxicity, environmental safety). An important property of rhamnolipids is the effect on the permeability of cell membranes and on growth of microorganisms [1]. The ability of rhamnolipids to enhance the effect of various biologically active substances, to stabilize liposomes for transporting substances into cells is known [2]

Promising antimicrobial compounds of a hydrophobic nature include thioesters of sulfonic acids, in particular esulan – ethyl ester of p-aminobenzenethiosulfonic acid (ETS) with antioxidant, antimicrobial, antiviral, and antitumor effects. However, its use is limited by low water solubility and bioavailability. Previously, it was shown that the antimicrobial activity of ETS in compositions with rhamnolipids was increased against a number of test microorganism’s cultures [3].

A modern form of ETS compositions can be rhamnolipid nanomicelles with ETS. Their advantages are a significant surface area of nanoparticles; protection of the biologically active substance; prolonged and controlled release of the biocide. So far, rhamnolipids as nanocarriers for hydrophobic drugs have not been sufficiently studied.

The aim of the work was the synthesis of ETS/rhamnolipid nanomicelles, determination of the optimal ratio of components for the maximum loading of nanomicelles, determination of antimicrobial activity.

Nanomiclles were obtained via mixing ETS in a rhamnolipid-ethanol solution, followed by the addition of a buffer and separation on a 0.22 μm PTFE membrane. The dimensions of the obtained nanomicelles were determined by the method of dynamic light scattering on a DynaProNanoStar device (Wyatt Technology, USA)

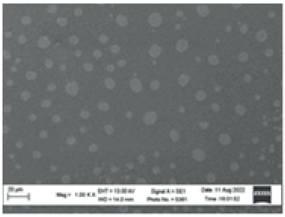

Fig 1. *Nanomicelles Scanning electron microscope analysis*

Table 1

ETS load in nanomicelles and encapsulation effectiveness

ETS:rhamnolipide ratio	Load %	Encapsulation effectiveness %
1:1	42	25
1:2	23	26
1:4	18	35

at 298 K. The dimensions of ETS/rhamnolipid nanomicelles were 157 nm and the polydispersity index were 0.40. Scanning electron microscope analysis showed that most of the synthesized nanomicelles have sizes from 3 µm to 14 µm, and are mostly spherical in shape.

The ETS load in the obtained nanomicelles decreased with decreasing of the ETS amount, but the encapsulation efficiency was increased (Table 1).

Determination of the obtained nanomicelles antimicrobial effect on *Staphylococcus aureus* test culture (Table 2) showed that the most active nanomicelles ETS-rhamnolipid have ratio 1:1. The minimum inhibitory concentration (MIC) is 1.47 µg/ml, the minimum bactericidal concentration (MBC) is 2.94 µg/ml. For nanomicelles of 1:2 ratio MIC is 6.07 µg/ml; MBC – 3.045 µg/ml, ratio 1:2 - MIC – 8.38 µg/ml; MBC – 4.19 µg/ml.

So, it was established that the optimal ratio of ETS-rhamnolipid in nanoparticles is 1:1, and the ETS loading was 42%. The nanoparticles showed effect against *Staphy-lococcus aureus.* Considering biosurfactants ecological safety and problem of pathogen resistance to antibiotics, nanoparticles is a promising tool.

Table 2

The minimum inhibitory concentration and minimum bactericidal concentration on Staphylococcus aureus.

Rhamnolipid-aesulan ratio 1:1	MIC, µg/ml	MIC, µg/ml
1:1	42	25
1:2	23	26
1:4	18	35

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Cytotoxic effects of *cis*-Palladium(II)3-(2-pyridyl)-5-methyl-1,2,4-triazole in combination with C_{60} fullerene on LLC cells

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Today, cancer mortality occupies another place after the disease of the cardiovascular system among all causes of death in Ukraine. For the treatment of cancer, classical chemotherapeutic drugs with a cytotoxic effect are used, which have a large number of side effects. The creation of less toxic structural analogues of known effective drugs and their modulation by nanostructures in order to enhance the cytotoxic effect is promising nowadays.

The aim of this study was to estimate the effect of *cis*-Pd complex on the viability and cell cycle distribution of LLC (Lewis lung cancer) cells separately and in combination with C_{60} fullerene.

Cis-Pd(HL)Cl_2 (the purity of compound was ≥98%) was synthesized at Taras Shevchenko National University of Kyiv (Ukraine) as described in. A highly stable water colloid solution of C_{60} fullerene (10^{-4} M, purity >99.5%) was synthesized at Technical University of Ilmenau (Germany).

By using computer modeling it was shown that compound *cis*-Pd(HL)Cl_2 form stable complexes with DNA separately and in combination with C_{60} fullerene.

LLC cells viability was estimated using MTT test at 24, 48 and 72 h after addition of cis-Pd complex in 0.2 - 10 μM concentration range. The cytotoxic activity of cis-Pd complex against LLC cells at 48h incubation was found to be higher as compared with cisplatin, IC_{50} value for cis-Pd complex was 2.744 μM, whereas for cisplatin - 27.79 μM. Cell cycle analysis revealed the increased LCC cells content in G2/M phase after treatment with cis-Pd complex and the increased cells content in apoptotic subG1 phase after combined treatment with *cis*-Pd complex and C_{60} fullerene.

Thus, the *cis*-Pd complex showed a pronounced cytotoxic effect, compared to cisplatin, which was enhanced by combined treatment with C_{60} fullerene.

Session 4. Physico-Chemical nanomaterials science

Tracking photopolymerization shrinkage in polymer-filler dental restorative nanocomposites by annihilating positrons

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Photopolymerization shrinkage in acrylic polymer-filler nanocomposites is identified at the example of commercially available dental restoratives of various packing, such as densely-packed ESTA-3 (ESTA Ltd, Kiev, Ukraine) and loosely-packed Charisma (Heraeus Kulzer GmbH, Germany). Observed changes in atomic-deficient structure of these composites are parameterized with PAL (positron annihilation lifetime) spectroscopy applied in positron-Ps trapping conversion mode, the model-independent estimate of volumetric shrinkage being done in terms of average positron lifetime. Under saturated light curing, fragmentation of Ps-hosting holes is shown to prevail in polymer sub-system of these restoratives, predetermining polymerization-driven inverse (positron-to-Ps) conversion in their unconstrained three-component PAL spectra. The Ps-hosting holes get to be more fragmented in light-cured composites owing to cross-linking of monomer chains, they being merged into holes smaller in volumes but larger in numbers. Meaningful description of these transformations is presented employing the Positronics approach based on the x3-x2-CDA (the coupling decomposition algorithm). In densely-packed composites, polymerization shrinkage occurs mainly in filler sub-system owing to disappearing of free volumes in junctions between filler particles, while in loosely-packed composites this process occurs in filler-polymer sub-system owing to preferential disappearing of free-volume cavities at the interfaces between filler particles assemblages and surrounding polymer matrix.

Properties of PSBTBT lower oligomers as electron donors of the active layer of organic solar cells

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Recently, intensive research on the use of conductive conjugated polymers in organic solar cells (OSCs) has been undertaken due to the systematic increase in the cost of energy resources and the emergence of new sources of electrical energy. Their main advantages include lightweight, ease of manufacture, flexibility, low in cost, and the possibility of fairly simple adjustment of the main parameters of the electronic structure of OSCs molecules, such as the energies of the lowest unoccupied and the highest occupied molecular orbitals, donor (D) and acceptor (A) materials of the active layer and width of their band gaps (E_g).

In this work presents the results of quantum-chemical calculations of the main properties of lower oligomers n = 1–8 of the conductive polymer poly[2,6-(4,4'-bis(2-ethylhexyl) dithieno [3,2 - b:2',3'-d] silole) – alt - 4,7 - (2,1,3 – benzothiadiazole)] (PSBTBT), which is used as an electron donor in OSCs. All spatial and electronic structure calculations were performed in the DFT approximation (B3LYP, 6-31 G^{**}) and TDDFT. Exponential approximation of the data for oligomers to n gave a value of E_g=1.54 eV for the polymer. The main microscopic parameters of molecules of the active layer of OSCs based on PSBTBT (D) and (6,6)-phenyl-C61-methyl ester of butyric acid (A) are: E_{LL}=0.50; E_{LH}=0.21; E_{HH}=0.83 eV. The estimation of the value exciton binding energy shows that for the monomer it is 0.33 eV, and then with increasing n=2–8 it remains practically unchanged in the interval from 0.26 to 0.28 eV. If we use the formula given in [1] to determine the macroscopic operational parameter of the OSCs, the open circuit voltage VOC, we will get a value of 0.90 V, which is a good indicator for solar cells of this type. The obtained results and their analysis show that the computer modeling of the materials used in OSCs allows to optimally select their component elements to obtain the highest open circuit voltage values.

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New Approach to Obtaining of Nanosilica and Its Properties

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The development of new cost-effective methods for the synthesis of amorphous silica is of great practical importance, since highly dispersed silica is used in various industries in its initial or modified form both to improve the properties of materials and to create new composite materials. Therefore, special attention is paid to resource- and energy-efficient technologies, not requiring some special raw materials or the application of many expensive reagents and equipment [1].

The results of studies of a developed and successfully implemented new approach to the synthesis of highly dispersed amorphous nanosilica are presented. The proposed approach is based on the usage of ammonium fluoride, the physical effects of sublimation and desublimation of the silicon-containing part of the initial raw and is implemented on a pilot plant. The use of technogenic metallurgical wastes (copper slags) as the feedstock and ammonium fluoride as the only reagent, as well as the low synthesis temperature (400°C), makes this approach cost-effective and promising for implementation in manufacturing.

It is shown that this method makes it possible to obtain amorphous nanosilica with a purity of at least ~99.97% and a specific surface area of 10 (according to BET) and 110 (according to SAXS) m^2/g. The synthesized SiO_2 particles are characterized by a regular spherical shape with some lamellar structures, including small seed particles.

It has been revealed that the sizes of the synthesized particles can be controlled by changing the synthesis conditions: the concentration of ammonium hexafluorosilicate, pH, and temperature during the hydrolysis. It was also shown that changing the pH of the solution from 6 to 1 during hydrolysis before precipitation makes it possible to increase the specific surface area of the resulting hydrolytic SiO_2 by 4 times.

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Thermal and electrophysical properties of polymer composites based on silver and nickel alloys

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It was obtained samples of epoxy polymer (EP) and composites based on EP and magnetosensitive silver and nickel alloy, which were formed under the action of an external magnetic field and without it and subsequent thermal cross-linking of the samples. It has been found that in composites formed under normal conditions in the absence of an external magnetic field, the particles of the filler are discretely distributed in the polymer matrix. The formation of a composite under the action of an external magnetic field leads to the formation of continuous channels from the particles of the alloy Ag / Ni in the continous matrix EP. It has been established that discrete alloy particles do not significantly contribute to the resistivity and thermal conductivity of composites due to high intercontact electric and thermal resistance. This leads to the fact that the resistivity remains quite significant, and the coefficient of thermal conductivity is rather small for both pure of epoxy polymer and for a composite with a concentration of Ag / Ni filler up to 5%. When the Ag / Ni concentration increases above 5%, the particles of the ferromagnetic filler begin to contact each other. Subsequent application of the magnetic field leads to the formation of continuous conducting channels of the ferromagnetic particles of filler oriented along the lines of the magnetic field. The presence of continuous channels from the particles of the alloy Ag / Ni causes a significant decrease in the specific resistance and the growth of the thermal conductivity of the composites in the direction of orientation. There are grounds to consider the received materials as the modern composites with controlled anisotropy of electro- and thermal conductivity with the help of an external magnetic field.

The effect of an external magnetic field on the structure, thermal and electrophysical properties of polymer composites based on epoxy polymer and Fe_3O_4

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Abstract

This work presents the results of the study of the effect of an external magnetic field on the thermal and electrical conductive properties of composites based on epoxy polymer and magnetite.

The samples of the initial epoxy polymer (EP) and composites based on EP and magnetite (Fe_3O_4) were obtained. Epoxy oligomer (EDO) based on bisphenol A, with density =1150 kg/m^3 at 293 K (trade mark DER 321 from DOW Chemical) was used to obtain samples. Polypox H354 (manufactured by UPPC (Germany) was used as a hardener for EDO. As a filler, magnetite (Fe_3O_4) with a density of 5200 kg/m^3 with an electrical conductivity of $10^{-4}\div10^{-2}$ S/m and a particle size of $1\div5$ µm was chosen.

Such samples were formed under the action of an external magnetic field and without it. It is found that the formation of a composite under the influence of an external magnetic field leads to the formation of continuous channels from ferromagnetic particles of Fe_3O_4 in a continuous matrix of EP. It is established that, despite of the high intrinsic electrical conductivity of Fe_3O_4, the presence of continuous filler channels does not contribute significantly to the resistivity of composites due to high intercontact resistance within the filler channels. The thermal conductivity in the direction of the orientation of the Fe_3O_4 particles increases substantially.

Principal component analysis reveals new band of Raman spectra of reduced Graphene Oxide

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Raman spectroscopy is one of the most informative techniques that is applied in the structural analysis of reduced graphene oxide (RGO). Major bands in Raman spectra of RGO are located in 1000–1700 cm^{-1} interval and presented by high-intensity peaks D (at ~1350 cm^{-1}) and G (at ~1600 cm^{-1}). Minor bands of D* and D" were obtained as a result of curve fitting [1]. However, detection of minor-intensity bands may be performed using principal component analysis (PCA). Applying PCA allows increasing the signal-to-noise ratio significantly so that one may clearly indicate the signal. A set of 7 samples of hydrazine-reduced and thermally treated GO was synthesized for the revision of the Raman spectra of RGO. Obtained Raman spectra was processed by PCA algorithm. The analysis of the dependence of Loadings of the 1st component that contains 93.7% of total variance on Raman Shift given on Figure 1 clearly shows the presence of D* and D" bands as well as new broad band in the range of 1200–1300 cm^{-1} denoted as D^{Ar}. New band may be attributed to aromaticity disruption and formation of small aromatic domains.

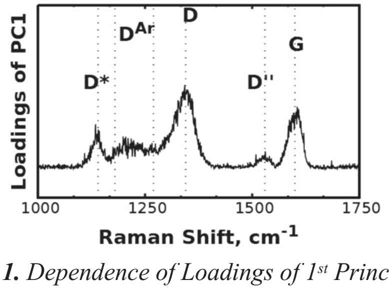

Fig. 1. *Dependence of Loadings of 1st Principal Component (PC1) on Raman Shift*

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KOH and NaOH biocarbnos from biomass: preparation, characterization and their applications in brilliant green adsorption

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Adsorption studies have been in the area of interest of contemporary science for a long time. The process of adsorption permits reduction of significant amounts of gas and liquid pollutants emitted to the environment, including pesticides, detergents, organic dyes and metal ions from mono- and multi-component solutions. A large group of effective adsorbents are carbon materials of which the most popular is activated carbon. Adsorbents of this type can be obtained by impregnation of an organic precursor with the activating agents such as sodium or potassium hydroxides followed by thermochemical treatment in a neutral gas atmosphere [1]. Industrial methods of production of carbon adsorbents are based on conventional heating, which, however, requires activation in high temperatures. An interesting alternative is the use of microwave radiation, which permits running the process at lower temperatures, shortening of the time of heating and energy saving [2].

The main aim was to develop low cost and effective adsorbent from biomass (thyme herb) to eliminate brilliant green from aqueous solution. The impact of different experimental parameters on the course of adsorption, like contact time, pH, and solution concentration, was studied. The thermodynamics of the sorption process was analyzed to establish the practical applicability of the adsorbent for wastewater treatment from liquid pollutants.

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Physical properties of the thin films based on germanium compounds with a supramolecular structure

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Complex compounds of metals and semiconductors with a supramolecular structure possess a number of interesting, often unique, physical, physicochemical, chemical, and biophysical effects at the same time that can be successfully used in the creation of promising micro- and nanoelectronic devices of various functional purposes [1]. However, the electrophysical properties and mechanisms of current transfer in them are not sufficiently studied and is the subject of research, the results of which are given in this report.

The resistivity, dielectric constant, tg, and current-voltage characteristics (CVC) of thin films of the germanium Ge(IV) complex (GC) with oxyethylenediphosphonic acid H_4Oedph were studied.

It is shown that the electrophysical properties of GC can be easily modified at the synthesis stage by introducing into their composition ions of other impurities that form salts with ions of other metals and organic cations [2]. In particular, the specific Ohmic resistance can thus be changed by 3 orders of magnitude - from 10^{10} Ω•m to 10^7 Ω•m.

On the basis of the analysis of the supramolecular structure and the temperature dependence of the conductivity of the complex compound based films and CVC, the possible mechanisms of current transfer are considered. The presented data assert the presence of several competing mechanisms of current transfer in GC, characteristic of complex compounds with a supramolecular structure and hydrogen bonds. In particular, depending on the properties of the modifying element or the temperature in the complex compounds, the so-called "relay" or "crew" current transfer mechanisms can be implemented.

The report also indicates the possible areas of application of GC in micro- and nanoelectronics when creating promising devices, in particular, in sensors for various purposes.

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Prediction of Isomorphous Substitution Limits and Thermodynamic Stability for $Y_{1-x}Ln_xVO_4$ (Ln = Ce–Lu, Sc) Solid Solutions with Zircon-Type Structure

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Solid solutions of orthovanadates of rare earth elements (REEs) are used as materials for matrices and activators for optical quantum generators, phosphors, scintillators, optical polarizers, LEDs. Solid solutions based on YVO_4, $GdVO_4$, and $LuVO_4$ are of greatest interest, since these orthovanadates do not have their own absorption bands in the visible and UV ranges of the spectrum. They can be used to create lasers for use in the treatment of cavernous and fibro-cavernous forms of tuberculosis, bone tuberculosis, upper respiratory tract diseases and in gynecology. Nd, Eu, Dy, Ho, Er, Tm, and Yb are most often used as activators.

The possibility of the formation of solid solutions in wide ranges between the matrix components and the matrix with activators is because REEs orthovanadates (except for $LaVO_4$) belong to a single structural type – a zircon-type structure. At the same time, the radius of the yttrium cation is slightly different from the REEs radii, as it occupies approximately the middle of the range of REEs radii. Phase relations and properties of solid solutions for most systems involving YVO_4 and other REEs remain insufficiently studied.

Using crystal-energy approach, in the approximation of regular solid solutions, the mixing energies (interaction parameters), critical decomposition temperatures Td, and substitution limits for $Y_{1-x}Ln_xVO_4$ (Ln = Ce–Lu, and Sc) solid solutions were calculated. It was established that with an increase in the REEs number, the contributions to the total mixing energies Q_{mix}, due to the difference in the sizes of the substituted structural units (Q_R), change regularly, significantly decreasing from 16.26 to 0.01 kJ/mol in the range from $Y_{1-x}Ce_xVO_4$ to $Y_{1-x}Ho_xVO_4$ solid solutions; and then slightly increase from 0.01 to 1.74 kJ/mol in the series from $Y_{1-x}Ho_xVO_4$ to $Y_{1-x}Lu_xVO_4$ solid solutions. It was shown that with REEs numbers increasing, the Td of solid solutions decrease for the orthovanadate systems of the Ce-subgroup and increase for the orthovanadate systems of Y-subgroup with maxima for the $Y_{1-x}Eu_xVO_4$ and $Y_{1-x}Yb_xVO_4$ systems. A thermodynamic stability diagram and decomposition domes for the $Y_{1-x}Ln_xVO_4$ (Ln = Ce–Lu, Sc) systems were constructed which allow graphical prediction of the Td for solid solutions at given substitution limits or equilibria substitution limits at a given Td, as well as ranges of thermodynamic stability of solid solutions.

Current state and prospects of using the high-speed evaporation-condensation method to produce dispersed and nanocrystal materials

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The possibilities of processes of high-speed evaporation and condensation of metals and non-metals in a vacuum for the creation of new composite materials are considered. Such materials include composite dispersion-reinforced layered and porous materials. Dispersion-strengthened condensates consist of a polycrystalline metal or ceramic matrix with dispersed particles of the second phase evenly distributed throughout the volume. By changing the temperature of the substrate, the deposition rate can be changed in a wide range, the average size of matrix crystallites from several hundreds of microns to several hundred nanometers, particles of the strengthening phase – from several nanometers to several microns.

The evaporative condensation method allows you to implement two typical approaches to the formation of structural microlayer condensates:

1. Carry out condensation at relatively low temperatures and, as a result, obtain condensates with a high density of the crystal lattice inside each layer.
2. To produce microlayer condensates with a sufficiently balanced structure at temperatures above (0.4-0.5) Tpl of the most refractory layer.

Electron beam technology can be successfully used for porous materials with adjustable sizes and volume of pores. Condensates based on Fe(Ni,Co)CrAl alloys deposited as coatings on gas turbine blades have gained wide practical application [1]. Electrical contacts are made from composite condensed sheet materials Cu-Mo, Cu-W, Cu-Cr; from the Cu-$A1_2O_3$ composition - electrodes for contact spot welding.

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Optical gap bowing parameter and spin-orbit splitting in $CdSe_{1-x}S_x$ thin films

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$CdSe_{1-x}S_x$ thin films are prepared by the method of high-frequency (HF) magnetron sputtering (13.6 MHz) using a VUP-5M vacuum station (Selmi, Ukraine). The target–substrate distance was 60 mm. The start and end of the process were controlled by means of a movable shutter. Before the sputtering process, the chamber was evacuated. The gas pressure inside the chamber was 4×10^{-4} Pa. This pressure is achievable when using a Polifenilovyi Efir 5Ф4E diffusion fluid in the vapor oil vacuum pump, which provides a low partial vapor pressure (9×10^{-7} Pa). The sputtering was carried out at a pressure of argon (Ar) in the range of 1.0–1.3 Pa. The power of the HF magnetron was maintained at the level of 100 W and the temperature of the substrate at 563 K. For heating the substrates, a high-temperature tungsten heater with a power of 300 W was used. The temperature was controlled by means of a proportional–integral–derivative (PID) controller for controlling heating and cooling rates, as well as for ensuring the temperature conditions of deposition.

The phase analysis and crystal structure refinement were examined with using X-ray diffraction data (DRON-2.0M) at the room temperature. The thickness of the films was measured on a Veeco profilometer (model Dektak 8). The mean value of the $CdSe_{1-x}S_x$ film thickness is ~0.5 μm. The X-ray fluorescence spectroscopy (XRF) and energy-dispersive X-ray (EDX) study were used for analyzing the chemical composition of materials. The spectral dependence of the optical transmittance (Shimadzu UV-3600) of the obtained sample in the visible and near-infrared regions is studied at room temperature.

The integral optical transmittance and the bandgap value of studied films are determined. The optical bandgap increases with increased sulfur concentration in the films. The spin-orbit splitting decreases with increase S concentration in the films.

Electrical properties of the p-CuNiO$_2$/n-Si heterojunction produced by radio frequency magnetron sputtering

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CuNiO$_2$ belongs to a group of materials called delafossites, which are known for their wide range of electrical properties. The conductivity of these materials can vary from insulating to metallic. CuNiO$_2$ as other delafossites have good photocatalytic properties and could possibly be used for reduce water in a solar water-splitting device [1].

Thin CuNiO$_2$ films (~ 150 nm thick) were obtained by RF magnetron sputtering on glass substrates and on plane-parallel n-Si plates. A stoichiometric mixture of CuO and NiO was used to make the target. Substrate temperature $t°_S = 350°C$, spraying was carried out with spraying time t = 30 min and magnetron power $P = 180$ W. Its resistivity was $\rho = 20\ \Omega\cdot$cm. The optical width of the band gap is $E_g = 2.81$ eV and absorption of light photons takes place by means of direct optical transitions [2].

Studies of I-V–characteristics of anisotype p-CuNiO$_2$/n-Si heterostructures at forward and reverse biases in the temperature range $T = 295 – 344$ K indicate the rectifying properties of the structures. The rectification ratio at $|V| = 0.7$ V and $T = 295$ K was $RR \sim 10^2$. The diode characteristics of the heterostructure are due to the energy barrier $q\varphi_k \sim 0.3$ eV from the n-Si side. At forward biases of $0.04\ V < V < 0.1\ V$ in the structure of p-CuNiO$_2$/n-Si the generation-recombination mechanism of current transfer prevails. At V > 0.1 V the tunnel mechanisms of current transfer with participation of surface states, with the activation energy $E_a \sim 0.13$ eV, prevail. The reverse current at biases $– 0.3\ V < V < – 3kT/q\ V$ is determined by generation mechanism of current transfer. At $– 2\ V < V < – 0.3\ V$ the tunnel mechanisms of current transfer. The p-CuNiO$_2$/n-Si heterostructure is photosensitive at reverse displacement under AM1.5 radiation conditions.

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Doped by NH^{4+}, Co^{2+}, Fe^{2+} Manganese(IV) Oxide electrode nanomaterial of OER processes

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Electrolytic doping is used to prepare nanosized oxide materials of transition metals. By adding cation additives in the electrolyte during electrodeposition, the phase composition, structure disorder, the nature of defect states, and their concentrations can be tuned [1-3]. In this work, MnO_2 was electrodeposited from 0.7M $MnSO_4$ in 0.1 M HF. As additives $(NH4)_2SO_4$, $CoSO_4$ and $FeSO_4$ were investigated.

XRD analysis shows that the addition of ammonium ions favours the formation of the hollandite phase, while Co^{2+} and Fe^{2+} promote the ramsdellite phase.

Besides the structure, also the morphology of the different doped samples varies. The ammonium ions favour the growth of nanoneedles in the hollandite phase, with a final diameter of about 12–24 nm. The further addition of cobalt ions in the range between 0 and 0.1 M reduces the size of the nanoneedles by almost a factor of two. Iron ions lead to the formation of aggregates with visible single acicular nanocrystals, which is consistent with the disappearance of the hollandite phase in XRD. The electrodeposition of lamellar microaggregates, covered with nanoneedles and nanowires, was also observed [2, 3].

Several synthesized materials are evaluated for their electrocatalytic activity for the oxygen evolution reaction (OER). Electrode inks are prepared and drop-coated as thin-film electrodes to be studied by rotating disk electrode (RDE). We optimized the protocol for electrochemical measurements on the RDE for these materials [4], and characterized the OER activity in alkaline and neutral media.

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BEDT-TTF molecular structural phases in dependence of doping molecule characteristics

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In this report, we describe a simple model of BEDT-TTF molecules. This model demonstrates how the doping molecules affect the alignment of BEDT-TTF molecules. This alignment is called a structural phase. Any change of the phase, which leads to the different positiont of molecules, is called a phase transition. This report is intended to explain a mechanism of this transition.

Firstly, the molecule is presented using the model of rectangular plates (see Fig.1). In this model a molecule in the shape of a rectangle parallelepiped is superimposed on the real structure of a BEDT-TTF molecule.

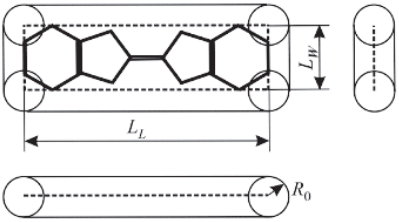

Fig. 1. The model of rectangular plates for BEDT-TTF molecules.

Secondly, we present three phases. These are the α-phase, the β-phase and the θ-phase [1], [2]. In the β-phase all molecules are placed parallel to each other. Introduction of a smaller charged molecules results in deflection of BEDT-TTF molecules and a slight increase of the equilibrium distance. This is caused by the quadrupole and electrostatic interaction between BEDT-TTF molecules and small dopants. These two types of interaction cause a molecular repulsion in BEDT-TTF.

In summary, the phase transition of the material occurs in order to stabilize the system and preserve its energy of intermolecular interaction.

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Novel photoswitchable azobenzene-based fluorinated aromatic polyether

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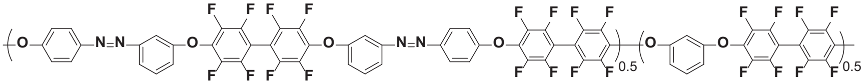
Among a number of functional poly(arylene ether)s (PAEs), azobenzene-based PAEs offer a versatile platform for developing thermo- and mechanically-stable materials with macroscopic properties that can be externally manipulated by light. Incorporating perfluorinated aromatic units into a polymer's structure not only enhances its chemical and thermal stability, but also upgrades its optical and electro-optical properties. However, the importance of fluorinated azo-containing PAEs (abbreviated as FPAEs) is still somewhat neglected in the literature, even though azo-free FPAEs themselves possess unique properties that are essential for effective functioning in modern high-tech applications.

In current work, a novel light-responsive FPAE copolymer with both azobenzene and perfluorinated biphenylene units as well as *meta*-linked fragments in the polymer backbone was developed:



The resulting copolymer exhibited complete solubility in chloroform, dimethylformamide, and dimethylacetamide, and was successfully cast into a flexible solid film (stress at break: 62 MPa; elongation at break: 5%; Young modulus: 1.45 GPa) using solution-casting techniques. Upon photoirradiation with typical UV light at 365 nm, photoisomerization occurred both in solution and in the solid film. Additionally, the copolymer film displayed light-induced birefringence changes when irradiated with polarized green light Azopolymer has potential as intelligent on-off photoswitches and in producing photonic elements, like gratings, polarizers, and plasmonic nanostructures. Its surface patterns can be used to microstructure or nanostructure other materials.

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Dielectric relaxation of solid water solutions of hydroxypropylmethylcellulose: the role of ions.

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We present the results obtained in the study of dielectric properties of water and NaCl-water solutions of hydroxypropylmethylcellulose. The dielectric permittivity at frequencies 5 kHz, 10 kHz, 20 kHz, and 50 kHz was measured for water and 0.9% NaCl-water solutions of HPMC with mass concentrations 0.1%, 0.4%, 2%, 2.5% and 3% in the temperature range from -190°C to 50°C.

All systems were found to undergo low-temperature dielectric relaxation. When HPMC is added to water, a hydration shell, affecting the network of hydrogen bonds in ice, is formed. Adding polymer impurities into ice leads to the increase in the entropy and energy of the activation process, shifting its maximum towards higher temperatures (Fig. 1).

When NaCl is added to water-HPMC system, ions in the solid state surround HPMC molecule and change the way hydration shell affects the network of hydrogen bonds in ice. These ions also affect the hydrogen bond network elsewhere in ice, shifting the relaxation process towards lower temperatures (Fig. 1).

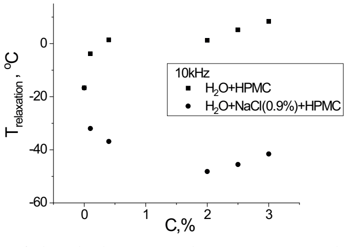

Fig.1 *Maxima of the dielectric relaxation at 10 kH for pure water, water-HPMC solution and water-NCl HPMC solutions of increasing concentrations.*

Conductivity and response formation of semiconductor gas sensors based on tin oxide nanomaterials

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The semiconductor sensors are widely used for detection of explosive and toxic gases leakages in air due to their high sensor response and low production cost [1]. Improvement of the main sensor characteristics (sensitivity, selectivity, stability, power consumption and other parameters) is a main task during development of new semiconductor nanosized gas sensitive materials for the sensor layers that are able to change amount of chemisorbed oxygen on their surfaces. The chemisorbed oxygen is known to be responsible for the sensitivity of the sensor because the oxygen is involved in the catalytic oxidation of the target gas molecules on the semiconductor surface [2]. In this work highly sensitive to methane semiconductor sensors were obtained with the use of nanosized tin dioxide synthesized via sol-gel technique. Experimental data of dependences of conductivities of the created sensors were used for approximation by a simple mathematical model of the sensor conductivity and its response formation mechanism. The model is based on features of gas oxidation reaction on the surface of the gas sensitive material and allows to connect sensor conductivity with surface processes occurred on its gas sensitive layer. The relationship between the oxygen surface coverage and gas content in air was used in the model of the sensor response formation.

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Surface modification for improving mechanical properties and corrosion behaviour of low carbon steel

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The influence of cationic and anionic surfactants and their binary synergistic mixtures on acid corrosion of steel has been investigated. The impact of corrosion process and combined multifaceted effect of application of synergistic binary mixtures on the mechanical properties of steel such as plasticity and microhardness of the surface layers during acid etching have been evaluated.

Divers synergistic compositions with oppositely charged functional groups are found to be more efficient compared to individual additives. Such binary mixtures tend to exhibit peak protective efficiency at molar concentration as 1:1 owing to the inhibition of both anodic and cathodic partial reactions. High protective efficiency peaks are also in line with improved mechanical properties of the samples.

Thermodynamic parameters of the studied systems within a synergistic extrema have also been evaluated and found to be in line with the protective efficiency and influence on the mechanical properties. Overadditive reduction of the surface tension on the air-solution interface, an increase in enthalpy ($\Delta H>0$, endothermic process), as well as an increase in the entropy of the system ($\Delta S>0$) has been observed at molar concentration ratio of the mixture components as 1:1.

The plasticity of the steel samples etched in the presence of the binary inhibitive mixtures are found to be improved both compared to blank acid solutions as well as compared to the state of delivery owing to reduced microhardness of the surface layer.

Phase change materials based on vitreous $Ge_{15}Sb_{40}S_{15}Se_{15}Te_{15}$

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Phase-change materials (PCMs) are known for their unique behavior during switching between the amorphous and crystalline states. Rapid and reversible transitions between highly resistive and conductive states occurring at moderately elevated temperatures is especially intriguing for new-generation devices. Thus, we introduce a new class of PCMs based on equichalcogenides - $Ge_{15}Sb_{40}S_{15}Se_{15}Te_{15}$.

In this work, a thermally-induced High-to-Low resistivity switching below 200°C is demonstrated in this glass. The nanoscale mechanism is associated with the interchange between tetrahedral and octahedral coordination of Ge and Sb atoms, substitution of Te in the nearest Ge environment by S or Se, and Sb-Ge/Sb bonds formation upon further annealing. According to DSC scans, the heating of the as-deposited thin films above 175°C leads to the crystallization of several phases at ~200°C and ~300°C. The XRD reflexes of these phases coincide with $GeSb_4Te_7$, Sb_2SeTe_2 and Sb_2Se_2Te crystallites, as well as some unidentified reflexes presumably $GeSb_4Te_7$, GeSTe (Fig. 1). The material can be integrated into chalcogenide-based multifunctional platforms, photonic devices and sensors.

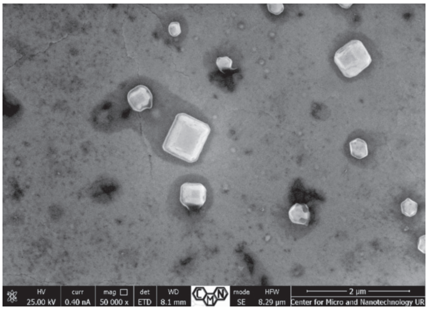

Fig. 1. *SEM image of crystallites formed on the surface of the film after annealing at 340°C*

Comparison of adsorption affinity of the plant derived activated carbons toward ionic polymers and heavy metal ions

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The nettle, sage, lemon balm and mint herbs were used for activated carbons preparation. In the first step the raw plant material were dried and cut into 1.5-2.0 cm pieces, and next subjected to simultaneous pyrolysis and chemical activation process. At the beginning the samples were impregnated for 24 h with 50% phosphoric(V) acid solution, at the precursor-activating agent weight ratio equal to 1:2. Then, the samples were dried at 110°C, next placed into the quartz boats and heated in a nitrogen atmosphere. In the first stage, the samples were heated to the temperature of 200°C at a rate of 5°C/min. Then, the materials were annealed at that temperature for 30 min. In the next step, the materials were heated to the final activation temperature of 500°C and again annealed for 30 min. After that time, the samples were cooled down to room temperature in a nitrogen flow.

The carbonaceous materials obtained differ considerably in the textural parameters. However, they can be all classified as mesoporous materials with well-developed surface area. The activated carbons obtained from the mint herb is characterized by the greatest specific surface area (1146 m^2/g), whereas the one derived from the nettle herb - with the smallest one (801 m^2/g).

The obtained carbonaceous materials were used as poly(acrylic acid), polyethylenimine, As(V) and Cd(II) adsorbents from single and binary solutions. The results proved that the precursor type has a significant impact on the activated carbons adsorption capacities toward examined substances. The macromolecules of both polymers exhibit the greatest affinity to the surface of materials derived from the mint and lemon balm herbs. In the case of metal ions, Cd(II) is greater adsorbed substance on the surface of all examined activated carbons than As(V). The presence of polymers have negative influence on the adsorbed amount of both metals. The impact of Cd(II) and As(V) on macromolecules adsorption is less noticeable.

Studies of indium nanostructures growth models on A^3B^6 layered template

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The A^3B^6 layered crystals structure [1] and morphology of indium nanostructures on A^3B^6 layered templates has been extensively studied in the last years [2,3]. The properties of a growing surface layer are closely related to its quantitative parameters, such as roughness, skewness and kurtosis. This makes it possible to determine the preferable models of growth while formation of nanostructures and in turn models of growth are very powerful tools that can help to predict and control properties of new hetero nano systems.

The growth kinetics of In deposited nanostructures on surfaces of 2D A^3B^6 layered semiconductor crystals was studied by Omicron NanoTechnology STM/ AFM System with acquiring of surface roughness parameters from a large scale 1x1 μm² images. In fact, the surfaces of the chalcogenide layered semiconductors, such as, In_4Se_3 InSe, InTe, Sb_2Te_3 were used as templates. We managed to estab-lish that the growth modes in the thermally deposited indium coating, and resulting formation heterogeneous metal-semiconductor nanostructures' arrays are determi-ned by the sequence of experimental procedures, namely: indium deposition, heating of the deposited layer, as well as the amount of In deposit on the surface.

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Peculiarities of phase composition, microstructure, and high-temperature (600–700°C) fracture toughness of Ti–Al–Cu composite

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Among advanced Ti-based composites, Ti–Cu–X alloys have an advantage in high-temperature electrical conductivity. Due to comparatively high electrical conductivity at elevated temperatures, their application area can include spring electrical contacts of power equipment and bipolar plates of solid oxide fuel cells (SOFCs).

This work is aimed at studying the phase composition, microstructure, and high-temperature (600–700°C) fracture toughness of Ti–Al–Cu composite. Ingots of the composite were prepared by melting in a vacuum induction furnace. The following phase fractions were determined using X-ray diffraction analysis of the composite: Ti_2Cu (58.3 wt%), TiCu (37.5 wt%), Ti_3Cu (4.2 wt%). Bar specimens were prepared by electric-discharge cutting of ingots, grinding, and polishing. The specimens with a sharp edge notch was undergone the fracture toughness test in a wide temperature range (20°C to 700°C). Based on the test results, it was concluded that Ti–Al–Cu composite is promising for applications in lightweight intermediate temperature (600–700°C) SOFC components.

Studies on microstructure and high-temperature (600–700°C) mechanical stability of Ti–Al–Mn–Si composites

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It is well known that $TiMn_2$-based alloys are widely used as high hydrogen storage materials. The purpose of this work was to study temperature-dependent mechanical behavior of Ti–Al–Mn–Si composite in which the Hexagonal Laves phase $TiMn_2$ dominated. The role of β-Ti content in improving microstructure and high-temperature (600–700°C) mechanical stability in terms of fracture toughness of the composite was also explored.

Ti–Al–Mn–Si composite was prepared by melting in a vacuum induction furnace. The X-ray diffraction analysis of Ti–Al–Mn–Si composite revealed two phases, namely β-Ti and $TiMn_2$ The phase fractions were as follows: β-Ti (18.26 wt%), $TiMn_2$ (81.74 wt%). Therefore, the last one dominated in material microstructure, and this was confirmed by the scanning electron microscopy analysis. Beam specimens were cut of ingots, grinded, and polished. Single-edge notch beam fracture toughness test of specimens was performed in a temperature range of 20°C to 700°C. It was revealed that fracture toughness of the composite is in a strong relation to its microstructure and phase composition. In particular, high-temperature (600–700°C) mechanical stability was attributed to the appropriate failure micromechanism. Therefore, the studied Ti–Al–Mn–Si composite is promising in terms of fracture toughness for high-temperature applications.

The effect of phase composition on microstructure and high-temperature (700–800°C) fracture toughness of Ti–Al–Fe composites

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Ti–Al–Fe composites attract the attention of researchers due to their high-temperature stability which is close to that of Cr–Ni and Fe–Cr–Al alloys. It is known, in particular, that Ti–Al–Fe composite of an appropriate chemical composition exhibits increased fracture toughness at high (700–800°C) temperatures. Thus, it is reasonably to consider such a composite for application in some critical components of state-of-the-art power equipment, in particular, bipolar plates of solid oxide fuel cells (SOFCs). This work is aimed at studying the impact of alloying elements Al and Fe on the phase composition, microstructure, and high-temperature fracture toughness of Ti–Al–Fe composites.

Materials of two chemical compositions (Ti–1.6 wt% Al–39 wt% Fe and Ti–0.6 wt% Al–79 wt% Fe marked as composite 1 and composite 2, respectively) were manufactured by melting using electric arc furnace. Fracture toughness tests of specimens with a sharp edge notch were carried out in a temperature range of 20°C to 800°C. It was found that composite 1 contained two phases, namely β-Ti (39.12 wt%) and $Ti_{50}Fe_{50}$ (60.88 wt%). Composite 2 contained α-Fe (45.84 wt%) and $TiFe_2$ (54.16 wt%). Drastical changes in microstructure of composite 2 resulted in a significant drop of its high-temperature fracture toughness.

Therefore, Ti–Al–Fe composite containing both the β-Ti and $Ti_{50}Fe_{50}$ phases can be regarded as promising for applications in lightweight intermediate temperature (550–650°C) SOFC components.

Improvement of the long-term strength and operating life of Ti-based composites for high-temperature applications

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Novel Ti-based composites are being developed for applications in power equipment and modern rocket and aircraft engines as they provide low specific weight simultaneously with high fracture toughness and strength in a temperature range of 20–700°C. In this work, the creep behavior of Ti–Si–X composites aimed at high-temperature applications in power equipment was investigated. The material of Ti–Si–X system (X=Zr and/or Al) was produced by melting using electric arc furnace with the addition of fine alloying elements. Three variants of the material, which differed in silicon and aluminum content, were obtained. Billets of material after casting were machined to prepare cylindrical specimens. Creep tests of specimens were performed at temperatures of 600°C, 700°C, and 800°C in air at various levels of engineering stress. It was found that at medium levels of engineering stress, all materials demonstrated classical creep behavior, and the creep curve contained three characteristic sections: deceleration, steady-state creep, and accelerated failure. Average creep rates for the applied levels of engineering stress were determined in the sections of steady-state creep. Based on the fracture analysis of the specimens, characteristic patterns of temperature-dependent creep of Ti–Si–X composites were noted. Using XRD analysis, the phase content and percentage of the main phases were determined and consolidated with the creep parameters (stress, creep rate) for the corresponding composites. The dominant micromechanisms of strengthening and the role of silicides in achieving appropriate levels of long-term strength and increasing the operating life of the Ti-based composites aimed at high-temperature applications are discussed.

Impact of microstructure on the mechanical behavior of Ti–Al–Ni composite in a wide temperature range (20–800°C)

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Titanium based composites are widely used for manufacturing critical high-temperature components of rocket and aircraft engines as well as power generation equipment. They have advantages over conventional titanium alloys in operating temperature which can be higher by 150–350°C exhibiting thus improved temperature stability and comparatively high fracture toughness at elevated temperatures. Therefore, they can operate in a temperature range of 20°C to above 700°C. This work is aimed at studying the effect of microstructure on mechanical behavior of Ti–Al–Ni composite in a wide temperature range (20–800°C).

Ti–Al–Ni composite was manufactured by melting using electric arc furnace. Chemical composition of the material was as follows: Al (1.8 wt%), Ni (40 wt%), Ti (balance). Single-edge notch beam specimens were cut of ingots, grinded, and polished to reach a satisfactory surface quality. Then, a fracture toughness test of specimens was performed in a temperature range 20–800°C. The microstructure and fractographic studies were carried out using a scanning electron microscope. The phase composition of the material was also estimated. Peculiarities of a temperature-dependent change in fracture toughness of the composite were then analyzed and related to its microstructure and fracture micromechanisms. A significant increase in fracture toughness of the material was revealed in a temperature range of 700–800°C. The role of separate phases in reaching such a high level of fracture toughness for Ti–Al–Ni composite was discussed. This material is regarded to be promising for high-temperature (700–800°C) applications.

Microstructural features causing an increase in high-temperature (700–800°C) fracture toughness of Ti–Cr–Al–X composite

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Lightweight titanium composites are considered as high-temperature materials for production of various components in aircraft and power generation industries. They can operate in a temperature range of 20–700°C, which is higher by 100–300°C than the operating temperature of conventional titanium alloys. In addition, these composites exhibit perfect temperature stability at elevated temperatures. The purpose of this work was to investigate the influence of test temperature on fracture toughness of Ti–Cr–Al–X composite and estimate changes in corresponding fracture micromechanisms.

Ingots of Ti–Cr–Al–X composite containing Cr (41 wt%), Al (1.5 wt%), C (5 wt%), and Ti (balance) were prepared by melting using electric arc furnace. Bar specimens were cut of ingots, grinded, and polished. Then, a sharp edge notch was machined in each specimen. Fracture toughness tests of specimens under three-point bending were carried out at temperatures of 20 to 800°C. The SEM microstructure and fractography analyses of examined specimens were performed. The X-ray diffraction analysis of the material was carried out and phase balance was evaluated. At temperatures up to 600°C, no discernible change in fracture toughness of Ti–Cr–Al–X composite was found (the average value of this parameter was about 5 MPa•m$^{1/2}$). A steep increase in fracture toughness up to 19.5 MPa•m$^{1/2}$ at 800°C was found to be a result of a change in the fracture micromechanism. Microstructural features causing an increase in high-temperature (700–800°C) fracture toughness of Ti–Cr–Al–X composite were suggested. In particular, the impact of the MAX phase and carbide phases was discussed.

The effect of low-frequency oscillation on the physicochemical characteristics of the industrial methanol synthesis catalyst

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The aim of our work was to study the morphological and structural properties of the industrial methanol synthesis catalyst trademark CHM-Y before and after exposure to low-frequency oscillations in situ. The samples were examined by various methods, including XRD, FTIR-ATR, DTG/TGA, DSC, low-temperature adsorption-desorption of N_2, SEM.

According to the XRD data, after the classical process, an increase in the size of the copper crystallite to 13.3 nm is observed compared to 12.7 nm for the original reduced CHM-Y. Interestingly, the crystallite size after low-frequency oscillations decreased to 10.3 nm. The FTIR-ATR spectra for the original and spent catalyst have almost the same appearance. The DTG method shows two sharp increases in the mass of the catalyst sample after low-frequency oscillations, corresponding to peaks at 147°C and 240°C, which may indicate the oxidation of copper to Cu_2O and CuO. The DTG peak at 485°C may correspond to accumulated carbon. This is also consistent with the XRD results, where the peak at 26.5° is attributed to the (002) plane of graphite. According to DSC, the use of low-frequency oscillations makes it possible to obtain reduced reactive Cu^0 at 145 °C against 165 °C after the classical process. The method of low-temperature adsorption-desorption of N_2 shows that all catalyst samples have an isotherm with a type IV hysteresis loop, which indicates the presence of mesopores. It was established that the pore volume of the recovered CHM-Y and after low-frequency oscillations is practically the same (0.22 and 0.23 cm^3/g, respectively), in contrast to the sample after the classical process (0.27 cm^3/g). It was found that similar values of the specific surface have the samples of reduced CHM-Y (72.1 m^2/g) and after low-frequency oscillations (71.7 m^2/g) in contrast to the catalyst after the classic process (66.5 m^2/g).

Oxidation of dihydrogen with oxygen over Pt/Niobia-phosphate aerogel catalysts

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The development of alternative energy involves finding ways of fuel switching to biofuel, biogas or dihydrogen-sourced fuel for the restructuring of energy-intensive industries. It should be mentioned that from an economic point of view, hydrogen fuel is the most promising alternative energy source among those available.

However, hydrogen release and subsequent accumulation of flammable dihydrogen-oxygen gas mixtures may occur during the operation of the hydrogen source engine. Therefore, for safety reasons and according to the paradigm of clean-up technology, platinum and palladium catalysts that operate with dihydrogen-air gas mixtures at low temperatures and low hydrogen concentrations can be used to recombine hydrogen leaks. To operate these converters, new highly active catalysts for the dihydrogen oxidation with oxygen should be developed.

The use of such a catalyst in the recombining converters could improve the recombination efficiency and reduce the severity of H_2 leaks to an acceptable risk level. Dihydrogen oxidation over PGM/Niobia-phosphate aerogel catalysts synthesized by aerogel drying methods, and PGM/alumina (PGM = Pt or Pd) catalysts has been investigated. The reaction performance in the presence of PGM/Niobia-phosphate aerogel catalysts for the H_2 oxidation with hydrogen is higher than that of PGM/alumina catalysts. It has been suggested that the enhanced activity of PGM/Niobia-phosphate aerogel catalysts is due to the interplay between Nb^{4+}/Nb^{5+} states in the solid matrix, which affects the oxygen activation on the catalyst surface.

The structures of the tested catalysts were investigated before and after exposure to the catalytic process by XRD, SEM, XPS and N_2 adsorption methods. The method of surface acidity analysis with probes adsorbed on the surface of the PGM/Niobia-phosphate aerogel catalysts was used to estimate the possible reaction mechanism.

Decorating carbon nanotubes with CdTe nanoparticles

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Many areas of nanotechnology application, especially in the creation of biomedical devices and sensors, require the creation of interfaces (transitional structures) that connect nanomaterials or nanoobjects with microscopic devices or tissues. One of the approaches to creating such interface nanostructures is the use of carbon nanotubes, modified with various nanoparticles (NP).

In this work, a microwave irradiation method, which is widely used to activate or accelerate chemical reactions, was used to modify COOH-functionalized single-walled carbon nanotubes (SWCNT) with CdTe nanoparticles stabilized by thiols.

The SWCNT with diameter about 1.5 nm were dispersed in separate containers in 1 ml of deionized water and 1 ml of CdTe NP suspension was added. The size of CdTe NP was about 2.6 nm. After that the containers were closed and loaded into a microwave equipped with a 700 W magnetron operating at 2.45 GHz. To minimize overheating of the solvent and increase the pressure in the closed vial, cyclic microwave exposures were performed with an on time of 30 s at 100% power, separated by 10-s off time intervals, with a total duration of 2400 s. The study of changes in the electronic structure of the samples was carried out by X-ray photoelectron spectroscopy (fig. 1). It was found that for SWCNT, the 1s spectrum of oxygen is characterized by two peaks at 531 eV and 533 eV, which correspond to the chemical bonds C O and C—O, respectively. During the interaction of SWCNT with CdTe NP, a significant decrease in the intensity of the peak responsible for the C—O bond is observed. This reduction is due to the decrease in the number of C—O bonds because of the formation of carbon bonds with CdTe nanoparticles.

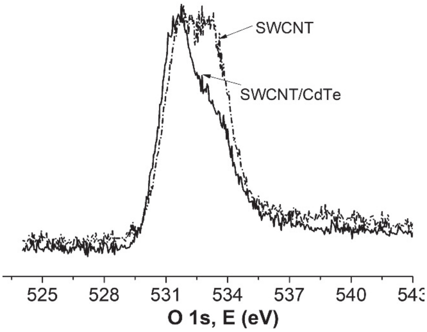

Fig. 1. *XPS O1s spectra of the samples*

Nanogold catalysts of dihydrogen oxidation in oxygen-rich gas-mixtures

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Gold NPs are considered to be a highly efficient candidate for heterogeneous catalysis. It is well known that Au NPs supported on reducible materials are more reactive than non-reducible materials unless specific modifications are made. However, non-reducible materials such as carbon materials, silica, and alumina have special advantages, including easily controlled surface properties, tunable microstructure, abundant reserves, and easy industrial fabrication. New strategies, influences and modification mechanisms to improve the catalytic performance and thermal stability of gold catalysts supported on non-reducible materials are among the most attractive research topics in gold catalysis.

However, to the best of our knowledge, reports & reviews focusing on gold catalysts for hydrogen oxidation in oxygen-rich gas mixtures supported on non-reducible materials are lacking. Herein, we discuss in detail several typical non-reducible supports, including the commonly used silica, alumina, carbon materials, and hydroxyapatite.

The currently prevailing modification strategies are summarized in detail from the aspects of theoretical conceptualization and practical methodology, including the ingenious synthesis method for catalysts with specific structure, and adsorption vs. colloidal immobilization with future thermal treatment in gas flow. The effects of physical and chemical modifications on the surface chemistry, electronic structure, Au support/promoter interaction/synergy, catalyst morphology, and water precipitation are also summarized. We will highlight important studies on unreduced supports in gold catalysis for catalytic promotion and anticipate the potential industrial demand for such catalytic materials. Furthermore, we will provide new insights into unreduced supports that can potentially be used as supports in gold catalysis.

Electrical properties of photosensitive n-$MnFe_2O_4$/n-CdTe heterojunctions

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Thin films of manganese ferrite $MnFe_2O_4$ grown by spray pyrolysis have a band gap $E_g \approx 2.1$ eV [1]. This value is in the range between the values for transparent conducting oxides (TCO) ($E_g > 3$ eV) and for effectively light-absorbing semiconductors (1.1 eV $< E_g <$ 1.6 eV), such as CdTe ($E_g \approx 1.5$ eV). Materials with energy parameters similar to $MnFe_2O_4$ are successfully used as a buffer layer in CdTe-based heterostructures. In this case, the material of the buffer layer forms a high-quality heterojunction with the base semiconductor.

The n-CdTe substrates with electrical conductivity $\sigma = 1.4\ \Omega^{-1}\cdot cm^{-1}$ were used to manufacture n-$MnFe_2O_4$/n-CdTe heterojunctions. The n-$MnFe_2O_4$ films with a thickness of $w \approx 0.5$ μm were deposited onto the n-CdTe surface by spray pyrolysis from 0.1 M aqueous solutions of $CoCl_2{\bullet}6H_2O$ and $FeCl_3{\bullet}6H_2O$ salts.

The current rectification factor of the n-$MnFe_2O_4$/n-CdTe heterojunction at $T = 295$ K is 10^4 at the voltage $|V| = 2$ V. The main component of the series resistance (RS ≈ 900 Ω) in the structure is a high-resistance n-$MnFe_2O_4$ film ($\rho \approx 10^6\ \Omega{\bullet}cm$).

In the region of forward biases $3kT/q < V < 0.36$ V of the n-$MnFe_2O_4$/n-CdTe heterojunction, the tunneling-recombination current flow mechanism is realized, which, at voltages $V > 0.36$ V, passes into recombination in the space charge region (SCR) with a diode coefficient A ≈ 2. At reverse biases in the voltage range -2.5 V $< V < -3kT/q$, the main mechanism of current generation is the generation of charge carriers in the SCR. The C-V-characteristics of the n-$MnFe_2O_4$/n-CdTe heterojunction are characterized by their frequency shift along the capacitance axis due to the presence of series resistance in the structure. The contact potential difference at the heterojunction determined using the dependences $C^{-2} = f(V)$ is $\varphi_k = 0.92$ V. The n-$MnFe_2O_4$/n-CdTe heterojunction generates ~0.56 V at 12000 lux illumination. The photocurrent density is 100 μA/cm². The fabricated heterojunctions are suitable for use as photodetectors of visible radiation.

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Potential of activated carbons from various sources as a low cost adsorbent to remove liquid and gaseous pollutants

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The main toxic gases emitted to the atmosphere are oxides of nitrogen, sulfur and hydrogen sulfide. They destroy the ozone layer, contribute to smog and hothouse effect so with the phenomena of great global concern [1]. On the other hand, we have to face the deterioration of the quality of water that is too intensive to be dealt with the natural self-cleaning processes [2]. Technological processes of removal of gas and liquid pollutants are usually very expensive so the search for cheaper methods is continued. Of particular interest are the methods based on adsorption and a large group of effective adsorbents are carbon materials, and among them activated carbon.

The primary objective of this study was to obtain a series of activated carbons by chemical and physical activation of residues after supercritical extraction of raw plants and to check the ability of the materials prepared to remove gas pollutants (NO_2 and H_2S) and liquid pollutant (crystal violet). Different experimental parameters, like contact time and solution concentration, were tested to identify their effects on crystal violet adsorption. Additionally, different isothermal models were analyzed with adsorption data to explain the mechanism of the adsorption process. Adsorption kinetics was studied by fitting the data with interparticle pseudo-first-order and pseudo-second-order kinetic models. Another series of experiments was performed to assess the effectiveness of the obtained activated carbons as adsorbents of gas pollutants. The effects of variant of adsorption process on the physicochemical and sorption properties of the activated carbons were also examined.

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Effect of impregnation ratio on physicochemical and sorption properties of biocarbons obtained by chemical activation

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Activated carbon is a highly utilized adsorbent for water treatment due to its exceptional sorption properties and developed specific surface area, which effectively eliminates pollutants such as organic compounds, heavy metals, and chlorine. However, the efficiency of the adsorption process is dependent on the physicochemical properties of both the adsorbate and the adsorbent. The adsorbate's specific surface area, surface chemistry, and pore size are critical factors that influence the adsorption process. Moreover, the precursor materials used to create activated carbon must have a high mass percentage of elemental carbon, be readily available and inexpensive, and have low mineral content and minimal biodegradability during storage [1]. Several properties of the adsorbate can also influence the adsorption process. Factors such as the concentration of the adsorbate, the size of its molecules, polarity, pH, temperature, and contact time can all play a significant role in determining the extent of adsorption onto the adsorbent surface. These properties interact with the characteristics of the adsorbent material to affect the overall efficiency of the adsorption process.

The aim of the study was to obtain a range of biocarbon from waste biomass (fennel seeds) by chemical activation using different impregnants such as sodium and potassium carbonates and different precursor:activator ratios. The study involved the determination of the specific surface area, iodine number, and sorption capacity of the obtained materials against organic impurities from the liquid phase. Additionally, the impact of pH and temperature of the aqueous solution on the sorption capacities of the biocarbon materials was assessed. Furthermore, the constants for the Langmuir and Freundlich adsorption models were calculated, and the kinetic model of adsorption was determined.

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Peculiarities of primary nanocrystallization of Al-V and Al-Hf alloys

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The progress of the aerospace industry stimulates the search for new metal alloys with both large plasticity and durability. It is known, these properties depend both on the phase composition of the alloys and on the grain size. As it was shown in many works [1-3], reduction of the grain of aluminum and aluminum alloys occurs after adding a small amount of vanadium, hafnium, zirconium, chromium. As it was established, the reduction of grains is due to the heterogeneous crystallization of aluminum on the crystal nuclei, which are the Al_3V, $Al_{10}V$, Al_3Hf compounds. However, in most cases, only the resulting effect of impurities on grain size has been investigated, without studying the process of formation of crystallization nanocenters, which affect the final grain size distribution.

In this regard, the mechanism of formation of nanocrystallization centers in Al-Hf and Al-V alloys from the liquid state was investigated in this work. Research on nanocrystallization was studied by the method of molecular dynamics simulations and by means of experimental methods. As a result of the work, the optimal conditions for the crystallization of alloys to obtain a dispersed structure with improved mechanical properties were established.

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Application of various reduction techniques for the improvement of microstructure and strength of YSZ–NiO(Ni) solid oxide fuel cell anodes

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Recently, solid oxide fuel cells (SOFCs) as devices for production of green energy are being intensively developed. An anode substrate used in such devices is predominantly fabricated by conventional powder sintering or tape casting of yttria stabilized zirconia/nickel oxide (YSZ–NiO) ceramics. The as-sintered YSZ–NiO anode ceramics should be preconditioned via reduction of NiO to Ni in a hydrogen-containing atmosphere. This also ensures appropriate level of electrical conductivity of SOFC anodes. This work is aimed at studying both the effects of preconditioning in a high-temperature (600°C) reduction atmosphere and cyclic treatment in reduction/oxidation atmospheres (redox cycling) on strength of YSZ–NiO(Ni) cermets.

The specimens of size of $0.5 \times 5 \times 25$ mm^3 were cut of 0.5 mm thick YSZ–NiO ceramic plates. The preconditioning modes were as follows: (i) one-time reduction in Ar–5 vol% H_2 mixture for 4 h at 600°C under a pressure of 0.15 MPa; (ii) redox treatment for three cycles in Ar–5 vol% H_2 mixture/air (each stage was 4 h) at 600°C with intermediate degassing. A part of specimens were then aged for 100 h at 600°C in Ar–5 vol% H_2 mixture under a pressure of 0.15 MPa. A series of as-sintered YSZ–NiO ceramic specimens and YSZ–NiO(Ni) cermet specimens after treatments were tested under three-point bending. Scanning electron microscopy was used to analyze peculiarities of changes in microstructure and fracture surface morphology of aged materials.

It was revealed that one-time reduction in Ar–5 vol% H_2 mixture followed by exposition for 100 h under such conditions did not cause a discernible change in mechanical behavior of the material. In particular, flexural strength of the cermet lowered by 12–15% as compared to that of as-sintered ceramics. In contrast, specimens after redox treatment followed by aging for 100 h exhibited significant drop in flexural strength (by about 33–40%). Features of microstructure degradation were substantiated based on a developed pore coalescence model of damage accumulation.

The effect of hydrogen concentration on the high-temperature (600°C) reduction performance and strength of YSZ–NiO(Ni) anode material for solid oxide fuel cells

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A ceramic material based on yttria stabilized zirconia and nickel oxide (YSZ–NiO) is widely used for fabrication of solid oxide fuel cell (SOFC) anodes. To make such anode ready for operation in a SOFC, corresponding treatment in a reducing atmosphere should be performed ensuring NiO to Ni reduction that provides electrical conductivity of the anode. The aim of this work is to study the effect of hydrogen concentration on the high-temperature (600°C) reduction performance and strength of YSZ–NiO(Ni) anode material. To obtain the corresponding YSZ–NiO(Ni) cermet structures, a series of YSZ–NiO ceramic specimens were reduced in various hydrogen-containing atmospheres for 4 h at 600°C under a pressure of 0.15 MPa. The atmospheres were as follows: (i) Ar–5 vol% H_2 mixture; (ii) pure hydrogen (99.99 vol% H_2). After reduction, the physical and mechanical behaviours of specimens were studied. Three different mechanical tests were performed: Vickers microhardness test, fracture toughness test by indentation method, and strength test under three-point bending. Microstructure of the cermets and fracture surface morphology of the specimens underwent the strength test were studied using scanning electron microscopy.

It was found that Ar–5 vol% H_2 mixture provided slow reduction of ceramic specimens with formation of thin fringes which cover nickel oxide particles. Exposure for 4 h at 600°C in this atmosphere did not ensure complete reduction of the nickel phase particles.

In contrast, specimens reduced in pure hydrogen exhibited distinct microstructure of completely reduced nickel particles. Energy dispersive X-ray microanalysis did not show any sign of nickel oxide in this cermet. However, comparatively low flexure strength, Vickers microhardness, and fracture toughness were determined for this material. In comparison, these mechanical charateristics were found to be higher for the cermet reduced in Ar–5 vol% H_2 mixture.

Synthesis and characterization of synthetic iron-modified mesoporous carbons: adsorption of phosphate ions from liquid phase

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Synthetically derived ordered mesoporous carbon (OMC) is a fascinating carbon material with precisely defined pore sizes ranging from 2 to 50 nm. OMC exhibits a high specific surface area, excellent thermal stability, and various oxygen-functional groups, making it a versatile material of interest. The key advantage of OMC lies in its well-structured mesoporous channels, which enable superior pollutant adsorption compared to natural activated carbons that have convoluted pore structures [1].

OMC synthesis offers the flexibility to tailor specific properties such as pore size and surface area, allowing for the design of customized sorbents for various applications. In this study, OMC and iron-modified OMC were synthesized using the hard templating method, with mesoporous silica KIT-6 serving as the matrix and sucrose as the carbon source. Iron incorporation was achieved by introducing appropriate amounts of iron salts during the synthesis process [2].

Comprehensive physicochemical characterization was performed to assess the obtained carbons, including determination of specific surface area, mesopore size, and structural confirmation using X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) analyses. Furthermore, the adsorption capacity of the materials for phosphate ions from aqueous solutions was evaluated. Langmuir and Freundlich adsorption models were utilized to calculate adsorption constants, providing insights into the sorption behavior of the materials.

Overall, this study highlights the unique properties and potential applications of OMC and iron-modified OMC, demonstrating their efficacy as promising materials for pollutant removal and other tailored sorption processes.

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Phase stability of nanostructured SiC ceramics under irradiation

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The study of ionic implantation effects in SiC is important because SiC is a wide-bandgap semiconductor and is used as a material for the first wall of thermonuclear reactors. It is also considered for applications in fuel matrices, twell shells, and other high-temperature structural components in advanced nuclear reactors. While the radiation stability of SiC has been extensively investigated in recent years, our understanding of it is still incomplete [1].

Our objective is to investigate how the saturation of vacancies induced by radiation affects the amorphization process and phase stability of 3C-SiC. The thermodynamic approach relies on calculating the Gibbs free energy for various phase states involving vacancy-type defects. Additionally, we consider the size dependence when estimating the concentrations of radiation-induced vacancies [2].

We explain the radiation stability of 3C-SiC by considering two competing effects: (i) the smaller grain size reduces the accumulation of vacancies inside each grain, thereby lowering the overall free energy; (ii) the decrease in grain size leads to an increase in the interphase surface area between the grains and in the free energy.

It is obtained that at a speed of defect generation $4\text{x}10^{-6}$ dpa/s (parameters of irradiation 2 MeV ions with fluency of about $1\cdot10^{15} - 2\cdot10^{16}$ ions/cm^2 for a temperature interval of 600-1500K zone of radiation stability (absence of amorphization) 3C-SiC corresponds to grain sizes less than 25-30 nm.

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Electrochemical bubble transfer of Graphene and optoelectrical characterization

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The first two-dimensional (2D) material that was obtained is Graphene (Gr), which is known for its unprecedented physical, mechanical, and thermal properties that often surpass similar properties of other materials. However, practical utilization still requires additional study.

To development biosensor (field-effect transistor - FET) was used high-quality Gr purchased in the company (6Carbon, Shenzhen, China). The Graphene layer from Cu foil on a SiO_2/Si substrate was transferred by the bubble method. Electrochemical bubbling transfer of Gr is a technique with high industrial potential due to its scalability, time and cost-effectiveness, and eco-friendliness. The Gr/Cu was spin-coated with poly-methyl methacrylate at 2000 rpm for 30 s and dried in air for 10 min, then put into the oven and dry for 30 min. 2 M NaOH aqueous solution was used in the electrolyte for constant current and voltage 2.3 V. The platinum wire electrode was 0.5 mm in diameter. The delaminated Gr/PMMA film was transferred to SiO_2/Si substrate. The transferred Gr was heated at 150°C for 5 min and then cleaned in acetone for 14 h and was washed in Deionized water.

Fig. 1 (a-b) shows that a complete and clean Gr monolayer film was transferred by electrochemical bubbling. It should be noted that the Gr/PMMA layer was separated from the Cu within seconds, achieving efficient transfer of graphene. The Raman spectrum confirms the high-quality transferred Gr layer. Fig. 1 (c-d) shows that a FET prepared with Gr film have a good electrical signal.

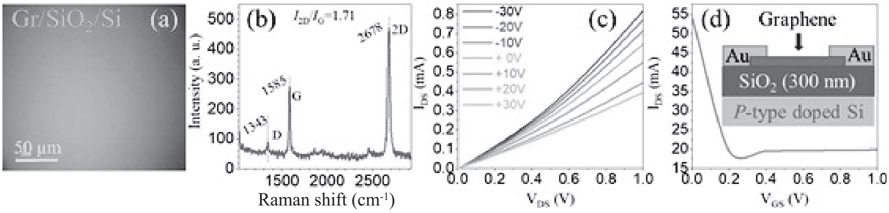

Fig. 1. *(a) Optical image of the Gr/SiO_2/Si sample surface. (b) Raman spectra of Gr with 532 nm laser excitation. (c) Output I-V characteristic curves within the bias ranging from -30 V to +30 V and (d) the transfer I-V characteristic curve at VDS = 1V. Inset: schematic of the device.*

Titanium-based alloys with a silicide nanophase

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The manufacturing of titanium and its alloys is a very important task, in particular for medicine use, due to its biological inertness and corrosion resistance. However, titanium itself is not robust, and the specific medical requirements are disallow to use traditional methods of its increase. Nowadays perspective and advanced work is aimed at the create of new titanium alloys without any toxic metals to replace traditional medical Ti_6Al_4V. This work proposes to do this by alloying titanium with Nb, Zr and Si, which increases its robustness and save the required plasticity.

The manufacturing of TiNbZrSi alloys ingots was by the method of melting on an electron beam unit by double remelting with using an intermediate container. The initial materials were sheet titanium, niobium and zirconium rods, lumped silicon. For high-quality fusion and homogeneity, small pieces of 40x40 mm, 2-7 mm thick were used. The amount of silicon in all samples was 0.9-1.1 wt.%, because its increase led to a dramatic decrease in plasticity. In one group of samples with 11-13 wt.% niobium and in another with 18-20 wt.% amount of zirconium varied from 1.9 to 15.2 wt.%.

As a result of the study of the structure, chemical and phase composition, as well as mechanical and corrosion characteristics of alloys of the Ti-Zr-Nb-S system, it have been fined the optimal content of alloy components, which causes the highest mechanical properties in the cast state. Studies of these titanium alloys were carried out in a wide range of concentrations of zirconium (1.9-15.2 wt.%) and niobium (11-20 wt.%). It was established that the optimal composition is 18-20 wt.% Nb, 1.9-2.2 wt.% Zr, and 0.9-1.1 wt.% Si. This method have been achieved the highest values of strength limit of 900-950 MPa, yield strength of 840-890 MPa, relative elongation of 0.3-2.5%, and Young's modulus of 70-100 GPa. It was established that the structure of this alloy consists of primary β-grains surrounded by a silicide nanophase Ti_5Si_3. In the middle of the primary β-grains there is a finely dispersed α-phase with highly dispersed nanosilicides that stand out along its borders.

Mechanisms of heteroassociation in aqueous solutions of BSA with curcumin

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Curcumin (Cur) and quercetin (Q), which have high antioxidant capabilities, are utilized as medicines to treat a variety of ailments. Both medications are hydrophobic macromolecules that are poorly soluble in water and degrade rapidly, resulting in a loss of useful biological activity. As a result, it is critical to attach them to bovine serum albumin (BSA), one of the most abundant plasma proteins that plays a key role in the transport of numerous substances, including medications. The presence of one of the amino acid residues, Trp212, in the macrochains, which is localized in the hydrophobic pocket, enables us to assess the degree of energy transfer from the fluorophore to the quencher and so establish the binding parameters in BSA-Cur and BSA-Cur/Q complexes.

The distance between the energy donor and acceptor, changes in thermodynamic parameters, and estimated binding parameters of docking modeling demonstrate that energy transfer happens in these systems via the FRET mechanism and that hydrophobic interaction predominates.

The complex formation of HSA with the medicine quercetin

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The three domains and two subdomains that make up the human serum albumin (HAS) protein’s intricate globular shape are joined by the Trp 212 amino acid residue, which is found in the globular pocket. This cavity’s size makes it easier for complexes to form with different biomolecules, including medicines, particularly hydrophobic ones. Such drugs include quercetin (Q), which is used as an antioxidant, cardiostimulating drug.

The docking modulation of the HSA-Quercetin system was performed, which indicates the localization of drugs in the hydrophobic cavity of the HSA. The study of the efficiency of radiation-free, resonant energy transfer shows that the value of r satisfies the condition of the Förster theory. The binding parameters and changes in thermodynamic potentials indicate the hydrophobic nature of complexation, which facilitates the transport of quercetin by HSA albumin.

Mechanisms of heteroassociation in an aqueous solution of ATP – Ag^+

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The fluorescence quenching of aqueous solutions of adenine-5'-triphosphate (ATP) molecules during their titration with $AgNO_3$ salt solution at varying concentrations at temperatures of 293, 303, and 313 K. Quenching and binding constants were determined using Stern - Volmer and Hill relations. The value of the quenching rate constant and the dependence of the Stern - Volmer constant on temperature indicate that the complex formation of ATP – Ag^+ occurs as a result of static PL quenching. Binding constants of heteroassociates for different temperatures were used to calculate changes in thermodynamic parameters ΔG, ΔH, ΔS, the signs and values of which indicate the non-specific nature of the binding forces in the studied complexes.

Complex formation in aqueous solutions of adenosine triphosphate with Mg^{2+} and Ca^{2+} ion

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Metal ions play an important role in biochemical processes occurring in living organisms. On the other hand, they have a real impact on the biological activity and functional properties of many biostructures when they are coordinated. The coordination of metal ions, including Mg^{2+}, during the coordination of adenosine-5'-triphosphate (ATP) affects the length of the final anhydride bond P-O-P, the charge density concentrated on this bond, and ultimately determines one of of important functions - ATP hydrolysis.

In the work, quantum-chemical modeling of ATP - Mg^{2+} and ATP - Ca^{2+} complexes was carried out. In addition to the optimized geometry, the alternation of charges and the electronic structure were determined. Fluorescence quenching for aqueous solutions of the considered systems was studied, quenching and binding constants were determined, and changes in thermodynamic parameters were determined, which indicate the predominant role of nonspecific binding in metal-ligand complexes.

The human serum albumin and the medicine curcumin heteroassociation in aqueous solutions

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For curcumin, as a hydrophobic drug, an important characteristic of its biological activity is the formation of complexes with one of the most important transport proteins, human serum albumin (HSA), to avoid degradation in plasma. In this case, the restructuring of the secondary structure of HSA is also of particular importance, which is responsible for the formation of complexes.

It has been found that the formation of heteroassociates of HSA with curcumin (Cur) is accompanied by static fluorescence quenching, the behavior of which is described by the distance between the fluorophore and quencher r, which satisfies the Förster energy transfer condition. The possibility of energy transfer in accordance with the FRET mechanism is confirmed by docking simulations and molecular dynamics modeling. As a result of the binding of HSA to curcumin, a hydrophobic interaction occurs with a significant decrease in the secondary structure component of the α-helix.

Binding parameters in ATP complexes with curcumin drugs

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Curcumin (Cur) belongs to the antioxidant medicines used for the treatment of many diseases. The molecular structure consists of aromatic rings, for which one of the important reasons for interaction with biomolecules can be its stacking as well as numerical interaction. It can also be expected that, as a result of its high hydrophobicity, Cur is able to form complexes with ATP, which includes adenine, a hydrophobic component.

The complexation of ATP with Cur was studied by determining the fluorescence quenching (FL) of the nucleotide at variable concentrations of the drug. From the PL quenching results, the quenching and binding parameters, the change in thermodynamic parameters, and the degree of energy transfer were calculated. These results, as well as quantum-chemical modeling of molecular dynamics, indicate the non-specific nature of binding in the ATP-Cur heteroassociation, which is dominated by hydrophobic interactions.

Synthesis of azomethine-containing methacrylates based on 3-aminopyridine and their radical polymerization

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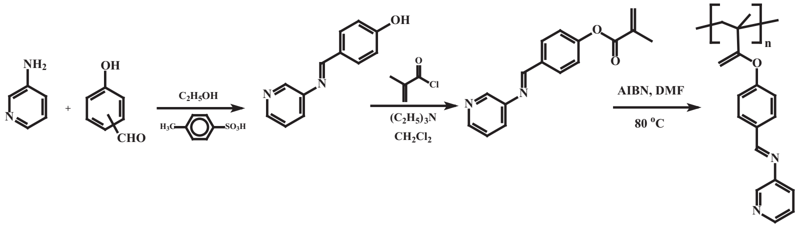
A special place among high molecular weight compounds is occupied by polymers with an azomethine fragment. Azomethines have found their applications in catalysis, analytics, photoluminescence, as thermal and anticorrosive objects, but relatively less research is known for pyridine-based compounds.

To create such polymers, we synthesized new methacrylic monomers based on 3-aminopyridine. In the course of our work, azomethines were synthesized using standard methods [1,2] from commercially available hydroxybenzaldehydes and 3-aminopyridine. The key stage was the methacrylation of azomethines.

The structure of all synthesized compounds was proven by 1H-NMR spectroscopy.

We have investigated the polymerization ability and determined the kinetic parameters of polymerization of new compounds in radical thermally initiated homopolymerization. The process was carried out in their 10 % DMF solutions in the presence of 1 % azobisisobutyronitrile (AIBN) at 80°C under argon atmosphere. Contractions were determined using a KM-6 cathetometer, and the conversion was found gravimetrically. The polymers were precipitated in ethanol and resedimentated from DMF to ethanol.



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Chemical plasticization of polymers without side groups

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We investigated the features of chemical plasticization of amorphous polymers for decreasing the polarity of the macromolecules, the replacement of the lateral polar groups on less polar and non polar or rigid fragments of the macromolecule chains to the flexible ones. For heterochained polymers whose chains contain no side groups, one of the methods of chemical plasticization is the reduction of the polarity of the macromolecule units. For polyoxides and polyiminates, replacement in polar groups on non-polar, for example, polyethylene oxide groups -O- with a dipole moment of 0.45 D, and in the polyvinylimine of the group -NH- - with a dipole moment of 0.4 D for the nonpolar group $-CH_2-$, leads to the loss of the polarity of the polymer and the dipole-dipole interaction, which is typical for polymethylene.

When replacing polar groups in the polyethylene oxide and polyimine with correspondingly certain values of the dipole moment (μ) to the nonpolar methylene group, the forces of intermolecular adhesion (E_{cog}), are weakened, the segments become more flexible and movable (decreases T_c), and the polymer is less elastic (G_a - decreases). For selected polar polymers, Tc polyethylene oxide and polyimine do not correlate with the values of their dipole moments. Tc of polyethylene oxide is lower than that of polyimine, and its link is more polar than the link of polyimide. The reason for higher compared to polyethylene oxide Tc, polyethylenimine has the higher value of internal rotational energy ($U_{во}$) around the -NH bond compared to the bond -O-. This corresponds to the phenomenon of plasticization. Agrees with the conclusion and an increase in the Van der Waals volume ($V_{вв}$) - the space taking the monomeric link, which can not penetrate other links with energy that corresponds to normal temperatures.

The chemical plasticization of simple polyeters by increasing the number in the chain of a macromolecule of non-polar $-CH_2-$ groups occurs effectively with a small size of the methylene fragment, when the polymer has a strong dipole-dipole interaction and these additional non-polar groups significantly weakens this interaction. With the increase in the size of the methylene fragment, when the distance between the polar groups becomes large and the dipole-dipole interaction of the macromolecules weakens, the addition of new non-polar groups does not significantly change intermolecular interaction, since it mainly determines the weak forces of Van der Waals.

Impedance spectroscopy of single crystals $CsPbBr_3$

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Lead-based perovskite (lead bromide $CsPbBr_3$) has good photovoltaic properties and is also heat- and moisture-resistant. This makes it a good candidate as a material for solar cells.

Impedance spectra were recorded using an automated system based on a Hioki IM3536 LCR meter. Alternating current impedance spectroscopy was performed on $CsPbBr_3$ perovskite single crystals. The dimensions of the samples were 3.3 x 4.2 x 6.0 mm^3.

A simulation model of the equivalent circuit of impedance-spectroscopy of alternating current was selected, which consists of elements of a constant phase, a resistance and a capacitor.

It is shown that the experimental samples have mixed ion-electron conductivity. The semicircle on the Nyquist stability diagrams (closer to the origin) is explained by the process in which electrons (or ions) oscillating around equilibrium positions. The inclined line at low frequencies refers to the impedance that occurs during mass transfer during ion diffusion.

Synthesis of Au-doped ZnO via polymer precursor method

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As a material for gas sensors, photocatalysts, transparent electrodes, and optic coatings, zinc oxide is highly appreciated for its physical and electrical properties. Since the development of the first metal oxide-based gas sensor in the 1960s, a lot of various methods for obtaining ZnO powders and layers have been discovered, including chemical or physical vapor deposition, RF sputtering, sol-gel methods, and solvothermal methods [1]. The polymer precursor method is a deviation of a sol-gel method that allows obtaining precursor solution of water-soluble metal salts suitable for obtaining both thin and thick layers of metal oxide, as well as a bulk powder.

In our previous work [2] we have studied applied layers and powders of ZnO, synthesized via the polymer precursor method with different solution compositions and annealing temperatures. Doping of zinc oxide with Au, Al, Co [1, 3], and other elements is often utilized to enhance its sensing characteristics, such as conductivity, sensitivity, and selectivity to certain gasses. In this research, we are exploring the possibilities of incorporating the doping of ZnO with Au into the polymer precursor method.

For synthesis, two polymer precursor solutions consisting of ethylene glycol, citric acid, nitric acid, and zinc nitrate were prepared. After the dissolution of zinc nitrate, 0.5% and 1% wt. of Au (as $HAuCl_4$) were added. Small portions (10 ml) of precursor solutions were annealed at 600°C for 2 hours, yielding gray and purple powders.

Preliminary analysis of the UV-Vis reflectance spectra suggests that synthesized ZnO powders contain gold nanoparticles at different concentrations with the approximate size of 100-110 nm for both powder samples. Absorption peak around 560-570 nm was present for both samples and was expectedly more intensive for the sample with higher dopant concentration.

This experiment confirms the ability to dope zinc oxide powders with gold (and, potentially, other elements) during the polymer precursor synthesis procedure in a reasonably simple and straight forward way.

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Effect of post-annealing on microstructure and corrosion behavior of additively manufactured Ti_6Al_4V titanium alloy

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Additive manufacturing (AM) is an evolving manufacturing method and has become a viable option for producing unique and complex shaped parts. This method is promising for manufacturing of titanium alloys, as it allows for significant cost reduction of titanium parts compared to conversational manufactured methods [1, 2].

In this work, the effect of post-annealing on the microstructure evolution and corrosion resistance of AM titanium alloy in a hydrochloric acid solution was studied by comparing it with a conversational manufactured one (wrought). As AM was chosen selective laser melting method which performed by 3DMetalTech company (Ukraine).

The results obtained via corrosion tests show that the anti-corrosion properties of AM titanium alloy was worse than for the wrought one, which was explained by the presence in AM titanium alloy of a non-equilibrium metastable martensitic phase and residual stress. Microstructural results showed that post-annealing led to the reduction of the non-equilibrium phase martensitic α', relief of residual stress, and formation of the β phase, which has a higher corrosion resistance. These changes lead to an improvement in the corrosion resistance of AM titanium alloy and result in appropinquate performance comparable to that of conventional wrought titanium alloy.

These results indicate that the selective laser melting AM method accompanied by the post-annealing processes can be used to produce AM Ti_6Al_4V parts in comparison to wrought ones.

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Electrochemical Synthesis of Branched $Al_xGa_{1-x}As$ Nanowires

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In the world of innovative technologies for solar cell manufacturing, there is an active search for new materials and methods to enhance the efficiency of light-to-electricity conversion [1]. One of these innovative approaches involves the use of nanostructured materials, often nanowires, which can deliver high levels of efficiency while keeping production costs low [2].

In this study, we report on the synthesis of the ternary compound $Al_xGa_{1-x}As$ on a GaAs substrate using electrochemical deposition with an $AlCl_3$-based electrolyte. The process incorporates an initial texturing of the GaAs surface, resulting in the formation of a system of branched $Al_xGa_{1-x}As$ nanowires, instead of a continuous film. The proportional content of As, Ga, and Al in the compound can be manipulated by modifying the synthesis conditions. It's essential to note that $Al_xGa_{x-1}As$ is a ternary compound, with boundary cases being AlAs at x=1 and GaAs at x=0.

Utilizing structures with well-studied morphology, such as nanowires, could lead to a reduction in energy losses caused by surface recombination due to their high surface quality. Additionally, these structures can be formed on like substrates using simple methods, as in our study using electrochemical deposition, thereby reducing the production cost of solar cells.

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Lanthanide contraction in mixed rare-earth orthovanadates

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A list of mixed $X_{0.5}Lu_{0.5}VO_4$ (X = Pr, Nd, Eu, Tb, Dy, Ho, Er, Tm, Yb) crystals have been investigated within *ab initio* calculations. Geometry optimizations have been performed within Broyden-Fletcher-Goldfarb-Shanno minimization. Initial lattice parameters and atomic positions were derived from analysis of X-ray powder diffraction patterns of the investigated orthovanadates prepared by solid state reaction with calcined temperature 1200°C. At this stage, we used GGA-PBE exchange-correlation potential [1] for the self-consistent procedure. Ground-state properties have been evaluated within PBE0 hybrid functional [2], based on the projector augmented waves (PAW) [3]. That means, the mixing of the exact Hartree-Fock exchange with the exchange-correlation functional GGA-PBE is performed for *d/f*-states of a lanthanide and only inside the atom-centered augmentation sphere. The ratio of the exact exchange (parameter alpha) equals 1/3.

Ab initio study of the crystals relaxed geometries showed a presence of the lanthanide contraction. However, there is no explicit dependency of the energy band gap on the lattice volume. We consider changes in the energy of *f*-states as the main impact on differences in electronic properties. Obtained results good agree with transition and diffuse reflectance spectra measurements. Thermal treatment of some samples shows changes in transition spectra intensities but not minima locations. That means there are changes in refractive index caused by changes in powder shapes, whereas crystal structure is stable.

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Experimental observation of light holes in CdTe

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Semiconductors A^2B^6 are a promising material for the manufacture of radiation photodetectors, solar energy converters [1], elements of telecommunication networks and a number of other solid-state electronic devices. Among the materials that are already used as uncooled semiconductor detectors of ionizing radiation, CdTe occupies a leading position [2]. The main requirements for materials for gamma and X-ray detectors are their high conductivity and high mobility of charge carriers [2,3]. In this case, electrically active intrinsic point defects must be in equilibrium, i.e. compensation must occur.

The aim of this work is to establish a theoretical method for calculating the basic parameters of light holes in cadmium telluride and their experimental detection, which would make it possible to take into account the influence of these current carriers on the transport phenomena in the presence of two types of current carriers.

The concentration and mobility of light and heavy holes in CdTe at room temperature were calculated based on the analysis of the experiment on the magnetic field dependence of the Hall voltage. The calculation was carried out within the framework of the semi-classical phenomenological two-band model. The presence of holes of two types in this semiconductor is confirmed by the law of dispersion, from the graphic representation of which it is clearly visible that in the valence band there are two branches of the dispersion curve with different curvatures [3].

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1. V. D. Popovych, F. F. Sizov, O. A. Parfenjuk, Z. F. Tsybrii (Ivasiv) The effect of inhomogeneous dopant distribution on the electrical transport

Modification of the surface layer of carbon nanomaterials using the Diels–Alder reaction

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Carbon nanomaterials (CNMs) are typical nanoporous carbon sorbents. These CNMs can be used in chemical engineering, environmental issues and nanomedicine due to their non-toxicity. The chemical properties of CNMs make it possible to modify their surface to improve specific properties and produce various functional materials. The Diels-Alder reaction is selective and takes place between a diene and an unsaturated compound, a dienophile. Carbon nanomaterials can contain single and conjugated double C=C bonds, i.e. they can participate in the Diels-Alder reaction as a diene and as a dienophile.

The aim of this work is to investigate the surface active centers of various CNMs, including multi-walled CNTs, carbon black, activated carbon, and carbon fibers, which are capable of participating in the Diels-Alder reaction. To address this issue, the reactivity of CNM active centers in the reaction with 3-sulfolene (Su) and 1,3-cyclohexadiene (CHD) was investigated. Barothermal treatment was used for the modification. CNMs were modified in an autoclave at temperatures between 90-250°C. The samples were analyzed by SEM, N_2 adsorption, TG/DTG, TPD-MS, FTIR and Boehm titration methods.

We showed that modification with CNM by the barothermic Diels-Alder reaction leads to the introduction of 1–1.5 mmol/g of specific functional groups into the carbon surface layer. The TG/DTG and TPD MS methods revealed at least two chemisorbed forms due to the addition of Su and CHD. The first chemisorbed form refers to the products of the grafting of the reagents onto the carbon surface by the classical Diels-Alder addition. According to TG/DTG and TPD MS data, the second chemisorbed forms decompose at a temperature higher than 250°C. These forms correspond to the thermal decomposition products generated by the partial pyrolysis of the chemisorbed modifier. The obtained materials have specific hydrophobic-hydrophilic surface properties and can be used in gas and water purification.

Photoluminescent properties in different gas ambient of ZnO nanopowders doped by Mo and V

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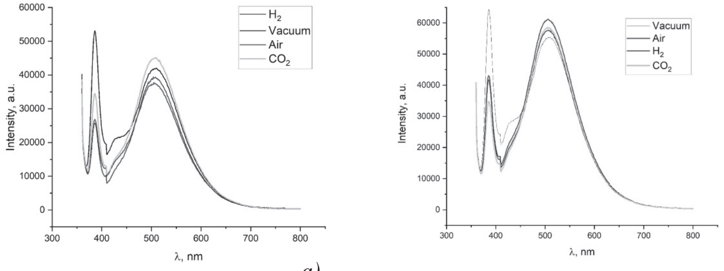
The researches structural, morphological and photoluminescent properties of *ZnO* nanopowders doped by *Co* and *V* obtained using pulsed laser reactive technology is carried out. Electron microscopy and X-ray diffractometry were conducted to determine the structure, shape, and size of the nanoparticles. Investigation the peculiarities of photoluminescence (PL) in different ambient of *Mo* and *V* doped *ZnO* nanopowders was carried out. Changing the gas environment leads to a significant change in the intensity of the PL spectra and its deformation, that can be used in the gas sensors. The PL spectra of all sample consist strong emission bands located in the UV-range and broad non-elemental emission band in the visible region from 410 to 600 nm (Fig. 1). The decomposition of PL spectra into elementary bands shows the presence elementary peaks of 430, 520 nm. The influence of the impurity and the gas medium on the redistribution of elementary luminescence bands intensities was investigated.



a) *b)*

Fig.1. *Photoluminescent spectra in different ambient of ZnO nanopowders doped by a) Mo b) V.*

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Study of morphological features of electrically conductive composite carbide-silicon ceramics

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During the martial law in the country, there is a need to develop radio-absorbing materials that would reduce the radar visibility of military equipment and weapons, protect medical equipment and buildings of critical infrastructure from the influence of side electromagnetic radiation, and also provide the ability to protect internal information. Therefore, the creation of composite ceramics and the study of its morphological features is an urgent task of materials science.

Based on the need to ensure the manufacturability of the mass, the amount of additives SiC introduced varied from 10 to 30 wt. % over 100 wt. % on dry matter. A further increase in the additive content in the ceramic tile led to the formation of defects. For the manufacture of test samples, SiC was added to the mass of the finished charge in amounts of 9.1, 16.6, and 23.1%. Briquettes were formed by the method of semi-dry pressing with a specific pressure of 20 MPa. The resulting raw material was dried to a final moisture content of less than 1%, after which it was fired at a temperature of 1120-1140°C with exposure for 20 minutes. The technology of manufacturing experimental samples was close to the factory one.

The paper investigated the morphological features of the obtained samples and evaluated their influence on the physical and mechanical characteristics. It was found that after firing ceramics with the addition of 9.1 wt.% SiC, its peaks are absent in the X-ray pattern, and when 16.6 wt.% and more are added, the peaks of primary SiC are already detected by X-ray diffraction. In the structure, when adding up to 20 wt.% SiC, elongated pores with a size of 15-20 μm are observed, at 23.1% SiC, the pores in the structure become more rounded and decrease to 10-12 μm, which significantly improves the properties of the products. According to the results of the research, ceramic samples with the addition of 23.1% SiC showed the best properties: water absorption – 5.7%, open porosity – 12.2%, apparent density – 2.13 g/cm^3, resistivity – $0.4 \cdot 10^6$ Om·m. According to the obtained X-ray phase analysis data, SiC in this series was preserved in its original form, which is an important condition for effective protection against electromagnetic radiation.

Synthesis and characterization of colloidal Ag–(In,Ga)–S semiconductor nanocrystals

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Colloidal semiconductor nanocrystals (NCs) of the I–III–VI family, in particular Ag–In–S and Cu–In–S, are promising in view of their non-toxicity, high luminescence efficiency, size-dependent optical properties, notable photocatalytic activity, and possible applications in biology and medicine as well as in light sources and photovoltaic elements. Much less studied are NCs of the Ag–(In,Ga)–S system obtained mostly by syntheses in organic media at elevated temperatures.

Here we report on the synthesis and characterization of a size-selected series of quaternary non-stoichiometric Ag–(In,Ga)–S NCs obtained from aqueous solutions in the presence of glutathione (GSH) ligand at mild conditions (below 100°C). The NC size selection was carried out by repeated fractioning of the colloidal solutions by precipitation at 4000 rpm with sequentially added poor solvent (2-propanol).

X-ray photoelectron spectroscopy (ESCALAB 250Xi XPS Microprobe) data confirm the presence of Ag, In, Ga, and S in the NC composition, the [In]/[Ga] ratio in the NCs being noticeably higher than the relevant precursor ratio.

X-ray diffraction (XRD) studies (Rigaku Smartlab) reveal broad peaks in agreement with the tetragonal structure of the NCs shifting upward with increasing Ga content in the Ag–(In,Ga)–S NCs. The average NC size estimated from the halfwidth of the XRD peaks using the Scherrer equation is about 2 nm.

Optical absorption spectra (Cary 50) and photoluminescence spectra (Black Comet) of the size-selected Ag–(In,Ga)–S NCs show a distinct shift towards higher energies with the NC size decrease.

New nanomaterials based on gadolinium (III) complexes

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For a long time, the interest of researchers in various compounds of lanthanides does not diminish. They are used in various fields of science and technology: as emissive and magnetic materials in molecular spintronics, as single-molecule magnets for quantum information processing, magnetic refrigerants [1-3]. One of the requirements for materials is a high-spin ground state, which significantly reduces the presence of additional exchange interactions in polynuclear complexes. Therefore, high-spin complexes of gadolinium with -diketones are potential precursors of magnetic materials.

Synthesized mono- and heteroligand coordination compounds of gadolinium with unsaturated β-diketones. The synthesized compounds were investigated by elemental analysis, FTIR, DRS, thermal analysis, dynamic light scattering, electron microscopy (SEM). Fluorescence spectra were studied under standard conditions, at 77K, 1.6K and at different values of the magnetic field (B=0-5 T). It is shown, that the introduction of axial donor molecules into the composition of the complexes has a significant effect on the properties of the compounds.

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Microwave properties of oxidized carbon fiber Busofit in X and Ka-band

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Carbon fibers are a modern structural material, although the scope of their use is limited by their properties and high cost. Therefore, many modern studies are related to the study various modifications of the properties of carbon fiber [1].

The low fiber density provides a strength-to-weight ratio incomparable to other modern materials. It is because of these properties that carbon fibers are widely used in the aerospace, automotive, energy, construction and other industries.

The purpose of this work was the synthesis and study of the effect of chemical modification of carbon material on the nature of interaction with electromagnetic radiation in the ultra-high-frequency range.

An industrial viscose-based fiber called Busofit, which has a large specific surface area and a developed porous structure, was used as the starting material.

Carbon fiber Busofit was oxidized with solutions of hydrogen peroxide and nitric acid to form oxygen-containing groups on the surface. It was established that after oxidation, various types of oxygen-containing groups are formed on the surface: carboxyl, lactone, anhydride and phenolic. The effect of the oxidant on the microwave properties of carbon fiber in the X and Ka bands was studied.

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Microwave properties of carbon fiber, modified with amino groups

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Physico-chemical properties of carbon materials can be significantly changed with the help of chemical surface modification [1]. There is very little information in the literature about the effect of chemical modification on the ability to interact with electromagnetic radiation.

The purpose of this work is to study the effect of PAN CFs amination (with preliminary bromination on the interaction with electromagnetic radiation in the X and Ka-band. It was found that the modification of PAN CFs with amino groups using KBr_3 ($\Delta S_{21} \leq 3.7$ dB) in comparison with Br_2 ($\Delta S_{21} \leq 2.7$ dB) is more effective for changing its microwave properties in the X and Ka bands. It was investigated that the microwave properties of the modified PAN CFs have a different dependence on the types of grafted amines, namely, the value of S_{11} reflection increases, and the value of S_{21} transmission losses decreases when modifying PAN CFs SuEn, unlike other amines. It was demonstrated the possibility of adjusting the amount of attenuation of EM waves S_{21} and the amount of reflection S_{11} depending on the mutual orientation, with an increase in the angle between the frame of the PAN CFs and the direction of the electric field. It was established an increase in the amount of reflected power to 1 dB and a decrease in the power of the wave that passed through the sample to 9.3 dB.

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Some features of electric and photoelectrophysical properties of new photosensitive film composites based on naphthalimide-containing methacrylic copolymers sensitized by organic dyes of different types

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The new naphthalimide-containing methacrylic copolymers were synthesized by by free-radical polymerization method. The structures of the respective copolymers were characterized by 1H NMR, elemental analysis and UV-vis-spectroscopy. The novel photosensitive thin film structures based on these copolymers doped with organic dyes of different types have been prepared. Their spectral, electric and photoelectrophysical properties have been investigated. It was shown, that all studied film structures exhibit photovoltaic effect and wavelength-dependent photoconductivity under illumination by light from the long-wavelength edge of the respective dyes-sensitizers absorption region. The features of electrophysical, photophysical and photoelectric properties of the obtained thin film structures, as well as the possible nature of the photovoltaic effect and charge carriers photogeneration mechanisms are discussed. The respective phenomenological model for internal photoeffect and photovoltaic effect in the investigated thin film structures was proposed.

The relationship between dielectric and optical properties of cellulose micro/nanoparticles with their spatial structure

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Cellulose is the basis of many materials of industrial use, in particular, such as dielectrics in electrical products. It is known, that cellulose can be obtained from plant raw materials, and it can also be a product of the vital activity of bacteria. Therefore, the study of the relationship between a cellulose dielectric and optical properties and the ways of its production is relevant.

The Cotton linters Sigma-Aldrich cellulose powder and two types of bacterial cellulose (BC) (synthesized with use of the *Gluconacetobacter* or *Komagataeibacter xylinus* bacteria) were used or the study.

The temperature dependences of complex permittivity as well as IR, diffuse reflection and luminescence spectra were measured and analyzed. It was found that in the temperature range of -140 ÷ -20°C, dielectric relaxation is observed for cotton cellulose. For bacterial cellulose, the region of dielectric relaxation shifts to low temperatures. The analysis of IR spectra at different temperatures showed that the nature of dielectric relaxation is related to the conformational movement *tg*↔*gt* of methylol groups on the crystallite surface. A two-level model of identical relaxers was used to describe dielectric relaxation. It was established that the concentration of relaxers is larger in cotton cellulose than in bacterial cellulose, which indicates a different structure of the surface of cellulose nanoparticles and a different fractal dimension of the spatial structure of these celluloses at the micro level.

Spatial distribution of strains, boron content, and surface potential near dislocation etch pits in HPHT-diamond

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Due to several unique physical properties, boron-doped diamond (BDD) is a promising material for high-power and high-frequency electronics. However, defects and their non-uniform distribution significantly affect the capabilities and properties of diamond-based devices. Using a novel approach of correlative micro-Raman and frequency-modulated Kelvin probe force microscopy (KPFM) mapping, this report studies nano-morphology, local structural, and electrical properties of dislocation etch pits (EPs) in BDD, grown under high pressure and high-temperature conditions (HPHT). This allowed precise measurements of non-uniform distributions of crystallinity, internal strains, boron doping levels, and local surface potential near the dislocation EPs developed during the early stages of selective etching. In addition, micro-Raman mapping revealed a distinct dislocation-induced distribution of elastic strains with compressive and tensile stress regions.

Moreover, the relative intensity of boron-induced Raman peaks was analyzed as a function of boron doping estimated by micro-FTIR mapping of corresponding BDD plates. This allowed for estimating the spatial distribution of boron content in individual dislocation EPs, which were found to be strongly non-uniform with boron-rich regions surrounded by areas with lower boron doping. The KPFM analysis demonstrated significant surface potential localization at the EPs and certain terraces. The correlation between micro-Raman maps of deformation fields and boron content distribution are discussed as the origins of related surface potential fluctuations at the EPs. The report emphasizes defects' influence on BDD properties, which may be crucial for the development of diamond-based devices. The study was supported by NRFU project #2020.02/0160.

The effect of short-term annealing on the physical and chemical properties of the Amorphous Metallic Alloys system Al-(Y,Gd)-Ni

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Amorphous metallic alloys (AMA) based on Aluminum are interesting because of a good corrosion resistance. In [1] it was reported that amorphous Al-based alloys are promising materials for the formation of electrodes with high conductivity in silicon solar cells. In [2] it was investigated that as a result of annealing the mechanical properties of AMAs are improved. The authors [1] report that during the annealing of the amorphous alloy $Al_{87}Ni_3Y_{10}$ a layer of amorphous oxide 100 nm thick is formed, and on the surface of pure crystalline aluminum the thickness of the amorphous oxide layer is 4 nm.

Temperatures of annealing of AMAs were determined by differential scanning calorimetry (DSC) phase transitions of amorphous metal alloys of the Al – Ni – Y(Gd) system. Annealing at T3 (temperatures of sustainable growth of nanocrystals and equal to 609 K and 611 K for $Al_{87}Y_4Gd_1Ni_8$ and $Al_{87}Gd_5Ni_8$, respectivly) and leads to the formation of an amorphous matrix intermetallic compounds causes a shift in the corrosion potential in the cathode direction.

As the results of electrochemical investigation show that protective oxide layers are formed on the surface of the initial AMAs. Replacement of 4 at.% Yttrium with Gadolinium leads to a shift of the corrosion potential in the anode direction, which indicates easier oxidation of the AMA surface $Al_{87}Gd_5Ni_8$.

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How effects on nano level can enhance analysis of metal ions traces in water by means of low temperature secondary ion mass spectrometry

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Rapid analysis of metal ion pollutants in natural water is an urgent task under current tense ecological conditions. A significant difficulty in such analysis is the necessity of concentration of trace quantities of pollutants to the limits of sensitivity of measuring equipment. Here we propose a method of water sample handling for analysis by secondary ion mass spectrometry (SIMS) based on dilute water solutions behavior at micro- and nano- levels under cryogenic conditions.

The phenomenon of phase separation in aqueous systems (with low content of solutes) on their freezing results in formation of heterogeneous solids composed of pure ice crystallites of average size of 10^{-4} m separated by intercrystalline (eutectic) channels of 10^{-6} m width filled by the solutes. Given that an impact of a single bombarding primary ion under SIMS conditions excites a zone of about 10 nm in diameter, the efficiency of sputtering of the concentrated solutes from the eutectic channels is practically the same as from the macroscopic solute samples [1]. Thus, a method of SIMS probing of frozen water samples is proposed, which advantage is a possibility to work with rather small, down to several micro liters, volumes of the initial liquid. The analysis technique does not require any cryogenic blocks or temperature stabilization, just freezing of the sample on a sample holder in vapors of liquid nitrogen is necessary. The informative mass spectra can be recorded in the mode of spontaneous thawing of the sample in the ion source in temperature range from about 160 K to 220 K (when sublimation of ice samples under vacuum conditions of the mass spectrometer takes place).

The results of the low temperature SIMS detection of various metal ions in the samples of water of different origin (distilled, tap, sea water, and medicines) will be presented. As it was expected, Na, K, Mg, Ca, Cu, and Fe were detected in natural waters, while Mn, Ni, Co, Zn were found in some medicinal drops.

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Water evaporation kinetic from different pore sizes cellulose based materials

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The water evaporation from the porous materials significantly depends on the material spatial structure and the pores geometric parameters distribution [1]. This fact is caused by the mass and heat transfer processes within the volume depend on such type parameters and can differ meaningly for materials with different pores types [2].

In the report it is represented data of experimental investigation of water evaporation from different materials with various thickness in the air for atmospheric pressure and different values of ambient temperature (50, 60, 70 and 80°C). For pore size influence investigation cellulose-based materials with various pore sizes were chosen: filter paper, fabric, and bandage.

In the experiments sample mass dependences on time were measured at the time during water was evaporating from its surface. By using obtained experimental data water concentration in material (moisture content) time dependences were calculated. By using simplified model of the water diffusion process inside the samples the activation energies of water molecules diffusion in these materials were determined.

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Relationship between the physico-chemical properties of "pompon" graphene and its electrochemical parameters

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Graphene is the most promising nanomaterial due to its unique combination of excellent properties, e.g., electronic conductivity, mechanical strength and large surface area, which allow one to reach outstanding results in the field of materials science. Special structural and morphological characteristics and the largest ratio of surface area to volume of graphene have great prospects for use in energy storage devices, batteries and supercapacitors [1]. Compared with graphite, a traditional anode material in lithium-ion batteries, graphene has higher theoretical capacity of 740 $mAh \cdot g^{-1}$, since Li^+ ions can be adsorbed on both sides of a graphene sheet, forming an intercalate of the C_3Li composition. However, the quality of graphene plays a crucial role in obtaining high electrochemical parameters of energy storage devices, since the presence of defects, impurities, grain boundaries, multiple domains, structural disturbances and folds in a graphene sheet can negatively affect its properties.

This paper describes the behavior of several modifications of "pompon" graphene as a LIB anode. Relationships between the specific surface area, porosity, degree of disorder and electrochemical parameters of graphene anodes are considered. The specific capacity of the "pompon" graphene obtained in our studies exceeds 600 $mAh \cdot g^{-1}$, which allows us to propose this material as an alternative to traditional graphite anodes.

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Spectroscopic and structural characterization of Mg and Zn spatial distribution in $Mg_xZn_{1-x}O$ solid solutions

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Zinc oxide is a promising material for the manufacture of photodetectors, transparent electrodes, varistors, and gas sensors. To increase its bandgap and to change the conductivity, the doping with isovalent magnesium can be used. However, under thermodynamic conditions, hexagonal ZnO and cubic MgO are enabling to form continuous series of $Mg_xZn_{1-x}O$ solid solutions due to the inconsistency of their crystal structures and limited solubility of Mg in ZnO and Zn in MgO. In this work, the $Mg_xZn_{1-x}O$ solid solutions were sintered by solid state reaction approach at 900-1200°C for 3 h in the air. Their structural characteristics, chemical composition, and spatial distribution of elements were studied versus content of both oxides in the charge and preparation conditions using the methods of X-ray diffraction, scanning electron microscopy, Auger spectroscopy, and energy-dispersive X-ray spectroscopy.

It was found that the morphology of the samples, as well as the mechanism of solid solution formation, depends on relative contribution of both oxides. It turned out that the hexagonal and cubic phases of the solid solution are formed simultaneously. Besides, an increase in the MgO content in the charge, the magnesium content in the hexagonal grains continuously increases and reaches ~13 at.%. It was also observed an enrichment of grain boundaries with Zn and Mg that plays an important role in doping of the ZnO and MgO grains, while their contribution affects the morphology of the samples.

This phenomenon can be explained taking into account two mechanisms: i) Mg and Zn diffusion along grain boundaries and their subsequent incorporation into ZnO and MgO grains, respectively, and ii) direct diffusion of Mg into ZnO and Zn into MgO in direct contact of the grains of both oxides. The first mechanism is realized mainly at a low content of ZnO or MgO in the charge, while the second one is observed at comparable contribution of both oxides when the probability of direct contact of ZnO and MgO grains increases.

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Biocompatible hybrid hydrogels based on natural polysaccharides with LaponiteRD nanofiller

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Hydrogels are widely used in various fields, such as agriculture, ecology, pharmacology, and medicine. Traditionally, synthetic chemically cross-linked hydrogels are used. But the application in the ecosphere requires the use of environmentally friendly materials, however synthetic hydrogels can pollute the environment with toxic components (monomers or cross-linking agents) when they destruct over time. Thereby, modern trends are focused on the search for bio-safe alternatives. This work is aimed at developing new hydrogel composite materials for sorption and prolonged release of bioactive components based on physically cross-linked natural polysaccharides. The natural polysaccharides, namely sodium alginate, kappa-carrageenan and chitosan were used for the synthesis. The use of nanofiller LaponiteRD creates prerequisites for forming a gel structure at the nano-level, which results in sufficient mechanical strength, high swelling capacity and additional adsorption properties in relation to pollutants such as heavy metal ions. The interaction between the biomacromolecules and clay nanoparticles, and the structural and functional properties of the synthesized hybrid hydrogels were estimated using X-ray diffraction, FTIR, SEM and differential scanning calorimetry. The XRD and FTIR data confirmed the formation of an intercalated structure of LaponiteRD in the hydrogels composition. Synthesized hybrid hydrogels showed a good balance between sufficient mechanical strength and high swelling properties (the swelling degree reaches 25-27 g/g) and the sorption capacity towards Cd (II) (the adsorption capacity ~ 250 mg/g). Their biocompatibility with respect to pea seeds and positive impact on soil microorganisms' balance was proven by the Nelyubov method and microbiological study. This makes it possible to offer such materials as biocompatible sorbents for water purification or soil conditioners with prolonged release of nutrients.

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Shell formation during alcohol-salt solutions droplet evaporation

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A significant quantity of nanomaterials obtaining methods created for their synthesis are characterized by using metal salt's alcohol solutions used as reagents [1]. The standard solvent used to receive such compositions is ethanol [1], but the other alcohol's potential usability for such goals also are in the area of modern researches. [2].

In the report it was represented the experimental data of the alcohol (butanol, pentanol, hexanol) solutions of metal salt (LiCl, $CaCl_2$) droplets evaporation kinetics. The experiments were conducted for 1 mol/1 kg (1 M) initial solution concentration and gas medium different pressure values (740, 400 and 200 mm Hg) and the medium temperature value of 20°C.

During themeasurement the experimental dependences of the droplet surface area on time were obtained. Also the pendant where the drop was suspended, served as a temperature sensor [3].

The experimental and the theoretically calculated time dependences of the droplet surface area were compared. It was shown that the modified Maxwell model can be used for modelling the salt solution droplets evaporation kinetic. It was observed, that during the evaporation of butanol, pentanol and hexanol $CaCl_2$ solution and in hexanol LiCl the forming of a shell around the droplet is possible when the solution inside droplets becomes oversaturated, and it leads to an almost complete cessation of the evaporation.

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Iron and Chromium influence on crystallization kinetics of Cobalt-based amorphous alloys

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Amorphous alloys are promising materials due to their unique properties and potential applications in various fields [1]. Studying the transformation of amorphous alloys into a nanocrystalline state is essential for controlling the material's structure and uncovering new possibilities in materials research [2]. In this study, we focus on exploring the influence of iron and chromium on the crystallization process of cobalt-based amorphous alloys, specifically $Co_{72}Fe_5Si_{11}B_{12}$, $Co_{68}Cr_9Si_{11}B_{12}$, and $Co_{72}Fe_{2.5}Cr_{2.5}Si_{11}B_{12}$. Differential scanning calorimetry (DSC) is employed to analyze the crystallization behavior at three heating rates. As a result, three exothermic peaks are observed, with the initial peak corresponding to the nanocrystallization of the amorphous matrix. Notably, the nanocrystallization processes exhibit significant activation energies ranging from 266 to 481 kJ/mol. The addition of iron and chromium enhances the thermal stability of the alloys and induces changes in the nanocrystallization mechanism. The X-ray diffraction method provided confirmation of structural transformations and the formation of nanoscale crystalline regions within the amorphous matrix during non-isothermal heating processes.

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Modification of amorphous alloys with oligomeric coatings

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Expanding the application of Fe-based amorphous metallic alloys (AMAs) in medicine, as implants or controlled drug carriers, requires their isolation from direct contact with the environment by oligomeric layers. This will save their surface from destruction, as well as form layers of bioactive substances with their prolonged release in the human body [1].

The quality of surface coatings will be determined by the nature of the substrate - AMA, as well as the oligoperoxide and the solvent from which it is formed. For this purpose, it was investigated the film formation of oligoperoxide based on vinyl acetate (VA), 2-tert-butylperoxy-2-methyl-5-hexen-3-yne (VEP) and maleic anhydride (MA), i.e. VA:VEP:MA=1:1:1, on the surface of AMA $Fe_{78.5}Ni_{1.0}Mo_{0.5}Si_{6.0}B_{14.0}$ (AMA-1); $Fe_{73.1}Cu_{1.0}Nb_{3.0}Si_{15.5}B_{7.4}$ (AMA-2) from 1% aqueous ammonia and isopropanol solution.

Using the chronopotentiometry, voltammetry and impedance spectroscopy, the formed coatings were investigated on the contact and external surfaces of the tape. Those surfaces are differed in their elemental composition, the degree of structuring and roughness [2]. It is shown that for both solutions, denser coatings are formed on the external surfaces of the alloys, which are covered with an oxide layer even during the synthesis of the AMA tape by ultra-fast melt cooling method.

A higher affinity of the investigated oligoperoxide from both solvents to AMA $Fe_{73.1}Cu_{1.0}Nb_{3.0}Si_{15.5}B_{7.4}$ was established, which is reflected by more positive potentials, lower corrosion currents, and higher resistance values of the surface layers. A comparison of the obtained parameters of the surface layers applied to the surface of AMA from different solvents showed a better result for aqueous ammonia solution. In the case of application oligoperoxide layers from isopropanol, competitive adsorption of alcohol molecules occurs. In isopropanol, protective surface layers are formed on the surface of amorphous alloys, which, however, are not durable.

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Structural Evolution of Nickel Atoms by Carbon Implantation into Nickel Films and Post-Irradiation Heating

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Electron-diffraction and electron-microscopic studies have been made into structural transformations in nickel films exposed to different doses of C^+ ions.

At first, with increasing concentration of carbon atoms, a diffuse spreading of diffraction rings of the initial face-centered cubic (fcc) structure of nickel and the appearance of additional blurred diffuse ring zones are observed. A further increase in the implanted carbon dose is accompanied by reduction in the intensity of the diffraction rings of the fcp structure, and also, by the appearance and growing intensity of the diffraction rings of the hcp structure. On reaching the stoichiometric ratio Ni/C=3/1, the diffractograms exhibit only the rings of the hcp structure with the lattice parameters a=0.266 nm and c=0.433 nm. Note that the diffractograms show the reflections of the metal-nickel sublattice only.

The smoothness of the Ni fcc structure transition to the hcp-phase, as the implanted carbon dose increases, and the completion of the transition only after reaching the stoichiometric ratio Ni/C=3/1 may bear witness to the chemical nature of the observed structural transition with nickel carbide Ni_3C formation. However, recognizing that the composite atoms do not form chemical compounds, it may be concluded that the implanted carbon atoms form the hexagonal structure from carbon atoms in the environment of nickel atoms and contribute to the rearrangement of nickel atoms to forming the hcp structure. That is, with an increase in the carbon atom concentration there occurs the graphene plane formation from carbon atoms in the environment of nickel atoms and, simultaneously, nickel atoms rearrange themselves by the law of carbon atoms with the formation of similar hexagonal planes, displayed in the electron-diffraction pattern as the process of hexagonal structure formation with the lattice parameter a=0.266 nm. In other words, the formation of a multilayer system takes place, consisting from successively arranged layers: one from carbon atoms, and the other – from nickel atoms.

At temperatures of about 670 – 690 K, the process of the hcp structure decomposition sets in, which culminates in the recovery of the initial fcc-Ni matrix and the formation of precipitates along the boundaries of graphite-structured crystallites composed of carbon atoms.

DFT study of rare-earth metal adsorption on the Mo(112) surface

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We report the results of a theoretical study of the rare-earth metal (Gd, Ce) adsorption on the Mo(112) surface. The chemisorption of rare-earth elements on the furrows surface of Mo(112) or W(112) has been the subject of considerable attention. Some of the rare earths metals form long-periodic chain structures at low coverage due to the long-range indirect interaction between the adatoms.

All calculations were carried out with the ABINIT code using Perdew – Burke – Ernzerhof (PBE) functional and the projector augmented-wave method. The binding energies (Eb) of Gd and Ce atoms on the Mo(112) surface were calculated. It is revealed that there is a significant quantitative difference between the binding energies of Gd and Ce atoms on the Mo(112) surface. The binding energies of Gd are near 1 eV lesser than Eb of Ce.

It is shown that at certain condition Gd atoms can form dilute chain structures on the Mo(112) surface, in agreement with the experiment [1]. The phase diagram analysis for the Gd/Mo(112) system has revealed that there are p(4x1) and p(7x1) diluted chain structures. Instead, there are no diluted chain structures in the Ce/Mo(112) system for Ce coverage less than 0.5 ML [2]. It is found that the most energetically favourable periodic structures are c(2x2) structures at coverage of half a monolayer (ML) of Gd or Ce atoms.

The dependence of the binding energy on the degree of coverage for the Gd/Mo(112) system is flat, without a well-defined minimum, in contrast to the Ce/Mo(112) system. For the Gd/Mo(112) system, the long-periodic structures at low coverage are only 0.02 eV higher than the c(2x2) structure. Whereas, for the Ce/Mo(112) system, this value is approximately 0.17 eV.

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Obtaining of dense, hard materials by sintering AlB$_{12}$ nanopowders of with carbon additives

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The work carried out was aimed at creating new composite materials based on higher aluminum borides with high (significantly increased compared to existing analogues) mechanical resistance, damping resistance and wear resistance, resistance to the action of high ablation energies, aggressive chemical environments, radiation and shock loads for use in armor and radiation protection of people and equipment, protection of objects related to the production of electricity, in tool production, for friction welding, for the manufacture of nozzles, etc. In order to ensure the creation of materials with a set of these properties, the physico-chemical basis of the processes for the synthesis of nanodisperse powders (and mixtures) with increased reactivity, a nanostructured component and partially formed solid solutions, as well as the purposeful formation of solid solutions of borides in the process of consolidation. All compaction processes were carried ин hot pressing (up to 30 MPa, 1600-2050°C), electrospark (SPS) sintering (attempts) and in conditions of high pressures and temperatures (2-4.1 GPa, 1200-1800°C). The using of initial nanopowders allows to intensify consolidation processes, reduce synthesis and sintering temperatures, i.e. to reduce the cost and simplify production technologies, as well as to improve the mechanical characteristics of materials. Features of the structure of boron carbide and aluminum dodecaborides (α-AlB$_{12}$ and AlB$_{12}$C$_2$), namely the presence of the same structural elements - practically regular icosahedrons of boron atoms, the possibility of modifying the structure and properties by introducing additives, was the reason for conducting research in this direction aimed at creating new impact-resistant composite materials based on them, in particular, with improved impact resistant characteristics.

It was used in the work nanopowders (50-150 nm, with a specific surface area of 21-15 m^2/g) of -AlB$_{12}$ (three types with different content of amorphous carbon impurities from the graphite crucible during powder synthesis) and $AlB_{12}C_2$, which were synthesized by ph. Dr V.B. Muratov (IPM NAS of Ukraine) from h-BN, Al and C in graphite crucibles and it was relatively cheap for our investigations [1].

Because one of the uses of our materials is ballistic barriers, such materials have high hardness, crack resistance and Young's modulus, but still remain quite brittle. Due to the formation of solid solutions, a large internal tension was observed in the materials, which is why the maximum mechanical characteristics increased in them, but the fragility also increased. We carried out work on the universalization of the characteristics of our materials with a given reduction in fragility in them by the purposeful creation of ceramic laminar structures in our composites. One of the ways to improve the mechanical characteristics of layered structures is the development of laminates with weak interfaces to deflect cracks [2]. Thus, the authors [3] showed that a thin layer of boron carbide mixed with carbon nanofibers can be used to create a weak interface in a layered structure and provides crack deflection. Residual tensile stresses formed in the first layer affect the viscosity of the laminate. Therefore, we also used C-containing additives - SiC, nano-SiC, ash and graphene, in our studies. And the addition of carbon had a positive effect on both the structure and the operational properties of the materials. But, also, if carbon appears in the structure of the material based on aluminum dodecaboride, a new phase is formed, the crystal structure of which has the same icosahedral structure as that of boron carbide [4]. However, such a material in itself has a number of advantages, was synthesized at much lower temperatures (1800-1950°C compared to B_4C - 2000-2200°C), has increased chemical resistance, crack resistance and wear resistance. In our research, we started with C, and then we reached silicon carbide.

One of the examples of the successful use of nanopowders and the selection of thermobaric conditions were hot-pressed samples of the AlB_{12}-SiC system, where the hardness and crack resistance increased with increasing additives. The additions of 15 wt.% SiC to -AlB_{12} resulted in the formation of 88 wt.% $AlB_{12}C_2$, 12 wt.% Al_2O_3 (with Si impurity) composition (according x-ray), where the material itself had such indexes: *HV*(49 N-load)=23.0. GPa hardness K_{1C}(49 N-load)= 5.0 MPa•$m^{0.5}$, fracture toughnes and =2.6 g/m^3 density. Also, with the addition of 20 wt.%, the material had composition (according x-ray): 85.5 wt.% $AlB_{12}C_2$, 13.5 wt.% Al_2O_3 (with Si and BN impurities), and mechanical characteristics such as *HV*(49 N-load)=25.6. GPa hardness, K_{1C}(49 N-load)= 5.7 MPa•$m^{0.5}$ fracture toughnes respectively.

Generally, in our research after X-ray phase studies with interpretation by the Rietveld method, the formation of new phases, such as $AlB_{12}C_2$ [5], $AlB_{40}C_4$, AlB_{10}, $AlBO_3$, $Al_3B_{48}C_2$, Al_3BC_3, Al_4O_4C, $Al_3(ON)_4$_Sigm, Al_4O_4C, $\delta A_{13}O_4$, $Al_3C(BC_2)$, Al_4C_3 was established, and whose influence whose influence on the indestructibility of materials is obviously.

Later, the influence of TiC and C additives on the properties of the obtained composites and features of ceramic rutting under impact loading were discussed [6].

The high strength characteristics of the obtained systems can be explained by many factors, including the small size of the grains and the high connectedness between them, as well as the formation of solid solutions in the structure of the compacted composites.

The developed lightweight dodecaboride dicarbododecaboride -based ceramic composites hold great potential for a wide range of applications in extreme conditions [7].

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Influence of Gas adsorption on photoluminescence in metal Oxide Nanopowders

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The study aims to investigate the photoluminescent characteristics of metal oxide (Ga_2O_3, TiO_2, WO_3, SnO_2) nanopowders synthesized by means pulsed laser reactive technology [1], under various gas environments including vacuum, air, O_2, N_2, H_2, CO, and CO_2. The nanopowders structural, optical, and luminescent properties were investigated using techniques such as X-ray diffractometry, electron microscopy, transmission spectroscopy, and photoluminescent spectroscopy. The luminescence properties observed in our study exhibit distinctive features specific to this material. In particularly, luminescence of Ga_2O_3, notably including a broad radiation band ranging from 400 to 550 nm. The origin of this broad luminescent band, containing multiple elementary bands, can be explained by the existence of various electron-hole recombination pathways. The blue-green band arises from the recombination of electrons with holes localized within gallium acceptor vacancies. The nature of visible photoluminescence is determined by the intrinsic defects structure of nanomaterial, which is dependent on the technological parameters employed during nanopowder synthesis. Changing the surrounding environment induces a pronounced variation in the intensity and deformation of the photoluminescence spectra. This phenomenon can be attributed to redistribution of existing luminescence centers and the emergence of new luminescence adsorption centers on the surface of the nanopowders. The CIE1931 chromaticity diagrams of the photoluminescence light emitted by the nanopowders were obtained. It was found that the color coordinates vary depending on the gas environment. Consequently, the investigated nanopowders hold promising potential as highly responsive materials for the development of gas sensor systems [2].

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Effect of nanoparticles on morphological parameters of wheat

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Nanoparticles have a significant effect on morphological parameters of wheat, which can lead to both positive and negative results depending on the type, concentration and duration of exposure to nanoparticles. [1]

Wheat is an important cereal crop and a major source of food for humans and livestock. With the increasing use of nanoparticles in various applications, including agriculture, the release of nanoparticles into the environment can potentially affect the growth and development of wheat. [2] Studies have shown that exposure to nanoparticles can affect various morphological parameters of wheat, such as root length, shoot height, leaf area, and biomass accumulation. [3]

On the positive side, nanoparticles can improve wheat growth and development by improving nutrient uptake, enhancing photosynthesis, and promoting antioxidant activity. [4] They can also increase the resistance of wheat to biotic and abiotic stress factors such as pests, diseases and drought. [5] On the other hand, high concentrations of nanoparticles can lead to stunted growth, reduced biomass, and altered root morphology, which may ultimately affect wheat yield. [6]

The duration of exposure to nanoparticles is also a critical factor that determines the degree of their influence on the morphological parameters of wheat. [7] Short-term exposure to low concentrations of nanoparticles can have positive effects, while long-term exposure to high concentrations can have negative effects. [8]

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In general, the effect of nanoparticles on the morphological parameters of wheat is complex and depends on various factors. Therefore, further research is needed to fully understand the mechanisms underlying these effects and to develop strategies to minimize the negative effects of nanoparticles on wheat growth and development. [9]

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Compositional dependence of structural and magnetic properties of Li-Zn spinel nanoferrite

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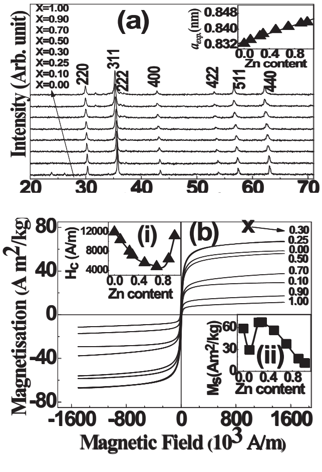
Magnetic properties of Li-based spinel ferrites can be tuned by a suitable substitution, e.g. Zn^{2+}. Low cost, high saturation magnetization (M_s), moderate coercivity (H_c), etc. makes Li-Zn ferrite promising for electromagnetic absorbers, and microwave devices, where control of magnetic properties is needed. We report the effect of Zn-addition on structural, magnetic properties of single-phase nanocrystalline $Li_{0.5-x/2}ZnxFe_{2.5-x/2}O_4$ (x = 0.0…1.0), prepared by sol-gel auto-combustion method, annealed at 450°C for 3 hours. Structural, morphological, and magnetic studies were performed using XRD, SEM, and VSM. Antistructure modeling was used to get active centers' concentration in tetrahedral (A) and octahedral (B) sites. Structural and magnetic data are shown in Fig. 1. SEM image analysis shows agglomerated particles and dissimilar particle size distribution. XRD reveals formation of *fcc* spinel structure: grain diameter 33.8 – 81.7 nm, strain 1.3 −3.7×10^{-3}, dislocation density 0.44 −1.6 lines/m². The linear increase of the lattice parameter (a_{exp}) is due to the replacement of Li^{1+} by Zn^{2+} ion with dissimilar ionic radii ($Zn^{2+} > Li^{1+}$). Fe^{3+} migration from A to B site leads to alteration of M_s: 11.4–67.3 Am²/kg), H_c (4775 – 11937 A/m).



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Session 5
Nanostructured surfaces

Optimization of bimetallic nanoparticle morphology for plasmon-induced polymerization

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As is known, an important application of metal nanoparticles in organic chemistry is plasma catalysis. Currently, this technology is increasingly used in the reactions of selective transformation of organic functional groups [1]. At the same time, one of the most interesting and poorly studied areas of plasmon-induced catalysis is localized and controlled polymerization. This type of transformation opens up new opportunities for the creation of functional plasmon-active substrates.

The plasmon-induced polymerization method allows you to monitor and track the growth of the polymer in real time. The polymerization of organic substances containingtheir metal nanoparticles occurs due to its heating. Of particular interest is the use of bimetallic nanoparticles, which is due to the possibility of more flexible regulationof their plasmonic properties in comparison with monometallic and shell nanoparticles.

As a result of the absorption of light pumping energy, the average temperature of the nanoparticle rises by ΔT, proportional to the absorption cross-section. At the same time, the dependence of heating on the volume content of the nucleus and shell meters, with their general character, may differ by an order of magnitude, which indicates the possibility of controlling thermal effects in the vicinity of a bimetallic nanoparticle by changing their geometric parameters and/or morphology.

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Study of surface roughness depending on the thickness of the Sn layer in Si-Sn-Si layered structures

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A surface relief of a-Si\Sn\a-Si layered films (which may use to produce silicon nanocrystals with quantum dots properties [1]) studied by methods of electron and atomic force microscopy as so as X-ray fluorescent microanalysis. We investigate the changes of shape and the scale of the periodic structuring of the Si\Sn\Si structure surface relief in depending on the tin layer thickness during the production of such films by vapor deposition.

Quasi-spherical formations with a diameter from 20 nm to 2-3 μm on such films' surface are found to be the main element of topography. We find that the structuring occurs in two stages: first, as a layer of hemispherical micro-droplets of tin gets formed and second, as a layer of silicon is deposited on the hemispheres. During the first stage, the layer of tin melts. A partial fusion of the droplets hemispheres occurs under the influence of radiation and the flow of silicon vapors from the evaporator. This process results in the tin hemispheres' size increasing by a factor of three. Silicon vapor deposition and amorphous silicon formation at this stage happens on the liquid metal surface. It turned out that the amorphous silicon obtained in this way has porous structure. It consists of grape-like dendrites of the fractal type on a scale of hundreds of nanometers. The elements of dendrites also have a quasi-spherical shape with a diameter of 20-50 nm. The existence of such nanostructurization of amorphous silicon is considered as a possible reason for abnormally efficient transformation of silicon from an amorphous state to a nanocrystalline state during further processes of tin-induced transformation of silicon in a-Si\Sn\a-Sn. The results obtained in this work are useful for understanding and control the surface roughness of Si\Sn\Si films, which is important for the technologies of nano-silicon film formation for solar cells.

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Charge Accumulation Processes in Chalcogenide Films under Electron Irradiation

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Irradiation of amorphous chalcogenide films with a thin electron beam leads to the formation of local space charge regions. We studied the processes of charge accumulation in films of the Ge-Se system using the Kelvin probe force microscopy. This paper presents the results of studying of the features of the interaction of thin films of the Ge-Se system with an electron beam under point irradiation. Ge-Se chalcogenide films have been pointwise irradiated with an electron beam using Tescan scanning electron microscope (SEM), model VEGA. The following irradiation parameters were used: accelerating voltage $U = 30$ kV, spot size $B = 0.64$ µm, electron beam current $I = 60$ nA. We performed irradiation at exposure times from 10 µs to 5 s. The point dose of irradiation varied from $1.86*10^2$ µC/cm^2 to $9.3*10^7$ µC/cm^2.

It was found that non-monotonic surface structuring of the films going upon irradiation with an electron microscope beam with an incident electron energy of 30 keV. Gaussian-type cones are formed on the surface of the films in the region of low irradiation doses (irradiation time 10–100 µs). The height of such a relief, the formation rate and sensitivity depend on the film chemical composition. Craters are formed on the surface of the films in the region of high doses. It was established by the KPFM method that a positive charge is concentrated on the surface of the cones (relative to the non-irradiated surface), and a negative charge dominates in the craters. The dynamics of the formation of an electron-induced surface relief in chalcogenide films is explained within the framework of a two-layer charge model. Parameters of this model have been determined. It is established that the relaxation time of the positive charge at the initial stage of irradiation is significantly (by a factor of 5–20) less than the relaxation time of the total charge in the space charge region at high doses.

Influence of strong magnetic fields on the temperature dependence of pseudogap in YBCO films

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The understanding the mechanism of electron pairing in high-temperature superconductors (HTSCs) will definitely indicate the direction of synthesis of superconductors with a desired high T_c. For this, it is necessary to study the properties of HTSCs in the normal state, especially in cuprates, where the pseudogap (PG) is opened at $T^* >> T_c$. It is worth noting that the PG state refers to a range of temperatures and energies where the density of states in a superconductor is suppressed, but superconductivity is not yet fully developed. This state is sensitive to the presence of a magnetic field, which can further modify the electronic and magnetic properties of the material. Obviously, applying of an external magnetic field is one of the excellent methods to study superconducting properties of cuprate HTSCs.

In our work, we studied a high quality 100 nm-thick YBCO film that has the T_c = 88.7 K in the absence of magnetic field. The resistive measurements were performed up to 8 T in $H||ab$ configuration. Having obtained reliable data of field- and temperature dependent excess conductivity below the PG opening temperature [1, 2], we plotted series of field- and temperature dependent pseudogap. The further details will be presented directly at the conference.

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Comparative study of RF sputtered Fe_2O_3- and Fe_3O_4-doped indium saving indium tin oxide thin films

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Indium saving iron doped ITO:Fe_2O_3 (PHS) and ITO50:Fe_3O_4 (PHS) thin films were deposited onto preheated at 523 K glass substrate by co-sputtering method at different oxygen flow rates and subsequently heat treated. In order to reduce indium usage in ITO films, an amount of indium oxide in the target was decreased from 90 mass% to 50 mass%.

Doping by both Fe_2O_3 and Fe_3O_4 resulted in increasing transmittance and crystallization temperature of indium-saving ITO thin films.

ITO:Fe_2O_3 (PHS) thin films showed lower volume resistivity (with exception of thin films sputtered at Q(Ar)/Q(O_2)=50 sccm/0.1 sccm at RF power 20 W) and higher transmittance than ITO50:Fe_3O_4 (PHS) thin films sputtered under the same deposition conditions.

We obtained ITO:Fe_2O_3 (PHS) and ITO50:Fe_3O_4 (PHS) thin films with volume resistivity of 930 and 1020 μΩcm, respectively, without any heat treatment when the oxygen flow rate was 0.2 sccm and RF power was 10 W.

The highest figure of merit ($6.8\ 10^{-3}\ \Omega^{-1}$) was obtained for ITO50:Fe_2O_3 (PHS) deposited at Q(Ar)/Q(O_2)=50 sccm/0.2 sccm and RF power 20 W and heat treated at 523 K.

Doping by iron oxides does not change structure of ITO50 thin films and they crystallize as $In_4Sn_3O_{12}$.

Arithmetical mean height (S_a) and root mean square height (S_q) of both as-depo. ITO:Fe_2O_3 (PHS) and ITO:Fe_3O_4 (PHS) thin films increased with increasing oxygen flow rate.

Catalytic influence of acetazolamide on the electroreduction process of In(III) in chlorates(VII) with varied water activity; the application of nanostructured cyclic renewable liquid silver amalgam film electrode (R-AgLAFE)

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The use of an innovative electrode with a cyclic renewable film of liquid silver amalgam R-AgLAFE is an excellent alternative to HDME, as it guarantees similar quality and performance parameters to HMDE [1] and fits into the current trend of green chemistry.

Acetazolamide (ACT) is one of the most important drugs used in the treatment of secondary glaucoma [2]. Therefore, there is a need to study the mechanisms of action of this drug or search for new systems of controlled release.

The effect of acetazolamide on the kinetics and mechanism of In(III) ions electroreduction in chlorates(VII) solutions under various water activities was investigated in aspect of the ,,cap-pair" effect. The results obtained with the innovative electrode using the different electrochemical techniques enabled to determine the magnitude of the catalytic effect of ACT and the correlation with changes in water activity. The multistep of In(III) ions electroreduction process in the presence of ACT is controlled by the rate of formation of the nanosized active complexes on the R-AgLAFE electrode, mediating electron transitions. Changes in the In(III) ions electroreduction mechanism and in the presence of ACT in high water activity solutions compared to low water activity solutions were demonstrated. Presented procedure may be of paramount importance for evaluating the progress of treatment and building a mechanistic model of the effects of this drug on the human body.

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Peculiarities of ZnO nanorod array crystallization at ion implantation of rare-earth elements

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Arrays of ZnO nanorods doped with rare earth elements (REE) are a promising basis for creating optoelectronic and sensor devices. The rectifying, emitting and absorbing properties of heterojunctions based on pure ZnO nanorods will be determined by the presence of intrinsic defects and, therefore, will depend on the deposition method, doping level and annealing [1]. Pure and doped ZnO nanorod films are deposited in various methods. Ion implantation can be used to introduce dopants into films with predictable parameters after film deposition. In this regard, the study structural changes in ZnO nanorod array films and the redistribution of implanted dopants during thermal treatments is a task of current interest.

In the present work 70 nm thin ZnO films were deposited on a p-Si (100) substrate by magnetron sputtering of ZnO:Al (2wt%) target at room temperature. The ZnO films had a columnar structure modified by implantation of Nd, Sm, Ho, Er or Tm ions with an energy of 75 keV and fluences of 3×10^{13} cm^{-2}. Annealings were carried out at temperatures from 300 to 850°C for 30 minutes in argon.

It is shown that the implantation of REE ions leads to an increase in the concentration and crystalline perfection of ZnO nanocrystals in nanorods. This phenomenon is more pronounced for heavier REE ions at the same implantation conditions. It is assumed that this phenomenon is due to the radiation-stimulated annealing during implantation and the low removal of thermal energy from the nanorods. A physical model of this phenomenon is substantiated and the characteristic heating temperatures of nanorods during implantation are calculated.

It has been established that low-temperature annealing (300-600°C) of implanted nanorods leads not only to an increase in the size of nanocrystals and a decrease in lattice parameters, but also to an increase in the degree of structural perfection of ZnO nanocrystals. At higher annealing temperatures, the crystal structure completely absorbs the amorphous phase, implanted dopants are displaced outside the ZnO nanorods and diffuse to the ZnO/Si interface.

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Modeling of optical characteristics of structures with Cu and Al nanoparticles and Si nanowires

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Solar energy has advantages in sufficiency and environmental friendliness, it is considered one of the most promising alternatives to traditional energy sources, in particular fossil fuels. The use of plasmon resonance is an effective method for increasing the efficiency of Si-based solar cells. Metal nanoparticles are promising for improving the efficiency of silicon photovoltaic devices by reducing surface reflection and increasing light trapping in thin-film devices. However, the use of metal nanoparticles can also reduce the efficiency of solar cells, for example, due to the absorption of light inside the nanoparticle or due to an increase in the front surface reflectance due to backscattering. Therefore, it is important to properly investigate metal nanoparticles with optimal optical properties for application in silicon photovoltaic devices. Al and Cu have attracted considerable attention from researchers due to their low cost, widespread use on our planet, high compatibility, and efficient scattering with a tunable plasmon peak.

To find the optimal geometric dimensions of the structure of solar cells, calculations of a large number of combinations of a flat structure with metal nanoparticles and a structure with nanowires and metal nanoparticles were carried out. The height of nanowires (h) varied from 50 to 3000 nm, the period of the structure (P) – 100 – 600 nm, the diameter of metal nanoparticles (d) – 50 – 400 nm. Spectra of absorption, reflection, transmission, short-circuit current and electric field strength were calculated.

Based on the set of calculations, the geometric dimensions of the samples with the lowest average reflection coefficient were determined. Namely, the diameter of Al and Cu nanoparticles is 150 nm, the period of arrangement of nanoparticles and nanowires is 300 nm, the diameter of silicon nanowires is 250 nm, and the height of silicon nanowires is 100 nm. Structures with such parameters give significantly lower reflection coefficients compared to a solid silicon wafer. The reflection coefficient is lower in structures with Cu-NPs in the wavelength range up to 600 nm. The worst result was in the sample without nanowires and nanoparticles, and the sample with Al NPs on a flat surface performed worse. The rest of the samples have almost the same indicators.

Features of ordered nanostructure formation in ultrathin FePd films annealed in hydrogen

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Magnetic materials on the base of FePd with large perpendicular magnetic anisotropy are perspective for use as ultrahigh density recording media in HAMR and development of magnetic tunnel junctions for future spintronic memory and logic devices.

The aim of this work was the investigation of the annealing environment (vacuum, hydrogen), temperature and duration of annealing on the phase composition, structural and magnetic properties of FePd(5 nm) films.

FePd films of equiatomic composition were deposited at room temperature by magnetron sputtering on SiO_2(100 nm)/Si(001) substrates. Heat treatment was carried out in a vacuum and hydrogen environment in the temperature range of (500-700)°C for 0.5 -2 h. The as-deposited and post-annealed films were investigated by X-ray analysis, RHEED, SQUID, FMR and AFM methods.

In as-deposited films, a disordered *A*1 FePd phase was observed. The ordering process occurs by a thermally activated solid-phase reaction of transition from the soft magnetic *A*1 to the hard magnetic *L*1o FePd phase. In this case, annealing in hydrogen significantly activates this process.

Thus, upon annealing at 650°C for 1 h in hydrogen, the *L*1o FePd phase with a coercivity value of 5 kOe is formed. In the same time, upon annealing in vacuum the ordering processes proceed much more slowly and the coercivity reaches ~ 1 kOe. In addition, hydrogen atoms affect the electronic structure of the film. During heat treatment in hydrogen (650°C, 0.5 h), in contrast to annealing in vacuum, a paramagnetic state appears in the film during the ordered *L*1o phase formation. With an increase in the annealing time to 1 hour, it is replaced by a hard magnetic state. A further increase in the annealing duration to 2 h or temperature up to 700°C, is again accompanied by the paramagnetic state formation. In this case, the crystal structure of the ordered L1o phase is mainly preserved. Thus, the annealing of the FePd(5 nm) film in hydrogen leads to a reversible change in the magnetic properties and states.

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Effect of nitrogen pressure during cathodic arc deposition on tribological properties of nanostructured V-Mo-N coatings

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Hard nanostructure V-Mo-N coatings are promising for tribological applications, due to enhanced plasticity and self-lubricating ability under dry friction conditions. The aim of this study was to investigate the effect of nitrogen pressure ranging from 1 to 3 Pa during cathodic arc deposition of V-Mo-N coatings on their mechanical and tribological properties. The coatings with the thickness of about 10 µm were deposited on polished 18Cr10NiTi stainless steel substrates. The hardness (H) and Young's modulus (E) of the coatings were determined by nanoindentation using a Nano Indenter G200 system. Tribological studies were carried out with the reciprocating ball-on-disk test using a load of 2 N and sliding speed of 0.01 m/s under dry friction conditions at two temperatures, 25 and 500°C.

According to the test results, all coatings are characterized by high mechanical properties (see Table). An increase in nitrogen pressure during deposition leads to an increase in the coating friction coefficient (k) and a non-monotonic change in the wear rate (w). The $V_{23}Mo_{25}N_{52}$ coating, deposited at a nitrogen pressure of 2 Pa, has similar wear resistance both at room and high test temperature.

PN_2, Pa	Composition, at.%	Crystallite size, nm	H, GPa	E, GPa	$k_{25°}$	$k_{500°}$	w25°, mm³/Nm	w500°, mm³/Nm
1	$V_{29}Mo_{21}N_{50}$	9.5	32	425	0.30	0.50	3.8×10^{-5}	5.6×10^{-4}
2	$V_{23}Mo_{25}N_{52}$	8.0	30	400	0.32	0.46	4.3×10^{-5}	3.5×10^{-5}
3	$V_{20}Mo_{26}N_{54}$	7.7	31	450	0.35	0.65	7×10^{-6}	1.9×10^{-4}

The work was financially supported by the National Academy of Sciences of Ukraine and The European Federation of Academies of Sciences and Humanities (ALLEA), within the framework the "European Fund for Displaced Scientists", Grant EFDS-FL2-04.

Quenching of heterogeneous electrochemiluminescence emission at micro/nanostructured glassy carbon electrodes

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Electrochemiluminescence (ECL) is a branch of electrochemical analytical techniques, possessing high sensitivity and broad dynamic range of detection. The technique is based on electron-transfer reactions between electro-active species, generated in the vicinity of electrode surface, that form excited states emitting light. Current progress in ECL has clearly demonstrated it is a powerful tool for ultrasensitive detection and quantification of various analytes in biology, medicine, environmental monitoring etc. [1].

ECL detection of a large number of biomolecules is mainly carried out with solid phase ECL assay formats, in which analytes/fluorophores are immobilized on a solid substrate (an electrode) – using ECL sensors.

In this work, we have studied aqueous ECL from diphenylanthracene in polyvinyl butyral film on the glassy carbon electrode surface in reaction with tetraphenylborate coreactant [2]. In this work it was demonstrated that periodic micro/nanostructuring of electrode surface by laser beam drastically affects the ECL response of the modified electrodes. We have found that laser-induced periodic surface structures [3] cause essential reduction of the ECL intensity from the polymer films incorporating fluorophores. The possible reasons for such effect are discussed.

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Crystallographic orientation of PbTe single crystal surfaces and ion induced surface structures shapes

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The ion-induced surface patterns are of great practical importance for various technical and technological applications. In many cases the ion bombardment significantly changes the state of surface of solids, their structural and physical properties. In this report we will discuss the results of our recent studies [1,2] of surface transformations that occurs when the surfaces of PbTe binary compound of different – (100) and (111) – crystallographic orientations are sputtered with normally incident Ar^+ ions. We revealed that the shapes of the surface structures forming the morphology of the sputtered (111) and (100) PbTe crystal surfaces are fundamentally different. Initially the ion-induced truncated cone-shaped structures are formed on the sputtering surface. In the case of (100) PbTe sputtering surfaces these structures resemble truncated cones, but in the case of (111) PbTe sputtered surfaces they resemble pseudo-hexagonal truncated pyramids. During prolonged sputtering the truncated cones on the (100) sputtering PbTe surface transform to tetragonal pyramids and the pseudo-hexagonal truncated pyramids on the (111) sputtering one transform to trigonal pyramids. The transformation of the conical structures into the pyramidal ones we explain by the impact of the main crystallographic planes of {100}, {110}, and {111} families, which for PbTe are the planes of easy cleavage and high reticular density. We also show that the lateral facets of the pseudo-hexagonal pyramids on (111) sputtered surface are formed by the crystallographic planes of the family {012}. These are the next highest reticular density crystallographic planes after the main PbTe crystallographic planes (100), (110) and (111). The transformation of the pseudo-hexagonal pyramids into the pyramidal structures we explain by the impact of the main PbTe crystallographic planes of {100}. Summarizing, we state that in the case of PbTe crystals the formation and transformation of ion-induced cone-shaped structures and pseudo-hexagonal pyramids under impact of Ar^+ ion sputtering is provided by the processes of self-organization of the planes of high reticular density.

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Modification of the aluminum surface by palladium nanoparticles by galvanic replacement

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One of the promising methods for modifying the aluminium surface with metal nanoparticles is galvanic replacement. This method is simple to perform and does not require a reducing agent in the solution [1]. However, the spontaneity of the process makes it difficult to obtain nanoparticles with a given geometry and size distribution. Therefore, it is important to establish the main parameters that affect these characteristics. In order to minimize the passage of undesirable processes on the surface of the sacrificial metal, interest in the study of galvanic replacement in the medium of organic solvents, in particular, aprotic ones, has increased in the last decade [2]. The aim of this work is to study the influence of the main process parameters on the sizes and shapes of palladium nanoparticles deposited on the aluminium surface by galvanic replacement in the medium of organic solvents.

The dependences of the geometry of the deposited palladium nanoparticles on the aluminium surface on the main factors of the galvanic replacement process were established: the concentration of palladium ions, the temperature, and the process duration. It was shown that spherical palladium nanoparticles with an average size of 100 nm are formed and uniformly distributed over the surface of the aluminium substrate.

The high catalytic activity of the modified aluminium surface with palladium nanoparticles (Al/PdNPs) in the cathodic reduction of CO_2 in organic aprotic solvents was detected.

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Multilayer Fe_3O_4 doped ITO indium saving indium tin oxide thin films sputtered on preheated substrates

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The multilayer Fe_3O_4-doped indium tin oxide (ITO) thin films (ML ITO50: Fe_3O_4) with reduced to 50 mass% indium oxide content were prepared by co-sputtering of the ITO and Fe_3O_4 targets in mixed argon-oxygen atmosphere onto glass substrates covered by very thin layer of conventional ITO90 (90 mass% In_2O_3) and preheated at 523 K. Optical, electrical, and structural properties of ML ITO90/ITO50: Fe_3O_4 thin films were studied in comparison to undoped ML ITO50 and SL ITO50: Fe_3O_4 thin films.

It was found that the transmittance of the ML ITO90/ITO50:Fe_3O_4 thin films was improved significantly in comparioson with that of ML ITO50. It was observed since Fe_3O_4 is an additional source of oxygen during filling of oxygen vacancies.

The volume resistivity of the ML ITO90/ITO50:Fe_3O_4 thin films sputtered at oxygen flow rate 0.1 sccm was 416 $\mu\Omega$ cm that is 2.5 times lower than that of SL ITO50:Fe_3O_4 thin films deposited under the same oxygen flow rate.

Introducing of Fe_3O_4 to the ITO50 thin films did not alter the ITO structure.

TEM image of the cross-section of ML ITO90/ITO50:Fe_3O_4 showed that thin film consists of two regions. ITO50:Fe_3O_4 layer formed of the individual columns. The selected area electron diffraction pattern shows spots making up rings corresponding to polynanocrystalline structure of $In_4Sn_3O_{12}$.

Influence of deformation force during vibration-centrifugal hardening on properties of nanocrystalline structure of steel 40Kh

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Vibration-centrifugal hardening (VCH) is one of the methods for forming a surface nanostructure by severe plastic deformation, which increases wear resistance [1] of the working surfaces of machine parts. The essence of VCH is that the tool with protruding balls fixed in it moves along the outer or inner cylindrical surface, which vibrates with a certain amplitude and frequency, creating shock dynamic loads (SDL) [1]. These SDL are characterized by the force of impact between the tool and the part, which is determined by the relationship [2]:

$$P\text{-}m\varepsilon\omega^2,$$

where m is the tool weight; ε is the tool eccentricity; ω is the circular frequency of part vibrations.

VCH creates an impact force from P = 477 N with a weight of the tool m = 3.5 kg, its eccentricity ε = 0.006 m to P = 2045 N with m = 7.5 kg, ε = 0.012 m for a ball diameter of 0.0135 m. This provides microhardness and hardened surface depth ranging from 3.4 GPa and 2.3 mm to 4.9 GPa and 6.2 mm. However, the optimal impact force is P = 1022 N, which allows you to get a maximum microhardness of 8.9 GPa and a strengthening depth of 5.8 mm on steel 40Kh.

The deformation force forms a high microhardness of the surface layer obtained due to high fragmentation of the structure up to 18 nm under the optimal treatment mode. The influence of the deformation force during VCH on the wear resistance of steel 40Kh, which increases to 2.8 times, has been established.

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Antibacterial properties of argentum nanoparticles deposited on different carriers

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Ag nanoparticles have especially been employed as antibacterials, antifungals, and antioxidants in agriculture and medicine. The Ag-containing sorbents, based on mineral carriers like alumina or silica systems possess with a meso- and macroporous structure. These sorbents can be used in gaseous or liquid media, for example, for thiophenic compounds and mercury adsorption [1, 2] as well as they can be utilized as the catalysts for some reaction [3].

The aim of this study was to obtain promising nanoscale silver-containing antibacterial sorbents based on natural zeolite, aluminum oxide, and activated carbon as well as to compare their efficiency.

The original carriers were gamma-alumina, activated birch charcoal BAU, and dealuminated Ukrainian clinoptilolite. The samples were doped with silver in the amount of 1 wt% using silver nitrate. Then silver was reduced utilizing glucose solution at 20°C for 1 h. The obtained samples were investigated by using low temperature nitrogen adsorption/desorption, XRF, and TEM. Ag nanoparticles of different size were identified: 5-10 nm with some of 20-30 nm for zeolite; 10-20-30 nm for alumina; 10-15-20 nm with big agglomerates of 50-100 nm for coal sample. Total viable count determination was used to investigate the antibacterial properties of the samples. Antibacterial activity due to the latter go up in the range zeolite-alumina-coal sample. The best Ag-zeolite performance can be caused, firstly, by the optimal size of silver nanoparticles, and, secondly, by the interaction of silver with cations or acid sites of zeolite.

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Elastic hysteresis of 40X steel with surface nanostructure

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The development of the modern technologies requires the design of novel structural materials with increasingly higher requirements for their physical and mechanical properties. Therefore, it is important to develop surface modification methods to obtain some required properties and structural stress state. Alongside with the improvement of heat treatment methods, progress in the protective and restorative coatings, the methods of formation of surface nanocrystalline structures (NCS) are being developed as well. The mechanical-pulse treatment (MPT) is among them. It forms surface strengthened layer with NCS by severe plastic deformation of the treated surface, providing the change in the structural-phase state, as well as in its chemical composition due to alloying from technological liquids during MPT. As a result of MPT of medium-carbon structural steels, their surface microhardness, resistance to wear, fatigue, corrosion-fatigue and contact fatigue are increased. The increase in modulus of elasticity of the surface NCS was also revealed. For the purpose of improvement of physical and mechanical properties, as well as serviceability of the machinery components, elastic properties of the surface NCS formed on 40X steel by MPT were studied. The elastic hysteresis of 40X steel was investigated by determining deflection and residual deformation of specimens depending on the applied loads. It was found that 40X steel with the surface NCS behaves like an elastic body after 1-2 cycles of loading compared to 5-7 cycles for untreated 40X steel. Residual deformation β_{res} was 30-40% less for 40X steel with the surface NCS. The elastic limit for 40X steel with surface NCS is σ 60 MPa, and for untreated steel it is 2 times lower, σ ~ 30 MPa. Increasing in elastic limit for the treated steel occurred due to high dislocation density of the surface refined structure. Therefore, the surface NCS formed on 40X steel due to significantly lower elastic hysteresis ω_h and especially low residual deformation β_{res} is expected to possess higher values of fatigue and service life than the untreated one, since these characteristics are inversely proportional to ωh and β_{res}.

The effect of chemical modification on the nanostructure of natural zeolites

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The widespread use of synthetic zeolites in the processes of adsorption and catalysis arouses interest in studying the possibility of replacing them with natural analogues. The preparation of effective sorbents and catalysts on the basis of natural zeolites occurs, as a rule, through the stage of formation of the hydrogen form (H-form) due to their polycationic composition. H-forms of clinoptilolite from the Sokyrnytsky deposit (Ukraine) were obtained in the work by chemical modification of natural zeolite (Kl-nat) by ion exchange from ammonium chloride solutions followed by thermal desorption of NH_3 (Kl-H-NH_3) and hydrochloric acid (Kl-H).

Methods of scanning electron microscopy, X-ray microanalysis, phase analysis by X-ray diffraction phase analysis, and IR spectroscopy were used to study the effect of various methods of chemical modification of zeolite on the nature of its surface and the ratio of frame-forming elements (Si/Al).

The results of the study of the original (Kl-nat) and modified samples ((Kl-H-NH_3 and Kl-H) by the method of raster electron microscopy showed the highest degree of crystallinity in the Kl-H-NH_3 sample, while the partial destruction of the crystal structure was observed in the Kl-H sample, which is characteristic for the process of dealumination in the presence of an acid. It is also confirmed by the data of X-ray diffraction phase analysis. At the same time, the Si/Al ratio increases in the samples in the following sequence Kl-nat, Kl-H-NH_3 and Kl-H – 2.5, 4.6 and 9.0, respectively.

An IR spectroscopy study showed that the Kl-H-NH_3 sample contains a significant amount of ammonium cations. Therefore, it is necessary to adjust the conditions of thermal activation of the samples to obtain a fully substituted H-form. At the same time, it is advisable not to increase the temperature but the time of thermal activation taking into account the low thermal stability of clinoptilolite.

Thus, the possibility of a purposeful change in the nature of the surface of the natural clinoptilolite of the Sokyrnytsky deposit is shown, which makes it possible to obtain sorbents and catalysts with predicted properties.

Nanostructuring of anthracite by high-temperature steam activation

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Activated carbons are used in many technical processes: purification of water and pharmaceutical products, removal of pollutants, as catalysts/carriers, etc. Anthracites are very suitable precursors for the preparation of activated carbons since they are high-rank coals, having a high C to H atomic ratio even without carbonization. However, the above-mentioned processes often require precisely nanoscale pores for the adsorption of large molecules (such as dye molecules, biomass, etc.). Conventional coal activation techniques are divided into physical using steam or CO_2, and chemical using oxidizing agents (KOH, $ZnCl_2$, H_3PO_4, etc.). The disadvantages of chemical activation are that the chemicals can be hazardous to the environment and carry a price, the activation process is corrosive, and a washing step is needed to remove residues chemicals. Physical activation, being free from the mentioned disadvantages, requires high temperatures, and has been poorly studied for obtaining mesoporous materials from anthracites [1].

In this work, the influence of the duration of high-temperature steam treatment (900°C) of anthracite on its structural and adsorption properties was studied. In the process of activation, a gradual decrease in the bulk density of the samples was observed, while the resistance to abrasion began to decrease only after 10 hours of activation. The method of low-temperature adsorption/desorption of nitrogen demonstrated a gradual increase in the average pore radius and the BET specific surface area in anthracite during the treatment. This was accompanied by an increase in the proportion of micropores in the sample during 10 hours of treatment, after which the latter decreased. The DFT pore size distribution showed the development of mesoporosity in anthracite during the activation process.

In this way, the possibility of structuring anthracite by the method of high-temperature steam treatment with obtaining of micro-mesoporous carbon material has been shown.

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The influence of deposition conditions on the surface morphology and luminescent properties of $(Y_{0.06}Ga_{0.94})_2O_3$:Cr thin films

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The influence of deposition conditions and substrate type on the surface morphology of $(Y_{0.06}Ga_{0.94})_2O_3$:Cr thin films and their luminescent properties was studied.

Thin films of $(Y_{0.06}Ga_{0.94})_2O_3$:Cr with a thickness of 0.2-0.8 μm were obtained by RF ion-plasma sputtering in an argon atmosphere. The deposition was performed on substrates made of amorphous fused quartz (υ-SiO_2) and high-purity alumina ceramic (99.8% Al_2O_3).

The analysis of the obtained microphotographs of these films indicates that the size of nanocrystallites forming thin films of $(Y_{0.06}Ga_{0.94})_2O_3$:Cr depends on the presence of thermal treatment and especially on the type of substrate. The average value of grain diameter on the surface of the thin film deposited on a fused quartz substrate without thermal treatment is of 181 nm, and the root mean square roughness of the film surface is approximately 1.2 nm. Thermal treatment in an argon atmosphere leads to a decrease in the average value of grain diameter to 123 nm and at the same time to an increase in the root mean square roughness to 2.9 nm. The investigation show that due to the growth and sintering processes, the average volume of nanocrystals after thermal treatment increases from 2.96×10^3 to 6.04×10^3 nm^3. The thin films deposited on polycor substrates are formed from significantly larger nanocrystals. In particular, after thermal treatment in argon atmosphere, the thin films are formed from nanocrystallites with an average diameter of 372 nm and a root mean square roughness of 9.5 nm. The average volume of such nanocrystals is 234×10^3 nm^3.

The investigation of the luminescent properties of the obtained thin films show that for films deposited on quartz substrates, the intrinsic matrix luminescence with a maximum near of 400 nm is observed at photo-excitation. The excitation peak is corresponding to this emission is located at 240 nm. For thin films of $(Y_{0.06}Ga_{0.94})_2O_3$:Cr deposited on polycor substrates, the activator luminescence of Cr^{3+} is observed. The obtained results have been discussed and analyzed.

Evaluation of the catalytic efficiency of metal-containing zeolite composites with separated phases in the conversion of n-hexane

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Traditionally, zeolites are widely used as a basis of catalysts for various types of reactions. One of the ways to increase their effectiveness is to change the properties of the zeolite component. In particular, different combinations of zeolites can be used. The combination of zeolites of various types and other materials into bi-zeolite catalytic systems allows of optimal use of their structural and acid-base characteristics, thus regulating the content and strength of active sites and their availability in the resulting material, which opens broad prospects for the use of such systems in catalysis.

Procedures for the synthesis of true zeolite composites are quite complex. In this work, composite catalytic systems with a natural mordenite component and a synthetic MFI zeolite phase were obtained by mechanical mixing (1:1). The samples were modified with Pd and Ni nanoparticles (1–1.5% by weight in total), examined using a number of physicochemical methods, and tested in the isomerization of n-hexane in a micropulse mode. Peculiarities of hydrocarbon conversion on the obtained composite catalysts were determined depending on the preparation procedure.

It was shown by N_2 ad(de)sorption that the MFI component of the catalysts has a microporous structure, and the MOR component is micro-mesoporous. The use of a binder (α-, γ-Al_2O_3) significantly increases the external surface of the catalysts and contributes to the appearance of mesopores with a radius of 3–10 nm, whereas the sample without a binder remained mostly microporous.

The formation of hexane isomers for all composites revealed a synergy of the two zeolite components, more effective in samples with an isotropic distribution of zeolite phases. Despite low mesoporosity, the composite catalyst obtained without a binder showed the highest efficiency among tested catalysts not only in obtaining of hexane isomers in general, but valuable dimethyl-branched isomers too. This catalyst is also superior to monozeolitic bimetallic catalysts with similar metal component content. The results obtained are prospective.

Crystal structure of oxide ceramic coatings formed on VT5 and VT14 titanium alloys

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An X-ray phase analysis of oxide ceramic coatings formed on VT5 and VT14 alloys in the process of plasma electrolytic oxidation in the electrolyte (KOH (3 g/l), Na_2SiO_3 (2 g/l)) was carried out. It was established that already at the beginning of the coating synthesis (after 5 min) in the surface layers of both alloys, titanium oxides are synthesized. The elemental composition of the obtained coatings was analyzed by electron X-ray microscopy. It was established that the element distribution in oxide ceramic coatings is almost the same. Oxide ceramic coatings on both alloys consist of oxygen, titanium, silicon, and aluminum. The phase composition of coatings was investigated by X-ray structural analysis. Quantitative phase content was calculated by the Rietveld method. It was established that the diffractogram of the oxide ceramic coating synthesized on the VT14 alloy consists of TiO_2 (brookite), TiO_2 (rutile), TiO_2 (anatase) and -Ti reflections, and on the VT5 alloy only of -Ti reflections. This indicates a major difference in the alloys coating thickness.

After 30 min of synthesis, the corresponding oxide ceramic coatings on VT5 and VT14 alloys contain the following phases: TiO_2 (brookite), TiO_2 (rutile), a significant amount of -Ti and traces of -Ti. The thickness of the oxide ceramic coating on VT5 alloys is 80-100 m, and on VT14 90-150 m.

Segmentation of the obtained images has been carried out and the distribution of pores by size has been calculated. The dependence of pore sizes in the coatings on the alloying of the original alloys was established. The minimum pore sizes for VT5 is 6.93 10^{-14} m^2 and for VT14 – is 2.77 10^{-13} m^2.

Thermal helium desorption of implanted in austenitic stainless steel 18Cr10NiTi implanted helium at temperatures 100 K & RT.

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Helium thermal desorption spectra were investigated on the samples of austenitic steel 18Cr10NiTi pre-implanted with 24 keV helium ions at current density 5 μA/cm^2 in the dose range from 5×10^{16} to 4×10^{18} He/cm^2 at the sample temperature T_{irr} ~ 100 K and 300 K.

The spectrum of helium thermodesorption from the samples exposed to doses ~ 5×10^{16} He/cm^2 represents the temperature-scale smeared region of helium desorption with maxima in the temperature ~1470 K.

The increase in a dose of the implanted helium is accompanied by advancement of a spectrum of allocation of helium in a direction of fall of temperature. For a dose 4×10^{16} He/sm^2 the spectrum helium thermodesorption represents to the area washed away on a temperature scale desorption with badly divided peaks in a range of temperatures 1000 – 1400 K.

At the further increase in a dose of the implanted helium there is a qualitative change of a spectrum thermodesorption the helium, shown in formation of peak to maximum temperature at T_m ~ 1000 K. The further increase in a dose of the implanted helium leads to growth of intensity of this peak of a spectrum thermodesorption and it becomes prevailing.

At doses above 1×10^{18} He/cm^2 (at temperatures T_{irr} ~ 100 K, RT) is formed low temperature region helium desorption in a kind washed away on a temperature scale of desorption region with a maximum at T_m~450 K. The quantity of the implanted helium is decreases.

Proceeding from representation that atoms of helium in a crystal lattice of a steel form vacancy – helium complexes, peak with temperature of a maximum ~1000 K corresponds to temperature of disintegration of such complexes. Thus the quantity of atoms of helium in a complex is strictly defined. Further energy of activation desorption helium will be calculated, the analysis of the received results of research is offered.

Analysis of temperature changes of the metal nanolayer caused by laser influence

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An improvement to the algorithm constructed on the basis of a gas-dynamic model of laser-induced impact on the surface of a solid surface been developed. The improvement of the algorithm is based on the consideration of the role of accompanying factors during the interaction of laser radiation with the surface. Special attention is given to the role of absorption and diffusion losses by the surface and the plasma formed near this surface during the interaction. Such refinements are aimed at improving the prediction of laser influence consequences.

The obtained temperature dependences in an analytical form are quite complex. In general, they depend on the coefficients of reflection and surface scattering of incident radiation. Their character is quite complex and depends on the structure of the irradiated surface itself. The specified coefficients, in turn, also have a significant dependence on temperature. Asymptotic approximations are used in the research. But they do not allow us to see the general picture of changes in the temperature characteristics of the surface. Therefore, there is a need to apply numerical methods to clarify the temperature dynamics of the surface under intense laser influence.

Theoretical and numerical prediction of the results of laser exposure, both destructive and non-destructive, on various surfaces of materials today is extremely important. Laser technologies are used in many areas. Currently, one of the important areas is research related to the use of optical sensors. Here the laser ray falls on a metal layer of nanoscale thickness. Considering that the thicknesses of the films used in surface plasmon resonance sensors are nanosized, the problem is further complicated. This is due to taking into account the dependence of the temperature of the nanosized metal layer on the absorption coefficient.

The paper calculates the temperature dependence of the heating of metal films applicable in SPR sensors. The obtained results are compared with previous results, where the temperature dependence of the optical loss coefficients was not considered.

Temperature range of deuterium retention from ferritic-martensitic steel implanted deuterium at temperature 100 K

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Deuterium thermal desorption spectra were investigated on the samples of ferritic-martensitic steel (16Cr12W2VTiAB) implanted deuterium at temperatures 100 K with deuterium ions in the dose range from 5×10^{16} to 4×10^{18} D/cm^2. It has been determined that for low implantation doses, the thermal desorption spectrum of ion-implanted deuterium is a wide temperature range of deuterium desorption in the temperature range of 400–1000 K. As the dose increases, this temperature range of deuterium desorption expands in the direction of decreasing temperature and at a dose of 1.6×10^{17} D/cm^2, a wide peak with a maximum temperature of 400 K appears. A further increase in the implantation dose of deuterium is accompanied by the appearance of a lower temperature region of deuterium desorption with a maximum temperature in the temperature range of 200–250 K. At doses above 8×10^{17} D/cm^2, a qualitative change in the deuterium thermal desorption spectrum occurs, which manifests itself in the appearance of a lower temperature region of deuterium desorption in the form of a clearly pronounced peak with a maximum temperature of ~180 K.

A further increase in the dose of implanted deuterium leads to an increase in the intensity of the lowest temperature peak of the deuterium thermal desorption spectrum, and it becomes dominant. The formation of a low-temperature intense peak in the deuterium thermal desorption spectrum may indicate the appearance of a new phase state, which can be considered as the formation of a hydride. The conclusion about the formation of a hydride was made on the basis of the data obtained by us in the study of the thermal desorption spectra of deuterium from Pd, Ti and ASS steel. These works show that the formation of hydrides is reflected in the deuterium thermal desorption spectrum by the appearance of lower temperature peaks. It is important that the formation of low-temperature deuterium desorption regions is accompanied by the appearance of a deuterium desorption region extended along the temperature scale in the temperature range of 200–1000 K.

Effect of thickness on the formation of grain boundary joints in undoped silicon films with a fibrous structure

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The structure of silicon films is the object of extensive research, since it has a great influence on the stability and reliability of devices in which polysilicon is used. Characteristic elements of the silicon film structure that affect the properties of the films are grain boundary joints. There are studies that are devoted to the analysis of the atomic structure of individual triple junctions in silicon [1]. But these studies do not give an idea of the role of film formation conditions and subsequent technological treatments in the formation of one or another type of grain boundary joints.

The aim of this work is to study the mechanisms of the formation of grain boundary joints in fibrous undoped silicon films of various thicknesses.

Silicon films were obtained by low-pressure chemical vapour deposition on thermally oxidized (100 nm oxide thickness) (100) Si wafers. The deposition temperature was equal to 630°C. The film thickness was ranged from 85 nm to 1500 nm. The structure of the films was studied by transmission electron microscopy. Surface morphology was analyzed by atomic force microscopy.

It is shown that in fibrous undoped silicon films, both triple and multiple junctions of grain boundaries of different types are observed, the ratio of which is determined by the film thickness. Multiple junctions of grain boundaries occur in films through such mechanisms as multiple twinning, splitting of grain boundaries, interaction of $\sum 3^n$ boundaries during film growth, and faceting of grain boundaries.

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Optical characterization of thin ferroelectric P(VDF-TrFE) films structural composition

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The ferroelectric polymer material P(VDF-TrFE) is promising in terms of applications in such fields of technology as wearable medical electronics, tactile sensors, and even nonlinear optical devices [1]. Among its advantages are flexibility, high chemical resistance and biocompatibility. Thin films are an important form of production this material for practical applications. Depending on the fabrication and operation conditions, this copolymer can exist in several molecular conformations or phases. Regarding ferroelectric properties, the beta phase attracts the greatest practical interest. Therefore, methodology of optimal manufacturing such material and its structural control is relevant.

Using the spincoating method, a set of polymer films samples was fabricated, differing in the speed of the substrate rotation (in the range of 2000...6000 rpm), as well as in the concentration of the solution from which they were formed (13%, 17% by mass). Copolymer powder with a molecular ratio VDF:TrFE = 70:30 and dimethylacetamide were taken as initial components. The formed material was controlled by the methods of atomic force microscopy, spectral ellipsometry, and was also subjected to annealing, in order to affect the phase composition (typical temperatures in the range of 140...170°C). A comparison of the obtained characterization results is presented in this work.

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The aligning properties of the sapphire with LIPSS in the twisted nematic cell

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We study aligning properties of the nanostructured surfaces with Laser-induced periodic surface structures (LIPSS). The usage of the surfaces with LIPSS (e.g. metals [1], transparent dielectric materials [2]) for the uniform orientation of different liquid crystals (LC) phases, namely nematics, blue phases, twist-bend and ferronematic phases, is the perspective branch of the LC alignment.

We investigate nanostructured sapphire surfaces with different characteristics (e.g. period of nano-grooves and width of unstructured gap) as one aligning layer in twisted nematic cells. To increase the anchoring energy of the LIPSS-treated sapphire, the surface was covered either with polyimide without using the rubbing treatment or with the coated photopolymer to obtain the 'command' aligning surface. We made measurements of the alignment properties with different UV light treatments of the photopolymer. The theoretical model of the twisted nematic cell with LIPSS on one surface is in progress.

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New electrode substrate for the construction of all solid state ion-selective electrode

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Ion-selective electrodes are low-cost and easy-to-use potentiometric sensors that selectively respond to a specific ion in the presence of other sample components. Electrodes without an internal electrolyte solution have recently become very popular, as they are more convenient to use and cheaper to manufacture and easier to miniaturise compared to electrodes with a conventional architecture. The direct connection between the ionically conductive membrane and the electronically conductive electrode substrate creates a phase boundary where charge transport is inefficient resulting in instability and non-reproducibility of the electrode potential. Known solutions to this problem involve the introduction of an intermediate layer, e.g. of a conductive polymer or carbon nanomaterial, between the membrane and the electron-conducting substrate.

In this paper, another solution will be presented consisting in the use of a new electrode substrate in the form of several hundred gold microelectrodes combined into one substrate electrode, on which only the ion-selective membrane is applied without an intermediate layer. The effectiveness of the new substrate was tested on two model systems in combination with a valinomycin-based membrane sensitive to K^+ ions and a membrane sensitive to NO_3- ions. For comparison, electrodes with the same membrane containing a gold disc electrode and a glassy carbon disc electrode were tested in parallel. The properties of ion-selective electrodes were examined by determining their parameters, such as: detection limit, linearity range of the calibration curve, characteristic slope, selectivity, potential reversibility, potential stability (potential drift) and sensitivity to redox potential changes. It was determined how these parameters change depending on the construction of a given electrode and the measurement conditions, such as the direction of concentration changes during calibration and mixing of the solution.

It was found that the SCISEs based on the new microelectrode array are characterized good analytical parameters, in particular, a significant improvement in the stability and reversibility of the potential was noticed compared to the electrodes based on conventional substrates.

Structure and mechanical properties of TiN coatings deposited by vacuum-arc method under high nitrogen pressure

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The vacuum arc method allows obtaining a wide range of solid nanostructured coatings on the surface of tools and parts for various industries. Most of the developed processes are based on the deposition of plasma flows at low gas pressure in a vacuum chamber (< 1 Pa). The deposition of nitride coatings in the area of higher nitrogen pressures appears promising, as it allows reducing the content of defects in the form of macroparticles of cathode material in the coatings.

In this study, the structure and mechanical properties of vacuum arc TiN coatings deposited at a nitrogen pressure of 2 Pa and a negative bias potential on the substrate ranging from 50 to 300 V were investigated. Atomic-force microscopy revealed that smooth coatings with a small number of uniformly distributed macroparticles were deposited on the surface of polished Ti-6Al-4V alloy samples throughout the entire range of potential changes. The surface morphology of the coatings is nanosized cellular with low roughness, which decreases from 15 to 6 nm as the potential increases. Somewhat unexpected is the increase in specific surface energy, indicating an increase in the adhesive interaction between the probe and the coating.

X-ray structural analysis revealed that a single crystalline phase, TiN nitride with a cubic structure of the NaCl type and strong axial texture [111], is formed in the coatings. As the potential increases, the texture in the coatings becomes more perfect, the crystallite size of the nitride increases from 46 to 86 nm, and the level of microdeformations and compressive macrostresses decreases.

According to the results of nanoindentation, all coatings are characterized by high mechanical performance. The most promising in terms of wear resistance is the TiN coating obtained at a potential of 150 V, which has an optimal combination of relatively low stress levels (6 GPa) and maximum values of hardness (32 GPa) and resistance to plastic deformation ($H^3/E^2 = 0.12$).

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Random sequential adsorption of mixtures of particles on a planar surface using the two-stage procedure

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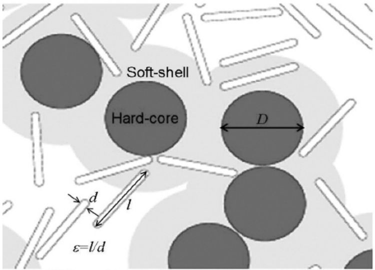
Model of random sequential adsorption (RSA) is widely popular to simulate formation of films on the two-dimensional (2D) substrates [1]. Such materials have shown promising practical applications in electronic, optical, magnetic and biomedical devices. This work studies two-stage RSA models for packing anisometric particles. In these models the 2D substrate was preliminary covered (pre-patterned) with particles of the first sort and then the particles of the second sort we added up to the jamming limit. Particularly, in so-called SD model, the discorectangles were initially deposited and discs were added and the situation was opposite in the DS model. The main parameters of the model are the disc diameter D, aspect ratio ε (length to width ratio) of the discorectangle, and level of preliminary coverage φ_ε (SD model) or φ_D (DS model). The dependences of the coverage of the adsorbed particles on the second stage on the model parameters were analyzed. For RSA processes on pre-patterned surfaces the particles were adsorbed in voids formed by the particles deposited in the first stage and there exist limits on the maximum values of $D_{\max}$ (SD model) or $\varepsilon_{\max}$ (DS model) defined by the level of φ_ε or φ_D, correspondingly. Percolation connectivity was also analyzed for particles with the core-shell structures.



RSA packing on the pre-patterned surface

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Effect of the surface nanocrystallization on the gas nitriding of two-phase titanium alloy

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Due to their excellent mechanical and anti-corrosion properties, high-strength two-phase titanium alloy (Ti–5Al–5Mo–5V–Cr–Fe) is widely used in the aircraft industry. However, this titanium alloy has low wear resistance, which limits its use in tribo-pair without additional surface treatment and, therefore, determine the need to develop effective methods of surface engineering. For these reasons, gas nitriding is a promising, technologically simple and economically efficient method of surface engineering for wear resistance enhancement of titanium alloy. Generally, the treatment temperature for the conventional gas nitriding of the titanium alloy is near 950°C with a processing time of several tens hours, resulting in high energy consumption and a significant negative effect on the matrix microstructure and mechanical and fatigue properties reduction of titanium alloy. Therefore, the issue of intensification of nitriding of titanium alloy becomes especially relevant [1].

In the work, the intensification of gas nitriding is provided by pre-surface nanocrystallization of titanium alloy. Ball burnishing was performed on titanium alloy to form surface nanostructures. By carrying out pre-surface nanocrystallization, it is possible to activate nitride formation on the surface of the titanium alloy, which leads to the texturing of the nitride layer from the nitride of lower valence Ti_2N into mononitride TiN. The intensification of nitriding is evidenced by an increase in surface microhardness and a thickening of the hardened layer compared to conventional gas nitriding under similar time-temperature parameters. This intensification can be attributed to high-density dislocations and grain boundaries that were introduced by pre- nanocrystallization and served as efficient channels for nitrogen diffusion.

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Heterolayers of cubic cadmium sulfoselenides with a surface nanostructure

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The basis of many functional electronics devices are CdS and CdSe crystals of the typical hexagonal (α) modification of the crystal lattice. At the same time, the question of obtaining their heterolayers (HL) with an atypical cubic modification with time-stable characteristics, properties and high radiation intensity in the short-wave region is important. Therefore, it is relevant to choose methods and modes of obtaining their nanomaterials, which provide fundamentally new properties [1].

The basic β-CdSe and β-CdS HLs were obtained by the method of isovalent substitution at T = 900-1100°C, which ensured the formation of β-CdSe/β-ZnSe and β-CdS/β-ZnS heterostructures (HS) of atypical cubic modification with stable properties. Based on studies of the differential spectra of absorption T'_ω and reflection R'_ω, the basic parameters of the energy structure $E_g = 2.02$ eV (β-CdSe) and $E_g = 2.90$ eV (β-CdS) were determined. Surface nanostructures were obtained by the chemical treatment of HS in etchant H_2SO_4:H_2O_2 = 3:1. The variation of time and temperature regimes of etching ensured the morphology of the surface layer characteristic of nanostructures. According to AFM topographies made on an atomic force microscope NT-206, the presence of pyramids with base sizes of 2-5 µm, which combine into nanopyramids with lateral dimensions of up to 10-100 nm, was revealed. A characteristic feature of the obtained HSs is the formation of two emission bands - A in the range of quantum energies $\hbar\omega \sim E_g$, as well as a broad band B with quantum radiation efficiency η = 7-15 % in the region $\hbar\omega >> E_g$ with maxima corresponding to HSs $\hbar\omega_m \approx 2.75$ eV (β-CdSe) and $\hbar\omega_m \approx 3.37$ eV (β-CdS) The properties of the band are determined by the quantum-dimensional effect, and the spectrum according to the well-known equation

$$\hbar\omega_m^B - E_g = \frac{\pi^2 h^2}{2d^2}\left(\frac{1}{m_n^* + m_p^*}\right)$$

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Thin CIGS films obtained by spray pyrolysis

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Nanostructured materials stand apart from their bulk counterparts due to their fundamentally novel and improved properties. Metallic nanostructures are among the most extensively researched nanomaterials. Nanostructured thin films consisting of metal nanoparticles have found application in solar cells. Today, the solar cell market showcases a variety of technologies, with solar cells based on CIGS ($Cu(In,Ga)(S,Se)_2$) attracting particular attention due to their high efficiency, durability, and the potential for economical fabrication methods [1, 2].

In this research, we report the synthesis of thin films using spray pyrolysis. Indium and gallium sources were derived from $InCl_3$ and $GaCl_3$ chlorides, respectively. Copper was sourced from $CuCl_2$ chloride. All components were mixed using both organic and inorganic solvents (oleic acid and selenous acid, respectively). H_2SeO_3 also served as a source of selenium. The components were blended with the help of a magnetic stirrer for a period of 20 minutes. The Ga/(In+Ga) ratio in the films was controlled by changing the Ga/(In+Ga) ratio of precursors from 0.4 to 0.6.

As a result, films were formed in all modes of operation. SEM analysis revealed that the films have a granular structure and consist of disordered crystallites. All samples exhibit X-ray diffraction peaks corresponding to the chalcopyrite structure of CIGS (JCPDS 35-1102). No other impurity phases were detected, except for the CIGS phase.

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Optimization of characteristics of laser-processed metal/semiconductor surfaces for sensor application

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Development and improvement of new or existing structures for sensorics application is perspective and challenging task. We elaborate the formation process of femtosecond laser-induced periodic surface structures (LIPSSs) on metal (Ag, W), semiconductor (Si) and dual metal-semiconductor (Au-Si) surfaces for sensor application. The resultant parameters and morphology of LIPSSs are determined by many laser parameters, that is irradiation wavelength, polarization, pulse power density, number of the laser pulses, surface scan speed. Each of the laser irradiation parameters stipulates certain characteristics of processed surface, namely the scale and direction of the LIPSSs, periodicity perfectness, depth, width, and micro-roughness of the LIPSSs, etc. In this report we focus on the methods of the characterization of laser-teated surfaces and byproducts of texturing (especially, ablated nanoparticles), ways of the optimization of crucial parameters of the surfaces. The scanning electron microscopy (SEM) and 2D Fourier transform of obtained SEM images of the laser-perocessed surfaces reveal the deviations from periodicity, the presence of nanoparticles (NP) and other features on the surfaces of all studied materials. We develop a method of a real-time monitoring of the LIPSSs formation which is based on the measurement of the emission from semiconductor (Si) during its laser structuring [1]. Thus the intensity ratio of the second harmonic generation on the modified Si surface to the sharp emission lines of the ablated Si atoms and ions indicates the quality of the formed LIPSSs. We also alalyzed measured time-resolved emission from the surface under structuring. We evaluated the NPs produced during femtosecond laser ablation of the studied substances using dynamic light scattering. We conclude wich charachteristics of laser treatment is essencial for enhansement in SERS and SEPL.

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Initial stages of Ce_xO_y film growth on Mo(112): structure and electronic properties

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Nowadays, rare-earth metals find many useful applications in electronics, catalysis, optics, medicine etc. These metals are rather expensive, but, fortunately, show their useful properties being present even in minor amounts (in combination with other elements). In our investigation, the atomic structure and work function changes of Ce and O films coadsorbed on Mo(112) were studied using low-energy electron diffraction (LEED), Auger electron spectroscopy(AES) and contact potential difference (CPD) methods. The adsorbate coverages (θ_{Ce}, θ_O) were defined as the ratio of the concentrations of adatoms to the concentration of atoms on the substrate surface. The coverage ranges for the formation of various ordered surface structures are determined. Based on these data, the stoichiometry of surface phases in the (Ce+O)/Mo(112) system was established and hypothetical hard-sphere models of atomic structures were proposed.

For coadsorbed (Ce+O) films with a significant predominance of one element, the structure of the main-component remains stable within the impurity content of 15-50% in various coverage ranges. At θ_{Ce} = 0-0.5 (submonolayer range), the new (Ce+O) structures, namely c(4 4) and c(2 6) were found. Such phases containing up to 75% and 100% of oxygen are specific just for the (Ce+O)/Mo(112) system, they have not been previously observed either for cerium oxides or for cerium and oxygen adfilms. In the range of θ_{Ce} = 0.75-1.5 (more than one physical layer), the formation of close-packed c(4 6) and (4 4) structures was observed.

The adsorption of Ce on Mo(112) leads to a decrease in the work function by 2.1-1.5 eV. No noticeable effect of oxygen on the work function difference of the Ce/Mo(112) film was detected. Both oxygen-enriched and oxygen-depleted (Ce+O) films show similar typical electropositive properties. This effect can be explained by the specific direction of the electrical dipole associated with the Ce-O bond.

Magnetic field effect on crystallization of glucose from aqueous solution

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The structure of crystallite films, obtained by epitaxy [1] from the water solution of glucose, was studied using “Intergra” nano-laboratory. The magnetic field applied to the solution was found to increase the rate at which crystals grow. A proposed mechanism of crystallization assumes the cluster structure of the solution. We believe the magnetic field breaks down the clusters in the solution, thus increasing the rate of crystallization. The experimental support for this hypothesis was found by analyzing light scattering, the kinetics of evaporation, and the temperature dependence of density of the water solution of glucose with and without the applied magnetic field. Considering the objectives of the research and its practical aspect, the magnetic fields used in our experiments are weak. The sample system we investigate is the epitaxy from the water solution of glucose, as the present paper builds up on our prior work [2].

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Peculiarities of plasma-electrolyte treatment of multicomponent alloys with the formation of heterooxide nanocomposites

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Alloys of valve metals are widely used as carriers of catalytic systems. But plasma-electrolyte treatment of such materials is complicated by the heteroresistivity of the surface of Al and Ti multicomponent alloys. So, establishing the features and developing the optimal method of PEO surface treatment of such materials is an important practical task. Alloys AK12M2MgN and OT4-1 were the model objects for experimental studies. It was established that varying the composition of the working electrolytes, PEO regimes, and adding dopant metals (Co, Mn, Zn, Mo, W) provide flexible control of the characteristics and properties of the formed heterooxide nanocomposites. We have established approaches for controlling PEO treatment of multicomponent Al (Ti) alloys. It is shown that the ratio of electrolyte components (c, mol/dm^3), PEO current density (j, A/dm^2), sparking and formation voltage (U_s, U_f, V), PEO time (t, min) are factors of the variability of plasma-electrolyte treatment of alloying alloys [1]. Changing these parameters allows to change the qualitative and quantitative parameters of the modified surface, as well as to determine the complex of functional properties of the synthesized coating. The practical significance of the obtained results is the developed variable technological schemes of plasma-electrolyte treatment of multicomponent aluminum (titanium) alloys in diphosphate electrolytes with minimization of alloying elements in the surface layers and the formation of heterooxide coatings with an increased content of active components and specified functional properties.

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Surface-modified layers CdTe of oxygen-doped

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Cadmium teluride is a promising material for the manufacture of various types of detectors, such as light, X-ray, electron, proton, and others [1]. Diode structures with a surface barrier that can be used in solar cells play an important role among such devices [2]. Thin layers in these structures determine the physical and technical characteristics of the devices and are the active region. Therefore, an important problem arises of minimizing the concentration of defects at the separation boundary between the contact and the semiconductor [3]. These defects form surface levels, which can be effective recombination centers, which as a result leads to an increase in loss currents and noise levels, a decrease in the breakdown voltage, and the appearance of various types of instabilities [3]. An effective technological approach to reduce the influence of these levels is the creation of modified surface layers that significantly improve the photoelectric properties of diode structures. One of the important aspects is the introduction of isovalent impurities that impart specific properties to the material [4]. In this paper, we consider the process of obtaining modified CdTe layers doped with an isovalent oxygen impurity.

In this study, n-CdTe single crystals were used as the base material. They were obtained using the Bridgman method and had a resistivity of approximately 40 Ωcm at 300 K. The studied modified CdTe:O layers were obtained by doping with oxygen during annealing of the CdTe samples in air at temperatures from 700 to 1000 K. Condition surface of the initial substrates and the doped layer were monitored using a Nanoscope-IIIa atomic force microscope in the periodic contact mode.

After annealing the output n-CdTe plates, a CdTe:O layer is formed on their surface, which leads to a modification of the microstructure. The initial surface looks like a mirror, but after annealing it becomes matte. Studies using an atomic force microscope revealed that after heat treatment of CdTe, large blocks with arbitrary orientation and sizes up to 800 nm are formed on its surface. These results are consistent with similar observations of the effect of annealing on the state of the surface.

The appearance of highly efficient luminescence in CdTe:O layers at 300 K is an important phenomenon both for theoretical research and for practical use. This phenomenon is not observed in the initial single crystals. The emerging radiation is predominantly localized in the edge region. It has the following features: the presence of photons with an energy exceeding the band gap Eg, the independence of the position $\hbar\omega_m$ from the photoexcitation intensity when the latter changes by three orders of magnitude, as well as similar temperature dependences of the positions $\hbar\omega_m$ and E_g in the temperature range from 77 to 450 K. These features indicate the participation of interband transitions in the recombination process. In this case, the emission spectrum can be described by a known expression.

$$N_\omega \approx (\hbar\omega)^2 \sqrt{\hbar\omega - E_g}\,\exp\left(-\frac{\hbar\omega - E_g}{kT}\right)$$

where k is the Boltzmann constant, T is the temperature, N is the number of photons in a unit energy interval.

The appearance of intense luminescence at 300 K in CdTe:O layers is explained by the isovalent character of oxygen as an impurity. This phenomenon is caused by interband recombination of free charge carriers.

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Graphene based electron emitters with low work function due to rubidium intercalation

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This paper describes the electrochemical methods of producing and the results of researching layered graphene structures on a metal substrate, which can be used both to reduce the work function of the cold field emitter's cathode material by intercalating its surface layers with alkali metal atoms, in particular rubidium, and to create surface elements with a large aspect ratio.

The graphene nanoplates (scales) obtained by electrochemical methods were deposited on the surface of a nickel substrate by electrolysis from a mixture.

SEM research has shown that graphene scales stick together in a uniform layer of about 100 nm thickness with good adhesion to the substrate. The contours of separate graphene layers are visible on the surface. Due to defects, some parts of the graphene scales are oriented almost perpendicular to the surface, which increases their aspect ratio. Accordingly, the electric field is locally amplified around them. In this case, the defects have a positive effect.

Intercalation of graphene layers with rubidium was also attempted. Varying the mixture concentration, deposition time and deposition voltage affected the type of structures obtained on the substrate surface.

In conclusion, we have developed a method for the electrochemical synthesis of uniform graphene layers with good adhesion to a nickel substrate, which are perspective for the production of cold field emission cathodes that will operate at a significantly reduced external electrical field voltage without reducing the emission current.

Sensitivity of positron spectroscopy to nanoclusters formation in the strongly correlated binary alloys

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When quantum and collective phenomena at nanometer scale in atomic and electron subsystems of solids define some observable physical properties, they can exhibit itself in macroscopic level. Occurrence of such many-particles phenomena in solids determines the most promising materials for modern technologies. One of the powerful methods, which allows an experimental observation of corresponding effects in the electronic structure, is the method of positron spectroscopy, namely, the method of angular correlation of electron positron annihilation radiation (ACAR). In addition, this method allows to determine the size and concentration of defects in crystal and to study their electronic properties. Thus, the theoretical consideration of the influence of some many-particles effects on the momentum distributions of conduction electrons recorded by the ACAR method is important.

The nanoclusters formation (from one of two atoms' types — A or B) in binary substitutional alloys with strong electron correlations are investigated in the single-band Hubbard model for systems inclined to segregation. As shown at temperature of 0 K, such nanoclusters significantly change the momentum distributions of electrons as well as the equilibrium values of magnetic moments at the atoms of different types (atoms in clusters are considered as the third component C of alloy) and the parameters of pair correlations in the arrangement of atoms of different types and in the orientation of electron magnetic moments at nearest sites. The more strong atomic scattering potential of alloy component B determined the partial density of states, which firstly filled by electrons, and the type of clusters (from atoms of type B) with biggest magnetic moments at corresponding atoms in comparison with clusters from atoms of type A. Because of differences in the spectral function summation in the reciprocal space, the ACAR dependences demonstrate a greater sensitivity to the effects of nanoclusters formation than corresponding dependences of the electronic density of states.

Mass transfer and atoms mobility in high-entropy alloy and steel under the force influence

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The study of the diffusion and mass transfer mechanisms is reasonable for the formation of parts and tools surface layers that will have improved performance characteristics. The existing theoretical approaches for diffusion parameter determination, including anomalous diffusion, are described by the authors [1,2]. In the frame of this work, an experimental approach has been designed for finding the parameters of anomalous mass transfer by the radioactive isotopes method using ^{60}Co and applied to the HEA (AlFeNiCoCuCr) and Steel 3 after electrospark alloying and shock treatment.

The generalized mean (defined by both diffusion and drift) and root mean square as the first and second normalized statistical moments of the distribution, respectively, were founded from the experimental concentration distribution. Shown, that when the contribution of drift to the total mass transfer is large, the resulting concentration distribution significantly differs from the random walk mechanism theory of diffusion [2].

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Effect of alloying on long-term oxidation resistance and electrical conductivity of nanolaminate MAX phases of Ti-Al-C system

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A solid oxide fuel cell (SOFC) is an efficient source of autonomous power supply. For long-term operation, FC materials must be stable under technological conditions of 600°C air. The solution to this problem is associated with the creation of oxidation-resistant materials that have a low density and allow the manufacture of thin-walled FC interconnects, which is proposed to be implemented by creating layered titanium interconnects (0.3-0.5 mm thick) with coatings based on MAX phases of titanium [1] to replace traditional interconnects based on Crofer steels.

The work is devoted to the study of the influence of alloying of the MAX phase of the Ti-Al-C system with such alloying elements as Nb and Sn on the long-term oxidation resistance at 600°C of coatings obtained by two methods: vacuum arc plasma and magnetron sputtering. It was established that doping Nb up to 10 at.% and Sn up to 50 at.% increases long-term oxidation resistance in air at 600°C. The electrical conductivity of the obtained coatings is at the level of 1...$2 \cdot 10^6$ S/m

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Deuterium desorption temperatures of Al-Ti and Mg-Ti composites Prepared by the method of atom-by-Atom component mixing

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Aluminium-based and magnesium-based alloys are promising in the view of present-day requirements to the metal-hydride hydrogen storage systems. Behavior of hydrogen in the aluminium-based magnesium-based alloys is of scientific and applied interest that is confirmed by many publications. However, the use of such alloys presents some difficulties because of the high hydrogen desorption temperature (550-600 K).

To manufacture Al-Ti composites the plasma evaporation-sputtering method was used enabling the atom-by-atom component growth. Thus, the composites with a wide range of the ratios of components were obtained. A composite was deposited on the molybdenum foils (0.2 mm thickness, 10 mm width, 250 mm length) placed between the cathode assemblies in the facility. Deuterium introduction into the samples was performed by the ion implantation method. Deuterium desorption temperature ranges and deuterium storage levels were determined by the thermal desorption spectroscopy (TDS).

A low aluminium concentration and, consequently, a high titanium concentration in the composite are demonstrated in the deuterium TDS as a single peak with a maximum temperature at 820-840 K as a function of the implanted deuterium dose and composite composition. A single-peak character of the deuterium TDS, observed for aluminium concentration values from 10 to 70 at.%, evidences on the homogeneity of composite structural state in this range.

As the aluminium concentration in composites increases the deuterium TDS is significantly changing and, as a result, the deuterium desorption temperature for $Al_{85}Ti_{15}$ composites sharply decreases (T_m~550 K). A step-like shape of the maximum temperature curve of thermoactivated deuterium desorption, as a function of the component concentration change, evidences on the existence of two different structural states of the Al-Ti system depending on the ratio of components.

Strong electron-electron interaction in epitaxial graphene induced by Bi(110) islands [1]

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Magneto-conductance and Hall voltage of epitaxial graphene formed on SiC and covered with ultrathin Bi islands were measured within the range of ±4T. The structure and morphology of Bi coverages of average thickness up to 4 bilayers, MBE-grown at RT as well as after-annealed, were determined by SPA-LEED and STM techniques. The coverage was found to consist of needle-like (110) islands with "magic" thicknesses.

The analysis of the low-field part of the magneto-conductance [2] reveals a transition from weak-localization (WL) to weak antilocalization (WAL) with increasing Bi coverage and allows to characterize the scattering of conduction electrons by determining electron scattering lengths, namely inelastic-dephasing, intervalley and intervalley symmetry breaking ones. The correlation of average sizes of (andǐor distance between) Bi(110) islands for different coverages with the characteristic lengths demonstrate the role of electron scattering on edges and within the islands in the WL-WAL transition. Calculated dependencies of Hall and magneto-resistance allow determining changes of electron density induced by Bi adsorption and reveal the substantial contribution of electron-electron interaction in electronic transport [3].

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Electronic structure of zinc oxide thin films doped with nitrogen and fluorine

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ZnO films are attracting attention due to their unique optical and electrical properties as well as their wide range of applications. A wide bandgap of up to 3.37 eV and a transparency of about 80% in the visible range and low electrical resistance make them a potential candidate for use in solar cells as a transparent conductive electrode. However, today, the transparency and electrical conductivity of ZnO films are still lower than that of the widely used and expensive tin doped indium oxide (ITO). Thus, the doping of Indium-Zinc-Oxide thin films with nitrogen increased the transparency and narrowed the width of the optical band gap due to the reduction of oxygen vacancies [1]. After fluorine doping of zinc oxide thin films, an increase in transparency and a decrease in resistivity were observed [2]. therefore, optimization of the processes of obtaining ZnO films by doping with various elements, in particular, fluorine and nitrogen, in order to improve physical properties is an essential task.

In this work, ZnO films were prepared by magnetron deposition and doped with fluorine by placing fluoroplastic in a chamber. Nitrogen was present in the plasma atmosphere by injection from the gas phase. The resulting films were analyzed by X-ray photoelectron spectroscopy (XPS). XPS revealed the presence of only Zn, O, C, and N and F in the doped samples, indicating a successful doping procedure. The value of the modified Auger parameter for Zn L3M45M45 was 2010.1-2010.3 eV, which, when compared with the corresponding parameters of the NIST database [3], indicates the presence of only Zn-O bonds. Thus, zinc does not interact with fluorine and nitrogen. The XPS spectrum of oxygen was decomposed into two components (Fig. 1), the peak with a lower binding energy characterizes ZnO, the peak with a higher binding energy corresponds to oxygen with broken bonds. After doping with nitrogen and fluorine, a decrease in the intensity of the high-energy oxygen peak was observed (Fig. 1 b), which may indicate a decrease in the number of oxygen vacancies. Given that nitrogen and oxygen have almost the same atomic radius, and fluorine has an even smaller atomic radius, it can be assumed that nitrogen and fluorine atoms diffuse into the oxygen-deficient regions, thereby reducing the number of defects in the film.

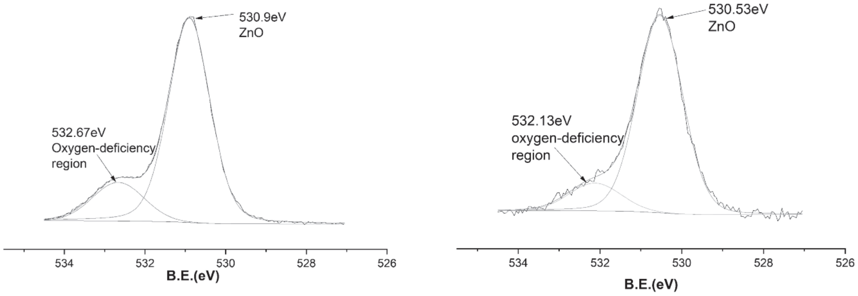

Fig.1 *a) XPS O1s spectrum of ZnO thin film b) XPS O1s spectrum of N and F doped ZnO thin film.*

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Development of frontal anti-reflecting nanotextured silicon layers using electrochemical and chemical etching methods

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The aim of this work was to develop and study frontal functional nanolayers of solar silicon (SC) using electrochemical and chemical technologies of porous silicon (PSi) to obtain efficient and cost-effective technological processes for the production of photoelectric converters. These technological processes should be adapted to the processes of production of silicon solar cells. Optimization of the technology of electrochemical formation of porous silicon layers has significantly improved their antireflective and passivation properties [1, 2]. Technologies for creating textures of the SC front surface are based on the process of dissolving the surface layer of silicon in solutions based on hydrofluoric acid. As the surface is covered with Si-O-Si bonds, the dissolution reaction becomes less active and stops with the formation of a continuous oxide film [3].

However, in order for porous silicon to be effectively used as an anti-reflective coating in the structure of silicon SC, its parameters and production technology must meet the following two requirements: a) the parameters of the translucent porous layers should not negatively affect the output electrical characteristics and efficiency of the SC; b) the technological processes of forming and hydrogenating layers of porous silicon should be compatible with the technology of creating silicon SC and not complicate it.

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Session 6

Nanooptics and photonics

Electrophysical properties of InGaN/GaN LEDs with quantum wells

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Traditional lamp-based lighting systems,such as filament bulbs and fluorescent tubes, have been progressively replaced by LED-based solid-state lighting (SSL). LED emits lights when forward current is applied to its p-n junction. Small and energy efficient LEDs have quickly conquered the field of microelectronics and optoelectronics. Commercial LEDs are made of III–V group compounds, which are GaAlAs (red-emitting), AlInGaP (yellow-orange), InGaN (blue, green), AlInGaN (ultra violet). Among them InGaN/GaN heterostructures with quantum wells (QW) as the core light-emitting region define an important standard for SSL [1].

The purpose of the study was to investigate the temperature dependence of electroluminescence and current-voltage characteristics (CVCs) of the InGaN/GaN heterojunction assembly in comparison to the homojunction ones (GaP, GaAsP).

The InGaN/GaN heterostructure with QWs was grown on sapphire (Al_2O_3) and demonstrated the maximum emission of electroluminescence at 505 nm [2]. It was found that at 290 K the single band splits into two peaking at 500 and 506 nm, the latter is of lower intensity. The separation of ~30 meV between them is close to the energy of acoustic phonone in GaN. The rise of injection current leads to a blue-shift by 0.043 eVdue to the band filling effect. It is a distinct feature of the heterojunction. The quantum yielddrops twice in a linear interval from 1 to 20 mA.

CVCs were acquired in the current generator mode for the 77-290 K temperature range. They demonstrate a power-law dependency. The negative differential resistance region most evidently appears at 77 K.Some decrement in the *dI/dU* slope before the S-shaped region is indicative of increment in the diode's differential resistance. The S-type regions are immanent to the systems with positive feedback [3]. The presence of instability within $dI/dU<0$ implies a variation in the current flow mechanism. The phenomenon might occur due to the resonant tunneling of carriers along the quantization levels, enhanced by the effect of their quasi-ballistic transfer through QWs.

We believe that both the appearance of a negative differential resistance and a decrease in quantum yield are manifestations of discrete levels in QWs.

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Differences in emission spectra of pristine and irradiated with 2 MeV electron beam InGaN/GaNLEDs with quantum wells

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The InN-GaN solid solutionsare used for the production of efficient InGaN LEDs emitting in the UV and Vis ranges thanks to their direct and wide band gap. They are typically fabricated on a sapphire substrate resulting in a lattice mismatch of ~12% between GaN and Al_2O_3. The development of mismatch dislocations especially in the quantum wells (QW) region introduces piezo-fields through the mechanical stress and additionally strengthens the natural polarization in the (0001) direction of growth [1]. The quantum-confined Stark effect is becoming more pronounced resulting in larger space separation of charges due to distortion of the energy zones and lower probability of their radiative recombination [2].

The permeable radiation is known to affect the electrophysical properties of materials by introducing structural defects and reducing the lifetime of minority charge carriers. The impact manifests in reduction of the emission intensity and of the current as it has been demonstrated for both the homo- and heterojunction LEDs [3]. The degraded characteristics might be partially restored by the thermal annealing [4].

In the present study we will focus on changes in electroluminescence spectra of InGaN/GaN LEDs with QWs caused by the 2 MeV electron beam irradiation with the flux up to $2.25•10^{15}$cm^{-2}. The blue color (λ_{max} = 470 nm) emitting $InxGa_{1-x}N$/GaN (x = 0.2) LEDs were grown on sapphire substrates. Thetemperature-dependent emission study was performed in the temperature range of 77–300 K for both the pristine and the irradiated LEDs and results are presented in Fig. 1.

As can be seen from Fig. 1, the emission spectral line has the Gaussian type profile perturbed by a phonon repetition peak (the phonon energy is $\hbar\omega\Phi = 65$ meV) in the low-energy side. It was also observed that the intensity of the LED glow can be amplified by increasing the injection current. Although, this can be done within a certain interval only, because for the current value exceeding 20 mA, there is a tendency to saturation caused by the filling of QWs and rising ballistic transfer of carriers through them. These effects are even more prominent for the irradiated LED, where the characteristic maximum appears at currents much smaller than the nominal one (≈5 mA), and followed by a steady decrease in quantum yield.The luminescence intensity diminishesdue to the introduction of deep non-radiative levels in the QW.

The observed performance decrement of the heterojunction LEDs under study after being irradiated with the 2 MeV has been found less pronounced in respect to what was observed for the correspondent homojunction LEDs according to the literature [5], thus, suggesting a better radiation resistance.

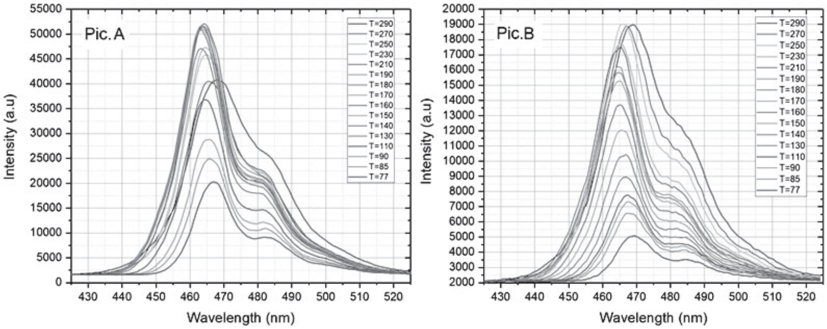

Fig.1. *Temperature-dependent (77–290 K) emission spectra of pristine (A) and irradiated with 2 MeV electron flux (B) InGaN/GaN LEDs with QWs.*

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The ellipsometry of chromium-glass, nickel-glass, and nickel-chromium-glass nanosystems below and higher the Néel temperature

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In this work, an investigation of the optical properties for the nanoribbons of nickel on chromium nanofilm is proposed in terms of Mueller ellipsometry. At the higher temperature than the Néel temperature for a macroscopic bulk of chromium, it was observed the abrupt change in the magnitude and sign of the first element of the fourth row in the Mueller matrix, characterizing the circular polarization of the scattered beam. The corresponding change in the ellipsometric parameters of the nickel nanoribbons on the chromium film is the pretendant to be discussed as the confirmation of the phase transition in the ordering of the internal structure of system with the ferromagnetic-antiferromagnetic interface.

Critical Voltages and Coulomb Blockade in Single-molecule Transistors

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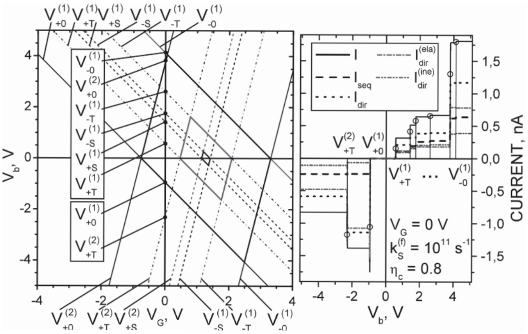
Electron current $I=\sum_m I_m P_m$ through a single-molecule transistor is specified by its contributions associated with the lowest neutral *(m=j=0,S,T)* and charged *(m=*α*=+,-)* electronic states of the molecule. Contributions are weighted with the corresponding occupation probabilities P_m. We show that due to the Coulomb blockade, probabilities and, consequently, the current exhibit a stepwise behavior at certain critical bias voltages

$$V_b=V_{\alpha j}^{(r)}(V_G)=\left[\alpha\left(\Delta E_{\alpha j}^{(0)}/|e|\right)+V_G\right]/\left(\delta_{r,2}-\eta_c\right) \qquad (1)$$

where $|e|$ and η_c denote, respectively, the electron charge and the voltage division factor whereas

$$\Delta E_{\alpha j}^{(0)}=E_\alpha-E_j+\alpha E_F$$

[1,2] are the transmission gaps. Eq. (1) determines the Coulomb parallelograms (diamonds for the symmetric transistor). This could be seen from the figure, which shows the voltage boundaries at which stepwise behavior and Coulomb blockade are observed for the current in a Zn-based transistor.



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Quantum Cone - Nano source of light with dispersive spectrum, distributed in time and a space

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Nanostructures (NS) are the most studied object in solid-state physics, especially the quantum size effect in the systems of quantum dots – 0D, quantum wires – 1D and quantum wells – 2D. Twenty years ago, a new quantum system was discovered, the so-called quantum cone in a Ge single crystal [1, 2], which has unique optical properties: a huge “blue shift” of the photoluminescence (PL) spectrum by 1.1 eV with an increased intensity of more than a million times, with period of 1 μ of the C6i template of the point symmetry group and the "red shift" of the frequency of the LO-phonon line by 6 cm^{-1} in the Raman spectrum. The symmetry of the PL band and the sharp LO phonon line in the Raman scattering spectrum are proof of the presence of the OD quantum cone. The appearance of a new band in the PL spectrum of the CdZnTe solution is explained by the effect of the quantum size of excitons in quantum cones [3]. Irradiation of the SiO_2/Si structure with an Nd:YAG laser led to the formation of nanocones that have a unique PL spectrum: a "blue shift" of 1.1 eV, an asymmetric broad band from 1.1 eV to 2.2 eV with a gradual decrease in intensity in the red part of the spectrum, the rainbow spectrum and the maximum PL intensity increase more than a million times [4]. These properties of the PL spectrum system are characteristic of varison semiconductors. This means that a quantum cone with a solid angle at the top of the cone less than 60° is a one-dimensional system with a gradual decrease in diameter from the base to the top of the cone. Therefore, where the diameter of the cone is equal to or less than the Bohr radius of an electron or an exciton, the effect of quantum size takes place [5]. A colossal increase in PL spelter intensity and a shift of its maximum to the blue part of the spectrum occurs due to the transformation of the Si and Ge crystal from indirect to quasi-direct and the retention of the electron-hole pair in the quantum cone. These facts indicate the possibility of a gradual decrease in the lifetime of electron-hole pairs or excitons from the base to the top of the cone. The purpose of this study is to determine the change in the lifetime of electron-hole pairs depending on the height in the cone using the kinetics of the PL method. Studies of the PL kinetics of a sample of diamond-like carbon (DLC) with nanocones with a diameter of 100 nm at the base and 2 nm at the top and a height of 60 nm showed that the PL kinetics is described by a stretched exponent and the lifetime of excitons gradually increases from the top to the base of the cone. It has 50 ps at the top and 3 ns at the base.

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Theoretical modelling of photoluminescence from thermally coupled levels

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Temperature (T) dependence of green photoluminescence from thermally coupled levels (TCLs) $^2H_{11/2}$,$^4S_{3/2}$ to $^4I_{15/2}$ of Er^{3+} ions in AlN matrix was studied in terms of using in fluorescence intensity ratio technique of optical thermometry and modelled within a theory based on kinetic equations in a system of three levels (Fig. 1).

Dynamics of the concentrations of Er ions on the excited states $^2H_{11/2}$ and $^4S_{3/2}$, respectively, is

$$dN_H/dt = fW - r_H N_H - \ N_H + \ N_s$$
$$dN_S/dt = (1 - f)W - r_S N_S - \ N_s + \ N_H,$$

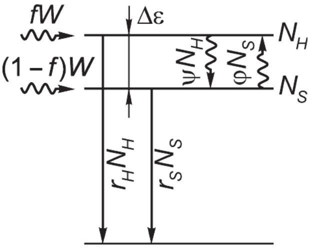

Fig. 1. *Transitions and their rates in a system with one ground and two excited levels.*

where W is the total rate of excitation of Er^{3+} to both $^4S_{3/2}$ and $^2H_{11/2}$, f is the fraction of the Er^{3+} centers being optically excited onto the level $^2H_{11/2}$, thus *fW* and (1 – *f*)W are the rates of excitation to the $^2H_{11/2}$ and $^4S_{3/2}$ levels, respectively. Parameters $r_{H,S}$ are the probabilities (reciprocal time constants) of the radiative transitions, and are probabilities of the excitation exchange. The effect of temperature on the system manifests through the dependence *(T)* = $\varphi_\infty \cdot \exp(-\Delta\varepsilon/kT)$, where is the energy distance between the TCLs and φ_∞ is the value for $T \to \infty$.

In the stationary mode, when *dNH/dt* = *dNS/dt* = 0, the luminescence intensity from the level $^4S_{3/2}$ reveals a usual dependence on temperature, following Mott formula, while that from $^2H_{11/2}$ is predicted to rise with *T*:

$$I_S = r_S N_S = \frac{r_S}{r_H} \cdot \frac{\psi + r_H[1 - f]}{\varphi(T) + r_S[1 + \psi/r_H]} W, \quad I_H = r_H N_H = \frac{\varphi(T) + f r_S}{\varphi(T) + r_S[1 + \psi/r_H]} W,$$

which was observed in the experiment. The value $\Delta\varepsilon$ = 76 meV was obtained within the simulation, which is close to that estimated from the spectrum.

(Tetrafluorovinylphenyl)carbazole as a multifunctional Material for OLED applications

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The multifunctional materials for application in organic light-emitting devices (OLEDs) based on a single structural motif are very desired but quite rare species. Such structures allow simplifying the chemical variety within OLED heterostructures and thus reducing their cost, manufacturing time, and logistic efforts. In this paper, we report the 9-(2,3,5,6-tetrafluoro-4-vinylphenyl)carbazole molecule (Cz4FS) utilized as a fluorescent emitter, host material for quantum dot based OLEDs (QLEDs), acceptor part of the exciplex active layer, and monomer that can be used for the preparation of emissive polymers and copolymers. The external quantum efficiency (EQE) of the corresponding fluorescent OLED based on a Cz4FS single emitter doped into a 1,3-bis(carbazol-9-yl)benzene matrix is 4.2%, which is close to the theoretical limit and maximum brightness at the level of 3600 cd/m^2. An OLED based on exciplex emission obtained utilizing Cz4FS as an acceptor demonstrates higher efficiency (5.3%) and much higher brightness near 25 000 cd/m^2. A QLED based on Cz4FS as a host for CdSeS/ZnS core-shell quantum dots demonstrates excellent energy transfer from the Cz4FS matrix that results in a clear spectrum of quantum dots with an EQE of 2.3%, maximum of 19 000 cd/m^2, and narrow spectral distribution. An OLED based on a Cz4FS-based polymer and copolymer demonstrates not extraordinary efficiency but low-efficiency roll-off in a wide range of current densities.

Optical properties of carbon-rich amorphous silicon carbide films subjected to annealing in air

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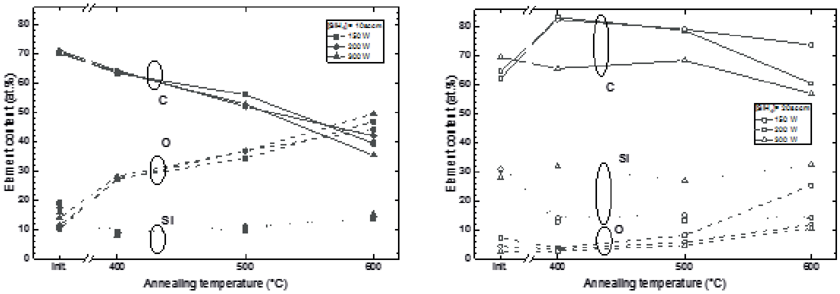
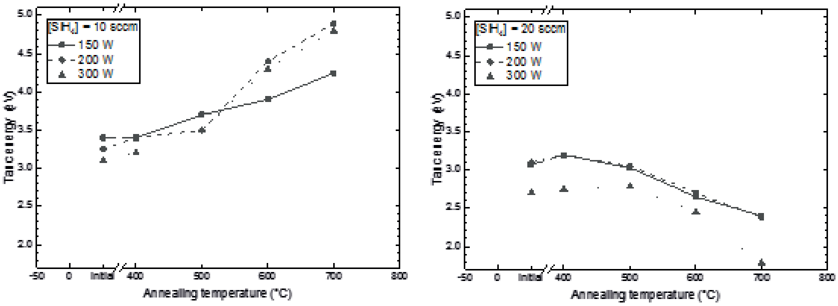
The purpose of the study was to evaluate thermal stability of the amorphous films under increased temperature technological treatments similar to technological stage of firing the screen-printing electrodes on solar cells in the aim to keep or even improve parameters of solar cells covered with antireflective amorphous films. The two series of amorphous silicon carbide films with lower and higher silicon content (11 and 20 at.%, flowrate 10 and 20 sccm during deposition, respectively) were deposited on silicon substrates, annealed in air and analyzed. It has been shown that annealing of the films at temperatures 400 - 700°C led to sufficient changes in optical properties. At the same time, behavior of low- and high-Si films is different during annealing. The high-Si films showed better stability against high temperature treatments with slower reduction of optical bandgap, refractive index values in comparison to low-Si films. Such behavior was explained by bigger number of Si-C bonds that resist to carbon oxidation and exodiffusion. Also, annealing of the films led to changes in thickness: at low



Effect of annealing temperature on composition of films deposited with silane flow 10 sccm and 20 sccm (b): ■ – deposited at 150 W, ● – 200 W, ▲ – 300 W.



Effect of annealing temperature on optical (Tauc) bandgap of films (calculated from R and T) deposited with silane flowrate 10 and 20 sccm, and RF power 150-300 W.

temperature annealing thickness increased and after some critical temperature decreases, because of oxygen incorporation into the film's matrix and then exodiffusion of oxidized carbon (CO_2). The obtained results can be used for analysis of the high temperature stability of such materials in applications on solar cells and other devices subjected to high-temperature treatments.

Kinetics of Optical Absorption Changes in Polymer Gas-Sensitive Nanostructures

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In recent years, there has been increased interest in the use of polymer films sensitive to various gases in optical gas sensors, in particular, electrically conductive polyarenes, due to their high manufacturability, ease of synthesis and use, and low cost [1,2]. At the same time, the peculiarities of changes in the optical properties of sensor elements under the action of gases, in particular, the kinetics of these changes and their recovery significantly affect the operational parameters of sensors based on them.

Gas-sensitive nanostructured polymer structures were obtained by the electrochemical deposition method, as it allows to vary the composition, topology, thickness, and properties of the synthesized layers within wide limits and to optimize them effectively.

The kinetics of changes and recovery of nanostructured films of polyaniline and binary nanostructures based on a mixture of polyorthoanisidine and polyorthotoluidine under the action of ammonia, carbon dioxide, sodium sulfide vapors and other volatile substances in a wide spectral range $\lambda = 350–900$ nm were studied, which ensures the use of synthesized combined structures for manufacturing optical gas sensors. Spectral and temporal ranges of sensitivity, speed and recovery parameters of active 2D nanoelements for smart optical gas sensors are established.

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Trapped-modes in non-Hermitian metasurfaces with gain and loss

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In this report, we discuss the possibility of incorporating active (gain) elements in the designs of all-dielectric metasurfaces. The studied metasurfaces support specific resonant conditions of operation associated with the excitation of the trapped modes [1]. We utilize the non-Hermitian effects, such as PT-symmetry breaking [2, 3], to realize an active control over the trapped mode by introducing loss and gain. In the lossless symmetric case (identical elements of the unit cell), the trapped mode cannot be excited and has an infinite quality factor. In the presence of asymmetry (unit cell contains elements of different sizes), it can be observed in the spectrum as a resonant state with a finite quality factor depending on the level of asymmetry. We show that introducing loss and gain into the system allows us to control the system's response in both symmetric and asymmetric structures. Our results demonstrate the capabilities of externally controlled gain media to vary the properties of optical resonances, which is extremely important for applications in sensing, nonlinear optics, and laser physics.

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Trapped mode control in all-dielectric metasurfaces composed of uniaxial anisotropic nanoparticles

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Metasurfaces are artificial structures based on the subwavelength resonant particles that allow to control the amplitude, phase, frequency, polarization state and angular momentum of electromagnetic waves in a desired way [1]. In this report, we demonstrate how one can utilize the anisotropic properties of bulk molybdenum disulfide (MoS_2), to achieve the excitation of trapped modes (also known as the bound states in the continuum, BICs) in all-dielectric metasurfaces [2]. Bulk MoS_2 is a novel material that is characterized by a thin-film structure. The electromagnetic waves interact with this media in the same way as with in the uniaxial anisotropic material possessing the form birefringence property. Studied metasurface is composed of disk-shaped resonant nanoparticles made of the MoS_2 material arranged in two-dimensional array. We assume that the anisotropy axis of MoS_2 can be tilted to the rotation axis of the disks. A detailed analysis of scattering characteristics and eigenwaves of such anisotropic resonant nanoparticles as well as the spectral behaviors of the metasurface, is carried out, revealing dependence of the conditions for excitation of the trapped mode on the orientation of the anisotropy axis of the MoS_2 material used.

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Side-chain azoquinoline polymers

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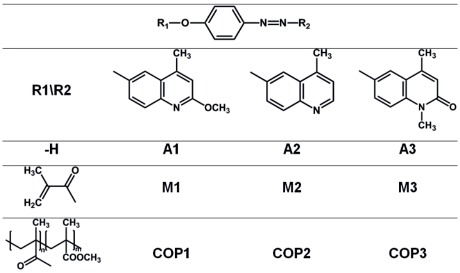
Synthesis of polymers with predicted and expected properties on the one hand and using specific features of interaction light with photoactive fragments in polymers, on the other hand, opens new prospects of application for new materials based on these polymers. The side chain methacrylic polymers with different active functional group have been well studied and widely applied in many fields, such as optoelectronics, nonlinear optics, optical storage materials, biochemicals, and medicine. Based on polymers with photoactive groups have been created materials also applied in many areas, key among which: nonlinear optical materials, core materials for optical waveguides, photoresists materials, field effect transistors, photoswitches, materials for optical memories, solar cells and so on [1].

The present work focused on synthesis new azoquinoline methacrylic monomers and copolymers with methylmetacrylate (MMA) based on these monomers. As previous research has shown the methacrylic copolymers with photochromic styrylquinoline unit has revealed NLO (nonlinear optical) properties, that were investigated by the second and third harmonic generation techniques which indicates on their potential in photonics applications. The common structure of synthesized azoquinoline containing compounds is presented in figure.



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Nanostructural impurity centers of organic molecules in Shpolsky matrices: appearance in quasi-linear luminescence spectra

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Phenomenon of quasi-linear luminescence spectra of complex organic molecules in solutions of n-paraffins at low temperatures, which was called the Shpolsky effect, was first observed in [1]. Later, these spectra have been found out to possess a multiplet structure with a different number of components, which are observed in the form of the similar band series located from each other at a distance of 10 100 cm^{-1} along the entire electronic vibrational spectrum. The qualitative phenomenological interpretation of this multiplet pattern in literature was associated with the formation of various types of impurity centers. Such centers were identified as individual impurity molecules located in different local fields of n-paraffin polycrystalline solutions. This work proposes a new approach to the explanation of the Shpolsky effect, based on the symmetry properties of the impurity molecule and the crystal matrix. It allows determining the number of components in the multiplet and modeling the structure of the impurity center, which is not taken into account in the previous interpretation. The procedure for determining the number of impurity centers **m** consists of three consecutive steps. As an example, a molecule of 2-fluoronaphthalene dissolved in n-hexane is considered. First, the number of optical isomers $\mathbf{n_m}$ of this impurity is determined. Applying the point symmetry operations of naphthalene $\boldsymbol{D_{2h}}$, we obtain two classes of equivalent positions (2, 3, 6, 7 and 1, 8, 4, 5), thus for 2-fluoronaphthalene in n-hexane, the number of optical isomers is 4 (positions 2, 3, 6, 7). The number of equivalent positions of this impurity in the n-hexane crystal with two symmetry elements, ***E*** and i is calculated. The action of symmetry operations of these groups causes determination of $\mathbf{n_k}$:

$\boldsymbol{E}(2) \rightarrow 2$ $\boldsymbol{E}(3) \rightarrow 3$ $\boldsymbol{E}(6) \rightarrow 6$ $\boldsymbol{E}(7) \rightarrow 7$
$\boldsymbol{i}(2) \rightarrow 6$ $\boldsymbol{i}(3) \rightarrow 7$ $\boldsymbol{i}(6) \rightarrow 2$ $\boldsymbol{i}(7) \rightarrow 3$

It equals to 2. The number of impurity centers of different types m is equal to the ratio $\mathbf{n_m}/\mathbf{n_k}$, in this case $\mathbf{m} = \mathbf{n_m}/\mathbf{n_k} = 4/2 = 2$.

The obtained results and literature data are discussed.

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Fluorescence enhancement of TCC aggregates by aggregation shifting to J-aggregates preferable formation

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The aggregation of organic dyes is a topic of great interest due to the unique properties and potential applications of the resulting aggregates. One particular type of aggregate, known as a J-aggregate, is characterized by a sharp and intense absorption band at a longer wavelength than that of the monomer. This is due to strong dipole-dipole interactions between the transition dipole moments of the dye monomers, which propagate electronic excitation in the form of a Frenkel exciton throughout the aggregate. J-aggregates can consist of several hundred molecules and exhibit a range of linear and nonlinear properties, including resonant fluorescence and exciton superradiation.

The exciton band of a J-aggregate can appear as either a bathochromically shifted J-band or a hypsochromically shifted H-band, depending on the molecular arrangement within the aggregate. The J-band is associated with "head-to-tail" molecule packing and is the lowest energy state of the exciton band, while the H-band is associated with "head-to-head" packing and is the highest energy state. In some cases, both H- and J-bands can be found for the same aggregate as a result of the Davydov splitting.

This study reports on the aggregation of thiacarbocyanine (TCC) dye in aqueous solutions and polymer films. The results show that H- and J-aggregates form in pure water, but with weak monomer and J-aggregate fluorescence due to the absence of electronic coupling between the H- and J-bands. To obtain more intense fluorescent species, the aggregation needs to be shifted towards preferential J-aggregate formation. The study demonstrates different methods for achieving J-aggregation of TCC dye in both aqueous solutions and polymer films.

Controlling mode degeneracy in a coupled waveguide system with loss and gain using exceptional points

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In this report, we discuss improving the controllability of an optical waveguide coupler by introducing gain constituents into the system [1]. A multimode approach [2, 3] is considered for studying multicomponent systems that can support both waveguide modes and surface plasmon modes. The presence of exceptional points in the plasmon-dielectric interaction of the modes is shown. These exceptional points are used to lift the mode degeneracy that occurs for hybrid waveguide and hybrid plasmon modes. At the same time, by controlling the parameters of the exceptional point, we control the transition of the system between the degenerate state and that with the lifted degeneracy, i.e., hybrid modes with different polarizations are separated. The influence of an external Gaussian beam on the excitation of modes in the waveguide system is also studied. It is shown that, by controlling the polarization of the external beam, it is possible to excite various types of modes. Thus, such a two-stage control of a plasmon-dielectric system allows one to significantly expand the scope of the system under consideration.

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Quadrupole versus dipole Brownian photomotors

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The operating properties of different-type Brownian photomotors [1] have been compared in relation to the symmetry interplay between their moving (particle/molecule) and immovable (substrate) units. As found, essentially different symmetry constraints and hence different motor behaviour are characteristic of molecules if their electron density redistribution on excitation involves only odd-order or only even-order multipole moments. The two respective types of molecules give rise to dipole and quadrupole photomotors [2]. Purely dipole photomotors can operate only on substrates with symmetric charge distribution and their ensemble with random molecular orientations undergoes equidirectional diffusion rather than directed motion. Purely quadrupole photomotors need substrates with antisymmetric charge distribution for directed motion to occur and they can move directionally in an ensemble. Also, quadrupole photomotors provide much smaller velocities of directed motion than their dipole counterparts (as a result of the much weaker interaction of quadrupoles than dipoles with an electric field). The generic distinctions between the two photomotor types are exemplified by donor-acceptor-substituted stilbenoids (dipole molecules) and symmetric squaraines (quadrupole molecules). The model used affords the rational design of photomotors by the selection of promising moving molecules and by the continuous wide-range tuning of charge-distribution symmetry in substrates.

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Light absorption by a composite with randomly arranged metal nanocylinders

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Currently, the optical properties of composites with anisotropic metallic inclusions are being actively studied. This is due to the fact that such systems can exhibit the effect of optical masking, as well as a negative, very large, or close to zero refractive index. In this regard, the study of the frequency dependence of the absorption coefficient of a composite with randomly arranged cylindrical nanoinclusions is relevant.

It is assumed that the concentration of inclusions is not small, therefore, to determine the effective permittivity T_{eff} of the composite, we use Bruggeman relation [1]

$$\sum_i \left\{ \beta \frac{T_{ii} - T_{\mathrm{eff}}}{T_{\mathrm{eff}} + \mathcal{L}_i \left(T_{ii} - T_{\mathrm{eff}}\right)} + \left(1-\beta\right) \frac{T_{\mathrm{m}} - T_{\mathrm{eff}}}{T_{\mathrm{eff}} + \mathcal{L}_i \left(T_{\mathrm{m}} - T_{\mathrm{eff}}\right)} \right\} = 0 \tag{1}$$

where β is the volume fraction of metallic inclusions in a composite; T_{m} is the permittivity of a matrix medium; L_i are depolarization factors; $i=x, y, z$.

The absorption coefficient was calculated using the formula

$$\eta\left(\omega\right) = \frac{2\omega}{c\sqrt{T_{\mathrm{m}}}} \operatorname{Im} \sqrt{T_{\mathrm{eff}}\left(\omega\right)} \tag{2}$$

The calculation of size-dependent parameters for cylindrical nanoparticles (depolarization factors and effective relaxation rate) was carried out within the framework of the model of an effective prolate spheroid [2].

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Initial temperature influence on the indications of optical sensors based on surface plasmon resonance

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The analysis of additional aspects of thermal influence on the sensory effect of the three-layer optical structure "prism - absorbing (gold) nanolayer - water" was continued. In previous studies, this effect was analyzed in relation to the change in the wavelength of the surface plasmon resonance (SPR) in two cases. First, in the approximation of the infinite absorption index of the sensor nanolayer, characteristic of metals. And, secondly, for the case of the finiteness of this index in view of the possibility of replacing the metal (usually gold) nanolayer with another material. But these studies did not take into account the influence of the initial temperature of the "absorbing (gold) nanolayer - water" system on the change in the SPR wavelength.

It was established that the change in the value of the sensory effect on the wavelength of the SPR when the initial temperature changes in the range of 20°C – 25°C is ~ 0.02% of the initial value of this wavelength (in our numerical experiments, it corresponded to the wavelength of the SPR at 0°C). Previous studies show that such a change in the wavelength of the SPR is practically not identified by the sensor. At the same time, with an increase in the initial temperature to ~ 100°C, the change in the SPR wavelength can reach 0.75% of the initial value of this length. As it was shown, such a value can already be detected experimentally. And the very effect that exists at low laser radiation fluxes (< 1 W/cm) can be the basis for the creation of alternative temperature meters in cases where other methods are unacceptable.

Optical properties of metal-dielectric composites. The role of electric and magnetic dipole absorption

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Metal-dielectric nanocomposites with unique optical properties are widely used in practice, in particular, to obtain structures with a negative, large or small refractive index, which are characterized by selective absorption or transmission of electromagnetic radiation. When creating such composites, a dielectric medium with metal nanoparticles embedded in it is used.

Due to the fact that with an increase in the size of nanoparticles in the infrared region of the spectrum, eddy currents, which are induced by the magnetic field of an electromagnetic wave, play a significant role, it seems necessary to go beyond the quasi-static approximation and, in addition to electrical, take into account the magnetic dipole absorption.

Therefore, the paper investigates the frequency dependence of the absorption coefficient of a metal-dielectric nanocomposite, taking into account the electric and magnetic contributions.

A comparison of the experimental results with calculations of the frequency dependence of the absorption coefficient showed a fairly good agreement in the infrared region of the spectrum.

Electromagnetic wave propagation through metasurface-dielectric-metal structure

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Metasurfaces in recent years have become one of the most important material advancing optic and nano-optic equipment that can not only reduce size and cost of existing elements, but offer a brand new functionality [1].

In this work we study how introducing uniaxial plasmonic metasurface on top of the layered structure that contains dielectric and metal is changing the behavior of incident under some angle p-polarized electromagnetic wave that propagates through the layers.

To observe changes caused by the modified structure we compose electromagnetic field components for each environment and inject the conductivity tensor that describes metasurface properties [2]. Considering boundary conditions between each layer the equations were used to express amplitudes for each part of the wave. It was found that p-polarized wave can be fully absorbed by the material composition or can be completely transformed to s-polarized one. For both cases we determined corresponding parameters of the system including dielectric layer thicknesses frequencies and angle of incidence of the electromagnetic wave.

Established effects and calculations can be used to enhance properties of existing optic and nanoelectronic equipment as well as to build new improved devices.

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Fast optical nonlinearity of copper oxide thin films synthesized by reactive pulsed laser deposition

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Thin structured films of metal oxides are interesting by their relative ease of creation and stability in air. Thin films of Cu_2O are attracting attention as advanced optically nonlinear structure. Previously [1], we investigated the nonlinearity of such structures excited by laser nanosecond pulses at wavelengths 1064 nm and 532 nm. A high value of the nonlinear refractive index was obtained (n_2 ~10^{-6} cm^2/W). It was shown that sign of the nonlinearity was changed depending on the structure of the film. Such structural changes were achieved by changing synthesis parameters. We have made an assumption that the mechanisms of this optical nonlinearity are related to electronic transitions in the semiconductor and have short action times. To confirm this, in this work we investigated the optical nonlinearity by exciting by femtosecond laser pulses at wavelength 800 nm.

The films were synthesized on SiO_2 (silica) substrates by reactive pulsed laser deposition technique at 293K or 800K under a different oxygen pressure of 1 Pa, 3 Pa or 5 Pa (to change the degree of oxidation of the film)

Optical nonlinearity parameters of the Cu_2O films were determined with the standard Z-scan technique. Nonlinear optical changes were induced using femtosecond pulse laser radiation at a wavelength of 800 nm, 280 fs pulse duration.

The experiment showed that the optical nonlinearity in Cu_2O thin films is fast enough to affect the femtosecond pulse.

We demonstrated that the change in the degree of oxidation has a significant effect on the value of the nonlinear refractive index n_2, which reaches its maximum value at the highest pressure (5 Pa) of pure oxygen in the deposition chamber. The value of n_2 is about 10^{-10} cm^2/W and has a positive sign. This value is significantly less than that obtained when excited by nanosecond laser pulses (see above). This may indicate the presence of several mechanisms of optical nonlinearity with

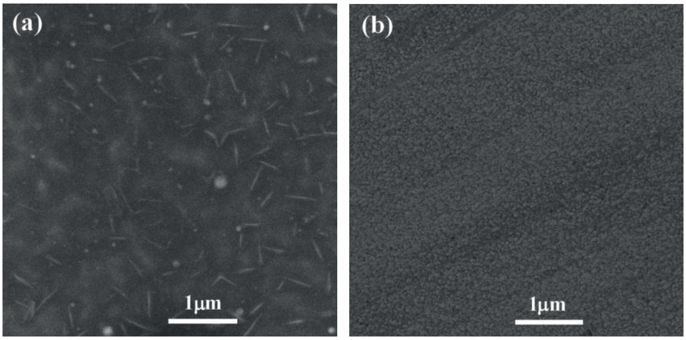

Fig.1 The structure of the surface of thin films depending on the temperature of the substrate during deposition
(a) – 293 K
(b) – 800 K

different action times. When we excited by femtosecond pulses, "slow" mechanisms of nonlinearity didn't affect.

We also observed the feature of nonlinearity for films deposited at an oxygen pressure of 3 Pa (we obtained a negative sign of the nonlinear refractive index). This may indicate the additional features of the structure of the films which appear at this pressure, for example, some additional defects in the crystal structure.

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1. V. I. Rudenko, N. Stefan, S. A. Mulenko, et al. "Optical cubic nonlinearity of copper oxide thin films synthesized by reactive pulsed laser deposition" Journal of Laser Applications 34, 032015 (2022)

Nanostructured fiber tip for enhanced light in-coupling

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Optical fibers are key devices of modern photonics and have been successfully applied in a variety of fields, including telecommunication and life science. While the actual light transport capabilities are excellent, the main problem arises at the beginning of the fiber where the light is to be collected. However, the disadvantage of commercial step-index single-mode fibers is the low refractive index contrast between core and cladding leading to the low numerical aperture. As a consequence, light may be efficiently collected into the fiber up to a maximum angle of incidence of 20 degrees [1].

In this work, we show both theoretically and experimentally that nanoprinted all-dielectric nanostructures implemented on fiber end faces allow to significantly enhance light in-coupling into fibers up to the unprecedently high levels.

The polymer axial-symmetric nanostructures are fabricated at fiber end face using the direct laser writing technique. Taking advantage of the unique properties of the nanoprinting technology, we outperform the functionality of bare fibers by orders of magnitude [1]. The various types of axially symmetric structures (e.g., single-pitch and double-pitch gratings or aperiodic arrays) were placed on the facet of SMF-28, resulting in structures of exceptional quality and coupling efficiency beyond all previously known devices [1]. We demonstrated the light in-coupling enhancement at the multiple selected angles and across the large angular intervals.

Applications can be found in a variety of cutting-edge fields that require highly efficient light collection over selected angular intervals, including endoscopy or quantum technologies.

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1. Yermakov O., Zeisberger M., Schneidewind H., Kim J., Bogdanov A., Kivshar Y., Schmidt M.A. Advanced fiber in-coupling through nanoprinted axially symmetric structures // Applied Phys. Rev. – 2023. – 10. – № 1. – P. 011401.

A defect containing feedback photonic structure for THz and infrared beams collimation

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Developing the idea to use the extraordinary narrow resonance peaks of transmission on the background of perfect reflection arising in a planar photonic resonator containing a unitary defect in the middle of the structure [1], we propose here a modified tool which can redirect the $-\varphi_r\ \boldsymbol{J_r/2}$ beam (Fig. 1) back into the resonator's electromagnetic field reservoir due to a feedback construction. This enables to obtain a collimated unitary outgoing $+\varphi_r$ beam of full intensity $\boldsymbol{J_r}$ instead $\boldsymbol{J_r/2}$ otherwise. The properties of standing modes inside the polyethylene (polypropylene)/ silicon plane resonators in the total intrinsic reflection region and unusual manifestations of THz transmission spectra in centimeter and millimeter wavelength range were studied in [2]. It was shown that the angle and frequency half-widths of the resonance peak can be less than 10^{-9} of the magnitude of angle and frequency in dependence on the number of periods. This allows one to form collimated beams with the divergence measured in a fraction of a microdegree. It is shown that a plane resonator containing a central defect transforms the frequency divided peaks into the outgoing-transmitted beams of various directions like a prism transforms light. In the talk, the way for precision measurements of angle and frequency distribution of THz radiation is discussed.

The idea of collimating device is presented in Fig. 1. A monochromatic diverged incident beam $\boldsymbol{J_t}$ passes from the source S into the resonator through an electromagnetic field reservoir (EFR). The latter allows one in a lossless process to concentrate inside the radiation of different directions with the angular white noise distribution.

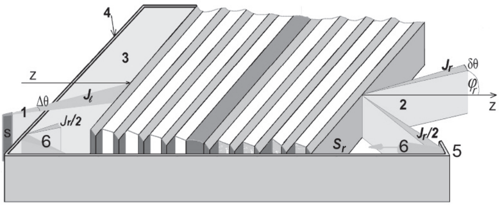

***Fig. 1**. A planar central defect containing photonic crystal resonator with feedback reflector. 1, monochromatic diverged incident beam $\boldsymbol{J_t}$; 2, collimated outgoing beams $\boldsymbol{J_r}$, 3, electromagnetic field reservoir; 4, mirror walls of the reservoir, 5, feedback reflector, 6, reflected $-\varphi_r\ \boldsymbol{J_r/2}$ outgoing beam; φ_r, output angle; $\Delta\theta$ and $\delta\theta$ are the input and output divergence of beam, correspondingly.*

For the THz frequency range, we consider a polypropylene-silicon $(Si/PP)_n$/D/$(Si/PP)_n$/Si defect containing photonic structure for various number of periods n. As a defect, the Si-layer was taken. To obtain collimation, the source frequency should be matched with the calculated resonant curve of transmission which occupies interval *(0.59076, 0.69275)* THz at chosen geometrical sizes of resonator Si - *40 µm*, PP - *70 µm*, D - *40 µm*, *n*=5. In the vicinity of 0.6 THz for the adopted parameters: $Il = 0.1\ W/cm^2$, source section 12.5 cm^2, output section 12.5 cm^2, EMW reservoir volume 1257cm^3 time of energy accumulation equals approximately 3.78 ms. The ratio of energy loss on the reservoir walls and the reverse flow through the source section was taken as 28%. As a result, the considered system issues a strongly collimated beam with angular HWHM δθ close to *0.123 µDeg* and output intensity $Jr = 0.07142\ W/cm^2$.

To operate inside the IR range we have chosen for consideration an optically enough contrast 10-period layered structure consisting of alternating 0.6 µm silicon films divided by 1.2 µm SiO_2 layers with a defect Si layer in the middle of structure and ending additional layer of Si. On the upper panel of Fig. 2, shown is spectrum of standing modes calculated inside the TIR angular region (shown is interval (17° – 23°). The considered interval of energies *(0, 1.0) eV* involves five bands divided by four gaps containing local (surface and defect) states. The first gap occupies interval *(0.148, 0.238)* eV and contains a defect and twin in vicinity of TIR angle 17°. Beginning with 18.2° incident angle of waves inside the Si layers, that quasi-degenerated surface state transforms into two detached band modes. We discuss perspective use of standing TIR modes in photonics applications.

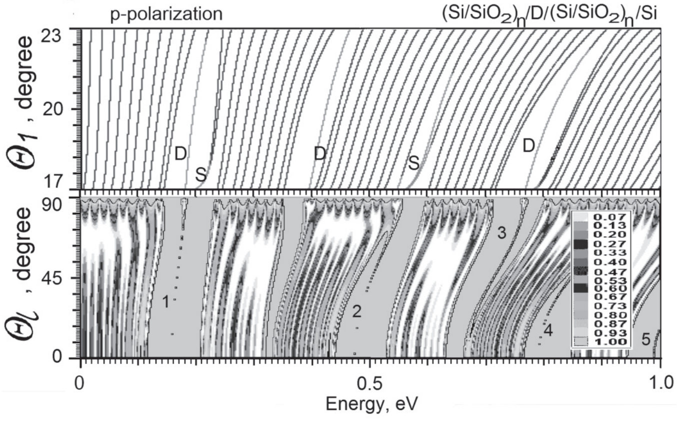

Fig. 2. Spectrum and reflection diagram of a defect containing photonic crystal resonator $(Si/SiO_2)_n/D/(Si/\ SiO_2)_n/Si$*, n= 5.* ***Upper panel:*** *D, defect modes; S, surface local modes.* ***Lower panel:*** *Color diagram of reflection in the external geometry of incidence. Six windows of perfect reflection. 1-5, local (defect) resonances of perfect transmission.* ***Inset:*** *color scale of reflection.*

On the lower panel of Fig. 2, the calculated color map of reflection is shown. Six windows of transmission divided by zones of perfect reflection correspond to bands and gaps of spectrum of the structure presented in the upper panel for the TIR angular region. The physical nature, properties and behaviour of local resonances 1 – 5 were analysed in [1, 2].

The proposed scheme of feedback redirection of electromagnetic energy allows one to avoid the doubled outgoing beam and to rise power of the beam outgoing in the needed direction. In this talk, we also discuss a new spectroscopy technique based on the existing sharp transmission resonances using the conception of accumulating reservoir of electromagnetic field. One more subject of discussion is an opportunity to form long and stable channels of communication and energy transportation in the infrared and THz frequency ranges.

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1. E.Ya. Glushko. "Collimation Effect on THz Transmission Resonances in Metalized and Defected Photonic Structures" in Research Trends and Challenges in Physical Science, edited by Prof. Shi-Hai Dong, vol. 1, Chapter 7, 83-89. B P International UK (2021).

2. E.Ya. Glushko "Local resonance based precision collimation of THz radiation in a defect containing 1D photonic resonator: spectroscopy and metrology" Eur. Phys. J. D (2022) 76:130

Exciton and trion emission at the edges and grain boundaries of monolayer MoS_2 grown by chemical vapor deposition

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Photoluminescence (PL) mapping of monolayer single- and polycrystal MoS_2 flakes grown by chemical vapor deposition (CVD) was studied along with AFM and Kelvin probe force microscopy imaging. Monitoring the main (A) PL band, a usual intensification and blue shift of the band at the flake edges and grain boundaries (GBs) between the single-crystal parts of polycrystal flakes were found and attributed to the tensile strains known to be present in CVD-grown material.

Detailed study of the PL spectral composition showed that the blue shift is enhanced by a reduction of the trion component compared to the exciton one. The latter observation contradicts to the results of Bao et al. [1] that found an increase of trion at the edges and GBs along with the widening of the total PL band and attributed that to Mo-zigzag type of the edges and Mo-rich defects at the GBs.

The surface potential mapping of the samples has shown a p-doping at the edges and GBs which allows to conclude S-zigzag type of the edges as well as S-rich GBs in our samples, which may cause an inhibition of the trion formation and the observed narrowing of the PL spectrum.

So, the PL distribution over the CVD-grown flake is governed not only by the local strains, but is also affected by the edge and GB types.

1.Bao W., Borys N., Ko Ch., et al. Visualizing nanoscale excitonic relaxation properties of disordered edges and grain boundaries in monolayer molybdenum disulfide // Nature Commun.-2015.-6.-7993.

Optical properties of Ag films on Ge underlayers in the vicinity of percolation transition

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The electron transport in thin metal layers under electromagnetic radiation is subject of interest of modern micro-, nanoelectronics and transparent electronics industries [1]. Metal films of nanometers thickness are promising as ohmic conductors with high optical transparency, both in the visible and in infrared wavelengths. They are very attractive for modern transparent electronics because they have more stable temperature and structural properties compared to ITO. Since thin metal layer can be both in continues and disperse phase (island) state, the question of transition conditions. The transition thicknesses from disperse to ohm conduction state is called critical percolation thickness d_c. At the region of critical transition, metal condensate exhibits abnormal optical and electrical properties that can be explained within the percolation model [2-3]. The controlled formation of silver nanoscale, stable metallic films at the vicinity of percolation thicknesses dc will solve the problem of new material for transparent electronics. Near thickness of percolation threshold ($d < 5$-10 nm) metal condensate can provide high ohm conductivity ($\sigma < 10^8\ (\Omega\cdot\text{m})^{-1}$) and extremely high optical transparency (T ~ 85-90%).

The Ag metal films or Ge underlayers with thickness 5 nm and 10 nm of 0,1-1 nm respectively were deposited on glass substrate at 78 K by vapor condensation of thermally evaporation metals on the bare glass substrate. All preparations were conducted under high vacuum condition (P ~ 10^{-7}torr) in the framework of “quench condense” regime [1]. A mass thickness of Ag films was monitored by the shift of quartz oscillator resonance frequency. Transmittance T and reflectance R spectra were investigated with Shimadzu UV-3600.

The transmittance size dependence analysis of Ag films (for 900 nm, 1000 nm, 1500 nm and 1700 nm wavelengths) deposited on glass substrate and glass substrate pre-coated with Ge underlayer with different mass thickness showed. That value of percolation mass thickness d_{Ge} for 5 nm Ag film is ~ 1,2 nm of Ge, while for 10 nm Ag samples, it is ~ 0,83 nm of Ge thickness.

The analysis of infrared absorption of Ag films showed the existence of maximum absorption for percolation transition thickness. In particular, it was found that for Ag 5 nm film deposited on glass substrate the absorption maximum is A = 0,52 for Ge underlayer $d_{Ge} = 0{,}8$ nm at $\lambda = 440$ nm. At the same time absorption maximum is A = 0,56 for Ge underlayer $d_{Ge} = 0{,}2$ nm at $\lambda = 858$ nm is observed for Ag 10 nm. The observed evolution of the silver film absorption maximum is due to the density of isolated silver clusters near critical thickness of percolation transition. The higher concentration of isolated metal islands, the more electrons participate in plasmon resonance, which increase absorption of dispersed metal film [3].

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2. Smilauer P. Contemporary Physics. 1991. Vol. 32, № 2. p. 89-102.

3. Kyoung J. Optical Materials Express. 2022. Vol. 12, Issue 3. p. 1065-1073.

Analysis of a specific design of a hyperbolic metasurface based on gold nanodisks

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Hyperbolic metasurfaces are known for their unique properties such as negative refraction, hyperlensing, enhanced spontaneous emission, etc [1]. With their help, it is possible to improve various areas of science and technology, for example, optical systems for processing and transferring data, quantum communications, biosensing. Hyperbolic regime of a metasurface is defined as the indefinite two-dimensional tensor of surface conductivity, i.e., its components have different signs. In this state the isofrequency contours in the wavevector space are hyperbolic [2]. The surface waves localized at hyperbolic metasurfaces are called hyperbolic plasmon-polaritons [2,3] and exhibit a lot of potential applications [4].

The proper designing of hyperbolic metasurfaces takes a lot of time and requires a substantial amount of efforts. Therefore, we develop the algorithm to engineer the hyperbolic metasurfaces for specific applications on demand. In other words, the properties of hyperbolic metasurface are analyzed depending on three main parameters such as the lattice period, the filling factor, and the stretching anisotropy factor. We fix two parameters and set the third parameter with a certain step to understand how the resonant wavelengths and the width of the hyperbolic regime change. We have also derived universal formula that combines all three parameters simultaneously to determine the difference in resonant wavelengths.

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1. Takayama O., Lavrinenko A.V. Optics with hyperbolic materials // J. Opt. Soc. Am. B: Opt. Phys.-2019.- 36.-P. 38–48.

2. Gomez-Diaz J. S, Tymchenko M., Alu A. Hyperbolic Plasmons and Topological Transitions Over Uniaxial Metasurfaces // Phys. Rev. Let.-2015.-114(23), 233901

3. Yermakov O. et al. Hybrid waves localized at hyperbolic metasurfaces // Phys. Rev. B.-2015.- 91(23), 235423.

4. Gomez-Diaz J. S., Alu A. Flatland Optics with Hyperbolic Metasurfaces // ACS Photonics.-2016.-3(12).-P. 2211–2224.

Investigation of ZnO/6H-SiC and ZnO/Al_2O_3 structures by means of infrared reflection spectroscopy

Melnichuk O.V.[1]***, Korsunska N.O.***[2]***, Melnichuk L.Yu.***[1]***,***
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Structures based on optically anisotropic materials, including ZnO, 6H-SiC, and α-Al_2O_3, exhibit unique properties that allow their use in optoelectronic devices. All these materials belong to the (P63mc) spatial group. However, ZnO shows significant anisotropy in the properties of the phonon subsystem and weak anisotropy in the properties of the plasmon subsystem, while 6H-SiC demonstrates an opposite behavior. Such a difference affects the plasmon-phonon interaction of these materials when they are combined in the structures.

This work presents the results obtained for ZnO films grown simultaneously on 6H-SiC and α-Al_2O_3 substrates by RF magnetron sputtering. Such simultaneous deposition of ZnO films on different substrates permits the separation of the effects of deposition conditions and type of the substrate on the electrophysical and optical characteristics of the films. The film thickness was ranging from 0.1 to 1 μm. The infrared (IR) reflection spectra were recorded in the range of 240 to 4000 cm^{-1} at room temperature using a Shimadzu IRTracer-100 spectrophotometer.

A theoretical model for the IR reflection spectra is proposed. It considers the quality of the substrate surface, as well as the semiconductor nature of ZnO and 6H-SiC, and the dielectric nature of Al_2O_3, which affects the phonon-phonon and plasmon-phonon interaction in ZnO/Al_2O_3 and ZnO/6H-SiC structures for the orientation of the electric field vector $E \perp c$ and $E \| c$. The fitting of experimental IR reflection spectra reveals the coincidence of the values of the carrier concentration and mobility, as well as the conductivity of ZnO films with different thicknesses grown on different substrates. This is and evidence of the main influence of the substrate nature on the phonon-phonon and phonon-plasmon interactions in such structures as it will be discussed further. These results offer the utility of IR reflection spectroscopy as a non-destructive and contactless method for determining the electrical and optical parameters of materials and structures.

This work was partly supported by the National Research Foundation of Ukraine (project 2020.02/0380). The authors thanks to all defenders of Ukraine, whose efforts made this research work possible.

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Structures based on optically anisotropic materials, including ZnO, 6H-SiC, and α-Al_2O_3, exhibit unique properties that allow their use in optoelectronic devices. All these materials belong to the C_{6V}^{4} ($P6_3mc$) spatial group. However, ZnO shows significant anisotropy in the properties of the phonon subsystem and weak anisotropy in the properties of the plasmon subsystem, while 6H-SiC demonstrates an opposite behavior. Such a difference affects the plasmon-phonon interaction of these materials when they are combined in the structures.

This work presents the results obtained for ZnO films grown simultaneously on 6H-SiC and α-Al_2O_3 substrates by RF magnetron sputtering. Such simultaneous deposition of ZnO films on different substrates permits the separation of the effects of deposition conditions and type of the substrate on the electrophysical and optical characteristics of the films. The film thickness was ranging from 0.1 to 1 μm. The infrared (IR) reflection spectra were recorded in the range of 240 to 4000 cm^{-1} at room temperature using a Shimadzu IRTracer-100 spectrophotometer.

A theoretical model for the IR reflection spectra is proposed. It considers the quality of the substrate surface, as well as the semiconductor nature of ZnO and 6H-SiC, and the dielectric nature of Al_2O_3, which affects the phonon-phonon and plasmon-phonon interaction in ZnO/Al_2O_3 and ZnO/6H-SiC structures for the orientation of the electric field vector $E \perp c$ and $E \parallel c$. The fitting of experimental IR reflection spectra reveals the coincidence of the values of the carrier concentration and mobility, as well as the conductivity of ZnO films with different thicknesses grown on different substrates. This is and evidence of the main influence of the substrate nature on the phonon-phonon and phonon-plasmon interactions in such structures as it will be discussed further. These results offer the utility of IR reflection spectroscopy as a non-destructive and contactless method for determining the electrical and optical parameters of materials and structures.

This work was partly supported by the National Research Foundation of Ukraine (project 2020.02/0380). The authors thanks to all defenders of Ukraine, whose efforts made this research work possible.

Structure and optical properties of AlN/AlCuFe/AlN sandwich films prepared by helicon-arc ion-plasma method

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Solar selective absorbers for thermal energy applications can be prepared using films of quasicrystalline AlCuFe alloys which exhibit high solar absorptance and low thermal emittance. The absorbers layers were deposited onto a silicon substrate using the helicon-arc ion-plasma method [1, 2]. Moreover, AlN layers were used as dielectric anti-reflective coatings, which are necessary for the required optical properties. Optical properties of the deposited AlN/AlCuFe/AlN heterostructures were investigated in the wavelength range of 0.4-25 µm. The initial amorphous-crystalline structure of the Al-Cu-Fe layer was transformed into quasicrystalline one through post-processing annealing. The effect of various processing parameters on the structure and optical properties of the deposited sandwich films is considered. Prerequisites to achieve optimal structure and properties of the heterostructures were found.

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Session 7
Nanoobjects microscopy

Thickness effect at crystallization of amorphous films of Yb_2O_2S

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Films with layer thicknesses $h = 20 - 50$ nm were grown on a cleaved (001) face of KCl single crystals by the method of electron beam evaporation of the weight of high purity YbS. The structural analysis was carried out by the methods of electron diffraction and transmission electron microscopy on EM-100L and PEM-100-01 electron microscopes operating at the accelerating voltage of 100 kV.

Fig. 1 illustrates the effect of film thickness on the fraction of the crystalline phase x at crystallization of amorphous Yb_2O_2S upon thermal annealing in vacuum (180 min at 575ºC). At this temperature, films of thickness with $h \approx 20$ nm remain amorphous. Crystallization occurs at $h \geq 25$ nm (Fig. 1a, b, c). The fraction of the crystalline phase in the film increases with the growth of film thickness and on the level of higher than 50 nm is equal to 1 (Fig. 1c).

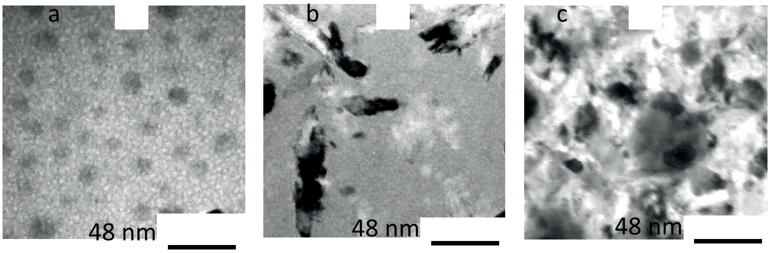

***Fig. 1**. The effect of thickness h on the crystallization of amorphous films of Yb_2O_2S upon thermal annealing in vacuum (180 min at 575ºC): (a) h = 25 nm; (b) h = 40 nm; (c) d = 50 nm*

The slowdown of crystallization at decreasing of the film thickness can be connected with increasing of the surface energy during crystallization. In addition, crystallization is associated with overcoming of the activation barrier, that separates the amorphous and crystal states. The height of the barrier increases with decreasing of the film thickness.

Electron microscopy of stacking faults in cementite after annealing of eutectoid steel

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The U8 steel of standard chemical composition (0.83% C, 0.2% Mn 0.25% Si) was studied by transmission electron microscopy using an EM-200 electron microscope at an accelerating voltage of 175 kV. Samples were annealed for a long time (100 hours) at subcritical temperatures. 680-700 ºC. After the end of the heat treatment, the samples were cooled with an oven.

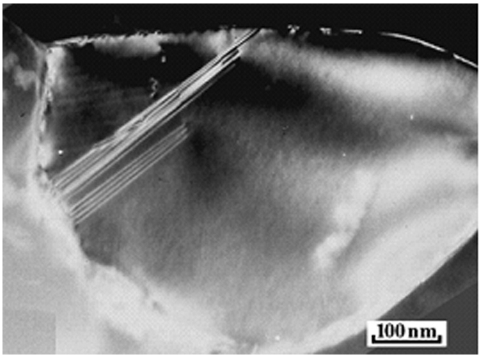

Fig. 1. *Packing faults*

At the formation and growth of defects in the crystal structure of cementite occurs in the process of dissolution and enlargement of Fe_3C particles (during spheroidization and coalescence) Fig. 1. This process is certainly controlled by the diffusion of carbon atoms.

CONCLUSIONS

The formation of large linear defects in the crystal structure (packing faults, twins) in cementite occurs in the process of growth on existing defects in cementite plates in perlite, or in the process of merging of two or more cementite particles.

Evolution of the structure and properties of Al-Mg-Si alloys processed by surface ultrasonic impact treatment

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The possibility of changing the structure and properties of the wrought low-alloyed, low-cost Al-Mg-Si alloy of 6060 type by surface severe plastic deformation has been studied. The alloy has high plasticity, the ability for hot extrusion, and high corrosion resistance, which are excellent characteristics for various applications. The low strength of the alloy, however, is its main disadvantage. Of great interest is the search for additional methods of hardening the alloy. The primary task of this research investigation has been to study the possibility of improving the mechanical properties of the alloy using surface severe plastic deformation in combination with different types of thermal treatments. One of the methods of surface plastic deformation is ultrasonic impact treatment (UIT). The use of high-power ultrasonic energy in the surface treatment of materials leads to fundamental changes in the structure of the surface and subsurface layers [1-3]. The study of the effect of ultrasonic impact treatment on the structure of Al-Mg-Si alloy surface showed that the initial structural state of the alloy significantly affected the mechanism of relaxation of internal stresses generated by shock-cyclic loading. Grain refinement was not observed during UIT of the Al-Mg-Si alloy. Strengthening was caused by internal stresses in the matrix. The increase in alloy microhardness after UIT was 24%. Also the UIT-treated Al-Mg-Si alloys exhibit improved corrosion resistance compared with their original state.

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STM investigation of ferronematic liquid crystal molecules on atomically flat Au(111) surface

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Recently discovered ferroelectric nematic phases (N_F) are of considerable interest due to their large spontaneous polarization, which reduces the electric reorientation fields of a liquid crystal cell by a thousand times compared to conventional materials [1]. However, their application is limited because a high temperature is required for practical use. 2,3′,4′,5′-tetrafluorobiphenyl-4yl 2,6-difluoro-4-(5-propyl-1,3-dioxan-2-yl) benzoate (DIO-CN) is an extremely prospective liquid crystal material which mixing with different NF might lower operational temperatures [2]. Here we report a STM study of the self-assembly of DIO-CN on the surface of Au(111). The absorbed DIO-CN molecules self-assemble into a monolayer film with regularly arranged molecular rows.

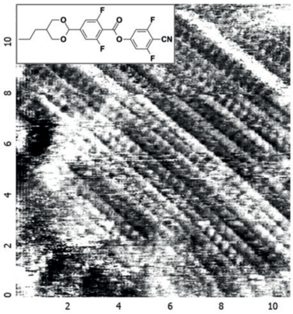

Fig. 1. *STM-image of DIO-CN monolayer on Au (111) surface. Parameters of scanning: 11× 11 nm*^{2}*,* I_t *= 107 pA,* U_t *= 629 mV.*

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Confocal Raman and scanning spreading resistance microscopy of coexistence and evolution of structural phases near metal-insulator transition in VO_2 films

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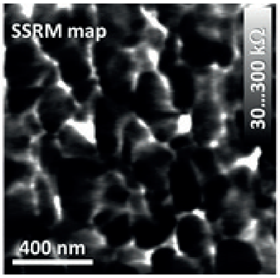
Vanadium dioxide (VO_2) is a strongly-correlated material exhibiting a near-room temperature reversible metal-insulator transition (MIT) accompanied by a dramatic change in the structural, optical, and electronic properties. It is a candidate for potential applications in optics and optoelectronics. The local distribution of the coexistence of different structural phases during MIT in magnetron-sputtered VO_2 thin films were studied by confocal Raman and Scanning Spreading Resistance Microscopy (SSRM). All of our films feature signature Raman modes of VO_2, and we did not find any obvious features corresponding to other vanadium oxides. Next, we presented the analysis of Raman Ag and Bg phonon modes of VO_2 thin films as a function of temperature, which are quantitatively correlated with electrical SSRM measurements of VO_2 films to provide insight into the relationship between the structural and electronic transitions. The critical role of the V-V and V-O vibrational disorder in the VO_2 phase transitions from an insulating monoclinic phase (M1) to a metallic tetragonal rutile (R) phase is established. The coexistence and evolution of the mixed (M1+R) phase in the vicinity of MIT might be caused by strains and defects within the grains of the film. The Raman mapping using to study the spatial distribution of crystallographic M1 and R phases depending on temperature. The SSRM maps show that phase localization in granular VO_2 films depends on strain distribution within grains and local thermal and electric field conditions. Grain surfaces, typically high-strain regions, are likely to adopt the rutile phase, while interiors, subjected to lower strain, may predominantly exhibit the monoclinic phase. Grain resistance measures approximately 104 Ω, with interior regions on the order of 106 Ω. Elevating temperature or/and adjusting local electric fields reduces grain resistance by an order of magnitude and diminishes the presence of the insulating phase. Results from our study showed that a combination of the Raman data with SSRM analysis is an effective tool for probing lattice and electronic structural dynamics.



Atomic force microscopy imaging of DNA onto surface under electrochemical control

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Deoxyribonucleic acid (DNA), the carrier and transmitter of genetic information in biological systems, has fascinated biologists, chemists, and physicists. However, current interest in DNA goes beyond its role in biology. In recent decades, nucleic acid-based research is also related to investigating the behavior of DNA under the influence of an external stimulus.

Scanning probe based microscopy methods, in particular, atomic force microscopy (AFM) with its unique capability to perform high-resolution imaging and characterize organic and inorganic samples at ambient pressure under air, liquid, and vacuum conditions, are valuable tools for understanding the complex architecture of nanoscale structures and for studying microscopic and submicroscopic objects below the diffraction limit of optical microscopy.

Despite of the fact that the imaging of single DNA strands immobilized on mica (which is a dielectric) by AFM has become routine , much of what was learned about the nanoscale conformations of adsorbed DNA on mica may not automatically translate to DNA adsorbed on conducting supports [1].

Here, we provide the results of AFM-based investigation of DNA at conductive surfaces in presence of electric fields shedding light on the current understanding of the behavior of such interfaces at the nanoscale.

Acknowledgements

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Session 8. Nanoplasmonics and surface enhanced spectroscopy

Plasmon-enhanced photodoping of $GeSe_2$ thin films with silver

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The most promising chalcogenide glass for use in non-volatile memory devices and photovoltaics are germanium chalcogenides, photodoped by silver. In addition, they are more compliant with environmental requirements compared to most investigated arsenic chalcogenides. In this work, photostimulated diffusion of Ag, enhanced by a plasmon field, into $GeSe_2$ thin films is studied. To ensure the excitation of surface plasmon polaritons (SPP) at the interface between Ag and $GeSe_2$, nanopatterned substrates in the form of silver diffraction gratings were used, on which chalcogenide layers 8.2 and 10.4 nm thickness were deposited by thermal evaporation in vacuum. The samples were exposed from its $GeSe_2$ side by the p-polarized radiation of a He-Ne laser ($\lambda = 632.8$ nm). The radiation of the same laser attenuated by two orders of magnitude was used to detect SPP, which made it possible to study the kinetics of photostimulated processes in the Ag-$GeSe_2$ structure.

It has been established that the photostimulated changes in the optical characteristics of the Ag-$GeSe_2$ structure, including the characteristics of the plasmon resonance, are significantly enhanced in the case of SPP excitation at the interface between silver and chalcogenide. The excitation of SPP during photodoping leads to an almost fourfold increase in the photostimulated Ag flux into the $GeSe_2$ layer in the initial period of exposure. The kinetics of the increase in the refractive index of thin $GeSe_2$ film due to photodoping with silver is well approximated by a logarithmic dependence. The concentrations of photodissolved silver in the chalcogenide layers are estimated.

It is assumed that the excitation of SPP during exposure can significantly intensify the electronic stage of photodoping due to an increase in the intensity of the electromagnetic field of the incident radiation near the Ag–$GeSe_2$ interface. In addition, in the case of SPP excitation at the metal-chalcogenide interface, plasmon-assisted hot carrier generation due to plasmon decay on the metal film surface is also possible. All this leads to an increase in the flow of drifting Ag^+ ions and an acceleration of the photodissolution of silver in $GeSe_2$, which is observed in our experiment.

Raman characterization of MoS_2/Graphene lamellar heterojunctions to develop flexible electronics

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The most typical member in the two-dimensional (2D) transition metal dichalcogenides (TMDCs) family, layer-dependent molybdenum disulfide (MoS_2) with a particular direct band gap in monolayer has been widely applied in various sensors with high sensitivity. The huge research interest in MoS_2 is caused by its similar properties to Graphene (the appearance of which turned the whole world of electronics). However, it is still challenging to achieve a large-area MoS_2 monolayer with desired material quality and electrical properties to fulfill the requirement for practical applications.

The growth of a high-quality defect-free monolayer depends on many factors, such as the type of substrate, quality of starting material, pressure, temperature, gas flow, etc. MoS_2 monolayer was prepared by chemical vapor deposition (CVD). MoS_2 layers are transferred from SiO_2/Si to a flexible substrate with Graphene using polymethyl methacrylate (PMMA). The solution was applied to the surface by spin coating to remove PMMA/MoS_2 buildup.

The use of Raman spectroscopy demonstrated the mono and few-layer MoS_2. Analysis of the Raman spectrum shows a high-quality MoS_2/Graphene lamellar structure (Fig. 1). The key issue is to ensure the integrity of MoS_2 films during large film growth and transfer.

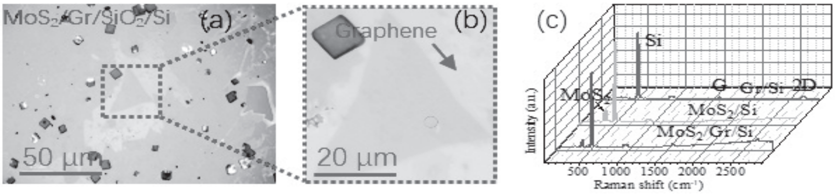

Fig. 1. (a) The optical photo of surface MoS_2/Gr film. (b) This is the Raman representation area. (c) This is the result of Raman characterization of Graphene, MoS_2 and MoS_2/Graphene.

Laser-induced breakdown spectroscopy as a promising nanotechnology for heavy metals detection in aqueous solutions

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Providing the population with clean drinking water is a priority task around the world according to the World Health Organization. This environmental problem is most acute today during the enemy shelling and hostilities in Ukraine.

Laser-induced breakdown spectroscopy (LIBS) is a novel atomic emission spectroscopic nanotechnology used to determine the elements composition of a sample. Method has several advantages, including easy sample pre-treatment, fast operation, chemicals free in process and identification of multi-state substances [1].

Experimental setup for the single-pulse LIBS consists Q-switched Nd:YAG high-power laser Continuum Minilite with a pulse duration of 10-15 ns, a repetition rate of 10 Hz, maximum pulse energy of 850 mJ, and output at the wavelength of 1064 nm with the USB 4000 Ocean Optics Spectrometer.

We primarily focused on the application of chemical replacement combined with surface-enhanced LIBS (CR-SENLIBS) for the detection of Cu, Pb, Cd and Cr in aqueous solutions. LIBS spectra containing information about all elements were collected immediately after microplasma generation. The aqueous solutions of 500 µg/mL $CuCl_2$, $Pb(NO_3)_2$, $CdCl_2$, $CrCl_3$ and NaCl as an etalon, were dropped into Al plates and dried. LIBS experiments for Al plates also were conducted [2].

These results show that CR-SENLIBS is a perspective method for improving the detection sensitivity of heavy metals in aqueous solutions, as well as for water quality monitoring around the world and for Ukraine in this difficult period of war.

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Hybridization biosensor system based on surface plasmon resonance for detection of the sequence of oligonucleotides of the Philadelphia chromosome

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The aim of this research was to show principal possibility of enhancement of SPR signal using gold nanoparticles modified with probe oligonucleotides and surface blocking molecules for detection of DNA sequences of the Philadelphia chromosome.

According to the aim of the study, 80 base pair long oligonucleotide of the site of the e13a2 junction of the Philadelphia chromosome [1] was used as the target molecule; in this study it is referred to as 80-mer BCR-ABL. The biosensor system employed for detection of target molecules consisted of two parts: the SPR sensor surface modified with probe oligonucleotides mod-Ph that are complementary to 24 base pair long region of 80-mer BCR-ABl and 13 nm gold nanoparticles (AuNPs) modified with the second DNA probe SH-DP which is complementary to another region of the 80-mer BCR-ABL target with a length of 18 nitrogenous bases. For hybridization of target oligonucleotide with immobilized probes, the target sequence solution of various concentrations in the 2×SSC buffer solution is injected into the measuring flow cell and exposed for 10 min.

Compared to the biosensor without AuNPs, the use of the proposed hybridization biosensor system made it possible to determine the concentration of 80-mer BCR-ABL in the studied solution with a much higher sensitivity and a much lower detection limit.

The linear operating range of the proposed system was shifted to low concentrations by two orders of magnitude, which is more promising for its use for analysis of real biological samples.

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Quantum plasmonics of achiral carbon nanotubes

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At present, the optical properties of carbon nanotubes (CNTs) are the subject of intensive theoretical and experimental studies. [1]. Particularly interesting from the point of view of their practical use are optical phenomena in the region of surface plasmon resonance (SPR), when there is a significant amplification of local electromagnetic fields. Therefore, the study of surface plasmons in CNTs is an urgent problem.

Due to the anisotropy of CNTs, their optical properties are characterized by the dielectric tensor

$$\tau_{ij} = \begin{pmatrix} \tau_{\perp} & 0 & 0 \\ 0 & \tau_{\perp} & 0 \\ 0 & 0 & \tau_{\parallel} \end{pmatrix}$$

Since the length of CNTs significantly exceeds their diameter, $\tau_{\parallel}(\omega)$ the classical Drude model can be used for research. At the same time, $\tau_{\perp}(\omega)$ a significant contribution is made by interband transitions determined by quantum size oscillations of conductivity [2].

The calculations were carried out for achiral CNTs of the "zigzag" and "armchair" types, which have a metallic type of conductivity. It has been established that the size oscillations of the transverse SPR frequency are characteristic of CNTs with radii ≈ 3 nm. In addition, these size oscillations take place in the vicinity of curves characterizing the classical size dependence of the plasma frequency.

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Size dependence of the polarizability of a metal nanosphere in a linear chain of nanoparticles

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One of the objects of study in plasmonics is plasmons in a chain of nanoparticles, which represent a transitional case between localized and propagating plasmons. First of all, the interest in chains of nanoparticles is due to the fact that they can be used as subwavelength waveguides of optical radiation.

Let us consider a linear chain of *N* metal nanospheres of radius *R*, located in a medium with permeability T_m. In the dipole approximation, the polarizability of the -th nanosphere can be written in the following form

$$\alpha_n = \left(\frac{\mathrm{T}_n + 2\mathrm{T}_\mathrm{m}}{\mathrm{T}_n - \mathrm{T}_\mathrm{m}} \frac{1}{R^3} - \frac{2}{3} \mathrm{i} k^3 \right)^{-1} , \qquad (1)$$

where $(2/3)\mathrm{i}k^3$ is the first nonzero radiation correction to the inverse polarizability, needed to ensure the conservation of energy of the system; T_n is the permittivity of the *n*-th nanosphere

$$\mathrm{T}_n = \mathrm{T}^\infty - \frac{\omega_p^2}{\omega(\omega + \mathrm{i}\gamma_n)} , \qquad (2)$$

Here ω is the frequency of an incident electromagnetic wave; T^∞ is a contribution of the crystal lattice to the dielectric function of a metal; ω_p is the plasma frequency; is the effective electron relaxation rate in a nanoparticle, which has the form

$$\gamma_n = \gamma_\mathrm{bulk} + \mathrm{A}\ (\omega, R) v_\mathrm{F}/R , \qquad (3)$$

where γ_bulk is the relaxation rate in a 3D metal; ν_F is the Fermi velocity, $\mathrm{A}\ (\omega, R)$ is an effective parameter describing the degree of loss of coherence upon scattering of an electron by the surface of a particle.

Expressions (1) - (3) make it possible to determine in the dipole approximation the size-dependent polarizability of a nanosphere in a linear chain.

SERS-substrates with self-localization of analyte in the hot-spots

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Surface-Enhanced Raman Spectroscopy (SERS) has been increasingly gaining popularity as a promising spectroscopic tool for detection and identification of trace amounts of various molecular species. The level of sensitivity claimed by many groups over a wide range of types of substrates and analyte compounds is sufficiently high for real-life application of this technique. Nevertheless, the wide commercialization of the SERS-based sensing technologies requires good performance at affordable fabrication costs of the sensing substrate. At the same time, the best performance is usually reported for SERS substrates fabricated by rather sophisticated routes. In addition, one of the important issues is reproducibility of the enhancement produced by the substrate. One of the conditions of achieving reproducible results is homogeneous distribution of the analyte over the substrate surface. On the other hand, the condition of obtaining high enhancement is localization of as much as possible analyte in the so-called “hot spots” – nanometer-scale space regions of high concentration of electric field between metal nanostructures.

In this work an original type of very affordable substrates is proposed that combines the possibility of self-localization of the analyte (deposited from solution) in the hot spots that are regularly arranged over the substrate surface. The basis of the substrate are self-assembled layers of highly monodisperse silica nanoparticles, synthesized by a facile and scalable route in water. The coverage of this nanoparticle layer with thin layer of gold or silver by thermal evaporation or some other methods creates numerous hot-spots in the places between silica particles. The efficiency of the developed substrates is demonstrated for several different types of analytes, in particular common dye molecules, small biomolecules such as aminoacids, as well as large biomolecules such as proteins.

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Developing plasmonic nanoparticles for application in stimulating ion channel activity in living cells

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Gold nanoparticles (AuNP) are widely used for biomedical applications [1]. Surface chemistry of nanoparticles in the as-synthesized state and its modification in the biological environments can underlie the precise mechanism of action and discrepancies between different studies.

In our previous studies [2,3] we have established that fluctuations in intracellular calcium can modulate plasmonic AuNP-induced gating of BKCa channels in smooth muscle cells and neurons through an indirect mechanism, probably involving the interaction of plasmon resonance with calcium-permeable ion channels.

In this work we optimized the synthesis conditions for highly stable AuNP with localized surface plasmon resonance (LSPR). We sought to obtain nanoparticles of the smallest size, preferably <10 nm, retaining their properties in biological buffer system for a long time, sufficient to study their effect on membrane ion channels and associated intracellular calcium signaling in isolated vascular smooth muscle cells and spinal ganglia neurons of the rat.

The work was supported by the Ministry of Education Science of Ukraine (project K-I-105).

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Influence of weak magnetic field preprocessing on plasmon absorbance of silver nanoparticles

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The ethanol solutions of the ZnO nanoparticles were placed in a constant and homogeneous weak magnetic field (B = 60 mT). Exposure time in the field was: 1 hour, 1 day and 5 days. These solutions were used for photocatalytic formation of ZnO/Ag nanoheterostructures under the action of UV irradiation. The production cycle was repeated during 30 days. During this time, the evolution of the obtained optical absorption spectra of solutions containing ZnO/Ag nanoparticles were measured. For reliability of the received results the solution which was not exposed in magnetic field, but stored together with all samples at the same temperature conditions was used as a reference. Under the UV action, photocatalytic reduction of Ag (I) and the formation of a ZnO/Ag colloidal heterostructure occurs, which is characterized by an absorption maximum at 400–460 nm. Moreover, increasing the UV dose leads to a long-wavelength displacement of this peak. These processes are characteristic for all studied samples. But the energy positions of the observed peak at low and maximum doses of weak magnetic field radiation do not match. It was found that within 30 days the final position of the maximum of plasmon absorption of the Ag nanoparticles, which were formed on ZnO solutions, that have been undergone magnetic field treatment, slowly shifts to the position of the latter in the reference sample. The latter circumstance indicates a "memory effect" that lasts for a month. It can be assumed that the observed spectral features upon irradiation of solutions containing ZnO NPs, silver nitrate, and sulfur are due to the photocatalytic reduction of elemental sulfur with ethanol and the formation of colloidal composite ZnO/Ag_2S (core/shell) NPs.

Correlation of Raman studies, X-ray and magnetic properties of $LuFeO_3$ nanoparticles

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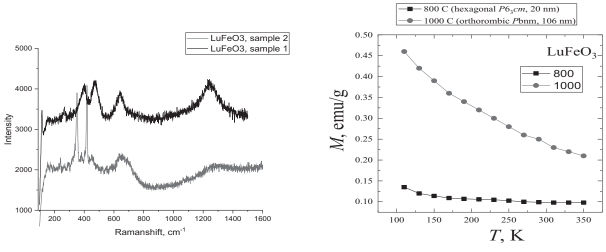
Using X-ray diffraction and Raman spectroscopy we revealed the gradual substitution of the hexagonal by orthorhombic phase in $LuFeO_3$ nanoparticles, which average size vary from 20 nm to 110 nm prepared, prepared at several annealing temperatures 800, 900, 1000 and 1100°C. A combination of Raman spectroscopy and magnetic measurements was used to explore the correlation of the lattice dynamics, structural changes, paramagnetic and antiferromagnetic properties of the nanoparticles appearing in dependence on their size and annealing temperature. As the next step, the phenomenological approach and numerical modelling were applied to calculate the phase diagrams, magnetic and polar properties of $LuFeO_3$ nanoparticles of various size. Special attention has been devoted to the possible appearance of magnetoelectric response, as well as to the comparison of modelling and experimental results. The combination of the Raman spectroscopy with X-ray diffraction, magnetic measurements and theoretical approaches allows to establish the physical origin of possible correlations between the lattice dynamics, microstructure, phase composition and magnetic properties of the $LuFeO_3$ nanoparticles prepared in different conditions.



Raman spectra (a) and temperature dependence of magnetization (b) of $LuFeO_3$ nanopowder after annealing at 800 (black curves) and 1000°C (red curves).

The work is supported by the Ministry of Education and Science of Ukraine, grant K-I-70 "Influence of dimensional effects on the electrophysical properties of graphene-ferroelectric nanostructures".

Quantum chemical modeling of vanadyl complexes with N,O-chelating Schiff bases grafted to silica surface

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Vanadium(IV) Schiff base complexes effectively catalyze a wide range of catalytic reactions. Catalysts containing complexes immobilized on solid matrices have shown great promise due to their ease of separation from the reaction mixture. However, determining their real structure by indirect physical methods can lead to ambiguous interpretations, so the application of quantum chemical methods to this task holds significant importance. In this work, the ROHF method with SBKJC basis set has been used to establish the structure of model vanadyl complexes with sterically hindered Schiff Base ligand – N-propyl-1’-hydroxy-2’-acetonaftonimin, immobilized on silica surface. Three types of structures are considered: (1) 2 ligands connected to silica surface by -$(CH_2)_3$- spacers surround one vanadyl ion; (2) 2 ligands connected to silica surface by -$(CH_2)_3$-SiH_2-O- spacers surround it; (3) 2 ligands connected to silica surface by spacers -$(CH_2)_3$-SiH_2-O- surround two distant vanadyl ions (one ligand, a water molecule and a chloride ion near each ion).

From the calculations results, it follows that model (1) could have a hypothetical structure with hydrogen atom transferred from a silanol group to the oxygen atom of vanadyl group, thereby reducing the vanadyl ion to vanadium(III), not observed in the experiment; so this structure is unlikely. Lengthening the spacer in model (2) alleviates strain, resulting in possible conformations with hydrogen bonds between the vanadyl oxygen atom and silanol groups. Triplet structure (3) could be formed in a presence of large excess of vanadyl ions. So the stable structures of vanadyl complexes may have different compositions. When the surface is densely populated with ligands, trigonal bipyramidal bischelate complexes are most likely.

Diffusion and phase transitions in anisotropic submonolayer adsorbed films with coherent structures

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The temperature-dependent processes of self-organization and degradation of adsorbed lithium films on the (112) faces of tungsten and molybdenum were investigated using the molecular dynamics method. The mathematical model was the most close to real Li-Mo(112) or Li-W(112) systems [1]. The aim of the work is to study phase transitions in submonolayer adsorbed films with strongly pronounced anisotropy, mutual influence of the structure and physical and chemical properties of the film and surface (2D) self-diffusion of adatoms. It is shown that the processes of temperature degradation of film structures are strongly blurred in strongly anisotropic chain structures formed with coherent coverages $\theta_{Li} = 0.25$ and $\theta_{Li} = 0.5$. That means the structures occur in wide temperature intervals (second order transitions). This corresponds to the main idea of the theory of 2D phase transitions KTHNY [2, 3]. Now many experimental facts are accumulating, which are quite difficult to explain within the existing theories of phase transitions. We found that with a stoichiometric coverage of $\theta_{Li} = 0.25$, a first order phase transition takes place in the process of temperature degradation. This manifests itself in the catastrophic destruction of adatom chains at T = 160 K (formation of kinks, an increase in the number of vacancies and a sudden increase in the number of interchain atoms). We consider the cause of such phenomena to be nonlinear effects in the propagation of longitudinal acoustic modes.

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Session 9.
Nanoscale physics

Combining the Modified Crystal Field Theory and ab initio calculations under nanosystem studies

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We suppose to apply a complex theoretical approach combining the semi-empirical Modified Crystal Field Theory (MCFT) [1] and the density functional theory for studying nanoscale systems.

The MCFT is a semi-empirical method for calculating the electron energy levels of paramagnetic ions embedded in a coordination complex. Thanks to simple parameterization, the MCFT makes it possible to investigate the coordination complexes with arbitrary symmetry and a set of ligands to study various types of distortions of the coordination complex by modelling their effect on the electron state of the system, as well as to investigate the evolution of the electron spectrum under the influence of pressure, temperature, or magnetic field.

The capabilities of the density functional theory code allow designing the supercells with the given dopant concentration to detect crystal structure distortions using a geometry optimization procedure. Based on the obtained information, the electronic structure of dopants is calculated using the MCFT.

EPR diagnostics of compounds combined with MCFT and the DFT-based structure optimization procedures is a very informative methodology that can use to develop synthesis modes for minimizing the impact of impurities and defects that impair the quality of the obtained materials.

The above methodology is applied to study the EPR spectra obtained from ZnSeFe samples in the temperature range from 5 to 300 K. As a result, a temperature-induced charge transfer from Fe^{3+} into Fe^{2+} on cooling is detected and explained. A theoretical model of the EPR spectrum formation due to two alternative paramagnetic sub-systems related to Fe^{2+} and Fe^{3+} ions is developed. The manifestation of structural defects occurring in the doping process in the EPR spectrum formation is studied.

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Effect of Temperature on the Nanocluster Structures in a Concentrated of Aqueous Solutions of Glucose

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The study of concentrated aqueous solutions of glucose is relevant because such solutions are used in medicine as hypertonic solutions. The light-scattering of aqueous solution of glucose with a concentration of 40% in the temperature range of 20-70°C is studied. The time dependencies of light scattering intensity (t) were obtained. It was established that the intensity undergoes significant fluctuations over time. It is shown that the function (t) is a quasi-periodic function.

The two phases coexist, namely, solution and glucose crystal hydrate in the studied temperature range. Accordingly, the interpretation of the experimental data was carried out within the framework of physics model. This model is a complex of crystal hydrate nanoclusters surrounded by a solution.

Such system is in a strongly unbalanced state, where the behavior of the nanocluster is determined by the local temperature. The changing of local temperature replace the structure of the nanocluster, namely, leads to an increase or decrease in its size. But there is also a feedback is releasing (or absorbed) of heat at changing of nanocluster size. The local temperature change during this process.

Accordingly, the time dependence of nanocluste size has an self-oscillation character [1,2]. As a result, self-oscillations of the dielectric constant occur and in the experiment significant fluctuations in light scattering are observed.

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Springer Science & Business Media.

Reduced resistance contacts to thermoelectric materials on the bi – te basis

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The reduction of electrical contact resistances is essential for increasing the efficiency of thermoelectric energy conversion. One of the ways to solve this problem is to create nanoheterostructures with a band spectrum described by the Fivaz model in the near-contact region. Within the framework of this model, the movement of charge carriers in the plane of the layers is described by the effective mass approximation and across by the tight bond approximation.

This is especially important in terms of miniaturization of thermoelectric energy converters. At the same time, it should be borne in mind that during the operation of thermoelectric modules in the mode of generating electrical energy, the formation of intermetallics, in particular nickel telluride, is possible in the contact areas. Such compounds can not only significantly increase the electrical contact resistance, but also lead to the destruction of the contact structure due to the formation of cavities and cracks in the intermetallic layer. This is possible because the specific resistance of the heterostructure is significantly lower than the specific resistance of the base material with a parabolic band spectrum.

The physical model, within which the degradation of the contact structure was considered, was as follows. It was believed that first the tellurium diffuses into the nickel to form nickel telluride, and then the nickel telluride diffuses into the base thermoelectric material and is distributed in it, forming a transition contact layer.

The results of the research are presented in fig. 1-3.

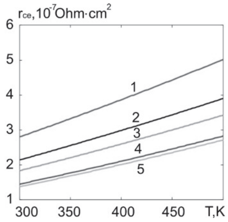

Fig. 1.

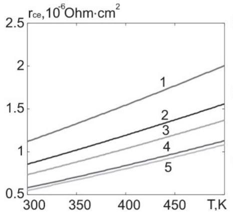

Fig. 2.

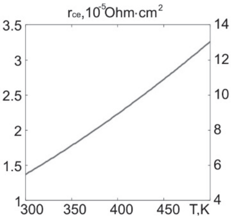

Fig. 2.

Fig.1. *Temperature dependences of the specific contact resistance in the Fivaz model for the rates of the non-parabolicity: 1-0.5; 2-1; 3-2; 4-5; 5-10 for the spent nickel layer thickness 5 µm. Fig.2 is the same as Fig. 1 for the spent nickel layer thickness 20 µm.*
Fig 3. Temperature dependences of the specific contact resistance for the parabolic band spectrum and for the spent nickel layer thickness 5 µm (left axis) and 20 µm (right axis)

From the figures we can see that thanks to the use of heterostructures, the electrical contact resistance can be reduced by 60-100 times even in the presence of intermetallics due to the effective blocking of the scattering of charge carriers across the layers.

Deformation-diffusion effects in CdSe-core – ZnS/CdS/ZnS-multilayer shell quantum dots for their biomedical applications

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Semiconductor quantum dots (QDs) have a wide absorption spectrum, narrow emission spectrum, large Stokes shift, high quantum yield and photostability, significant sensitivity and biocompatibility. Therefore, QDs have prospects for use in nanobiology and nanomedicine, in particular, they can be used as fluorescent labels to control targeted drug delivery. One of the current areas of research into the possibilities of using QDs in medicine concerns the reduction of their toxicity. Unitary doping with an isovalent impurity of QDs with a multi-layer shell allows creating nonuniform deformation in QDs, which induces deformation-diffusion flows that can limit the mobility of QD atoms, reducing their toxicity and increasing the degree of uniformity of their sizes [1]. The research of self-consistent deformation-diffusion effects in QDs with a multicomponent shell doped with an isovalent impurity is an urgent task in the context of their use in medicine.

In this work, researches of the spatial redistribution of defects of interstitial Cd in CdSe/ZnS/CdS/ZnS QDs and bionanocomplexes based on them were carried out. On the basis of the developed non-linear deformation-diffusion model, the method of "deformation-diffusion retraction" is proposed, which will limit the migration of cadmium beyond the QD boundaries and significantly reduce their toxicity for living organisms.

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The effect of thermal motion of a transverse domain wall on the magnetization of a cylindrical ferromagnetic nanowire in weak magnetic fields

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The study of ferromagnetic nanowires is one of the urgent problems of modern physics. Due to their unique properties, these objects are used for various technologies. An important problem is to control the magnetic and thermodynamic phenomena that occur in ones. Possible solution to this problem can be the use of domain walls (DWs) that are formed in nanowires. In this connection, in the works [1,2] it was established that thermal mouton of transverse DW can affect the thermodynamic properties of cylindrical nickel and iron nanowires. In this case, the values of critical diameters of nanowires (the maximum diameters at which the thermodynamic factor of DW is still actually) depend on their magnetization. Therefore, it is relevant to investigate the effect of thermal motion of DW on magnetization of ferromagnetic nanowires in external magnetic fields.

Using [3], it was found out that the maximum value of the relative average magnetization of the cylindrical ferromagnetic nanowire that is caused by the factor of the transverse DW is $\leq 1.2\ 10^{-2}$ in weak magnetic fields. The temperature corresponding to the given thermodynamic state was also determined [2]. Obtained result can find practical application in the production of highly sensitive precision nanoscale magnetic devices such as: relays, vibrators, resonators, stabilizers, etc.

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Effects of non-reciprocity in multilayer semiconductor nanowires with radial structure of the layers

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In recent time, a great attention is attracted by multilayer semiconductor nanowires which have become the basis of new generation of semiconductor electronics due to their outstanding electronic and optic properties [1,2].

In planar structure, it has not any meaning how this structure is orientated in space. At turning over it from left to right its properties do not change (if the voltage polarity is reversed). In nanowires with radial layer structure, its properties depend on in what direction the layers follow – from nanowire center or to it.

For illustration of non-reciprocity effects in semiconductor core-shell nanowires, a number of *p-n* junction structures are considered. In designation of the junctions, we stand conductivity type of the core material at the first place.

1. Depletion widths and capacitance of radial homo *p-n* and *n-p* junctions with the same doping levels are different.

2. Depletion widths and capacitance of radial *p-n* and *n-p* junctions are different even at symmetric doping if they are hetero junctions.

3. Density of saturation current in radial p^+-*n* diode is larger than planar value but smaller than it in radial *n*- p^+ diode.

4. In radial p^+-*n* diode, effective diffusion length of the injected current carriers approaches of 1.25 of the planar value while in radial *n*- p^+ diode, it equals to only 0.4-0.8 of the planar value.

5. Both in *p-i-u* diode and in *n-i-p* diode, spatial distribution of non-equilibrium carriers under double injection is asymmetrical even at equal electron and hole mobilities. At non-equal mobilities, character of the asymmetry changes to opposite one in *p-i-u* diode but become even more pronounced in *n-i-p* diode.

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Penetration of Abrikosov vortices into doubly connected superconductors

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We present the results of studying the spatio-temporal patterns of penetration of Abrikosov vortex flux into doubly connected bulk superconductors. Comparison of the obtained results with the patterns of penetration into single-connected superconductors (disk) showed significant differences. The limits of stability of the critical state, the magnitude of the magnetic flux entering the sample, and the duration of the vortex avalanches themselves change.

We measured the incoming magnetic flux using inductive sensors fixed on the sample, as shown in Fig.1. The outer coil registered the change in the magnetic flux in the entire sample, while the inner coil recorded the change in the cylinder (ring) cavity. The Hall sensor, located above the center of the hole, measured the local magnetic induction.

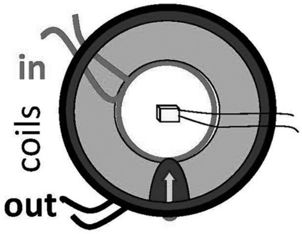

Fig. 1. *Placement of sensors on the sample.*

As a result of the studies carried out, it was shown that the limits of stability of the critical state in a disk and a ring of the same external dimensions differ significantly. The range of magnetic fields, in which the critical state in the ring is unstable, expands almost twice as compared to the disk, and the number of flux avalanches in the ring increases almost 7 times compared to the disk. With an increase in the external magnetic field, the magnitude of the magnetic flux introduced into the ring by avalanches decreases in inverse proportion to the induction of the external magnetic field, while in the disk the flux decreases almost linearly. Other features of the dynamic response of doubly connected hard superconductors to a changing external field are also discussed.

Tunneling of the quasielectrons in the single barrier structures based on the gapped graphene

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We consider the structure of the three graphene regions the middle of which is calculated as the potential barrier for electrons. Within the framework of the continuum model, based on the Dirac type equation, the transmission coefficient T of quasielectrons is calculated and analysed. We guess that the potential barrier is of rectangular shape. It is believed that there is an electrostatic barrier as well as the Fermi velocity barrier due to the fact that this quantity may acquire different values in the barrier and out of barrier regions (v_{F2} and v_{F1} respectively) of the considered structure. Presenting the solutions of the equation (1) in the standard form used in the presence of a barrier (incident and reflected waves), and matching the eigenfunctions and their derivatives at the interfaces we obtain the expression for the transmission rates in the following form:

$$T=4E^2(E-U)^2\cos^2\theta\cos^2\phi/\{4E^2(E-U)^2\cos^2\theta\cos^2\phi+\sin^2(qd)[\beta^2E^2\cos^2\theta-(E-U)^2\cos^2\phi]^2\},$$

where E is the energy of the falling particle, U the height of the barrier, θ, ϕ angles of falling and refraction respectively, q is the quasiimpulse in the potential barrier, d the barrier width , $\beta = v_{F2} / v_{F1}$. The presence of the energy gap can lead to significant reduction of T. This fact can be used in the development of the transistor-type devices based on graphene. The transmission coefficient T is very sensitive to the parameter β, so that we can choose its values to vary the situation. The Fabry-Perot type resonances as well as the critical angle play an important role in the formation of the transmission spectra. The analysis of the coefficient T on the qusielectron energy E and other problem parameters such as the energy gap, the barrier width is also provided.

Properties of spectral characteristics of quasi-stationary electron states in an open multi-cascade nanostructure

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With the appearance and development of nano devices, the functioning of which is ensured by the electronic transport through the resonant tunneling nanostructures, the relevance of the theory of physical properties of open structures has significantly increased. Despite the significant progress of experimental research, the theory is still not complete, as far as we know. The main problems are in the mathematical complexities caused by non-localized wave functions and the quasi-stationary spectrum of quasiparticles. Thus, in the majority of theoretical papers the research was carried out in simplified models.

In the proposed paper, we develop a theory of spectral characteristics of quasi-stationary electron states in a multi-cascade nanostructure, being an element of a quantum cascade detector. In the approximation of effective mass and model of rectangular potentials, using the transfer matrix method based on the solutions of the Schrödinger equation, an exact expression for the scattering S-matrix is obtained for open nanostructure with an arbitrary number of cascades. For the example of a multi-cascade resonant tunneling structure with GaAs wells and $Al_{0.33}Ga_{0.67}As$ barriers, the calculation of resonance energies and resonance widths of quasi-stationary electron states is performed within the complex poles of the S-matrix. The peculiarities of their evolution depending on the number of cascades are investigated.

It is established that in N-cascade nanostructure the resonance bands, each of which is formed by the energies of N quasi-stationary states, are observed in the electron spectrum. If the number of cascades increases in the interval of small values, the width of the bands increases too and at $N>10$ they almost do not change. It is revealed that one can see anti-crossings in the dependences of the resonance energies on N. States with energies on horizontal sections are characterized by significant constant resonance widths (small lifetimes), due to their location in the external left or right cascades. The widths of all other states localized in the internal cascades of the structure rapidly decrease rapidly when the number of cascades increases.

Renormalized spectrum of quasiparticle interacting with three-mode phonons in Davydov's model with damping at cryogenic temperature

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The investigation of broadband nano photodetectors functioning in far-IR range has been intensified recently. Considerable attention of researchers is aimed at optimizing of the operating parameters of nano detectors, which work in the current second window of atmosphere transparency, located in the far-IR range in the energy region of 90-160 meV. Detection of the electromagnetic field in this interval is provided by nano devices with active elements of cascades, which contain multi-layered quantum wells of isotropic compounds, where phonon-accompanied electron transport occurs as a result of their interaction with the three main phonons modes (confined optical mode and two interface ones).

In the proposed paper, the theory of the renormalized spectrum of a quasiparticle interacting with three-mode phonons in the Davydov's model [1] with damping at cryogenic temperature is developed. Analytical calculation of the shape-functions of the electromagnetic field absorption band is performed within the method of Green's functions, as in [2] with the introduction of phenomenological attenuation at T=0K.

It is shown that the shape-function is a superposition of Lorentz peaks, which contains, in addition to the main (without phonons) three groups of peaks of unmixed individual modes and all possible combinations of peaks of mixed phonon modes. The properties of the obtained spectrum are analyzed.

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Magnetotransport properties of BiSe whiskers

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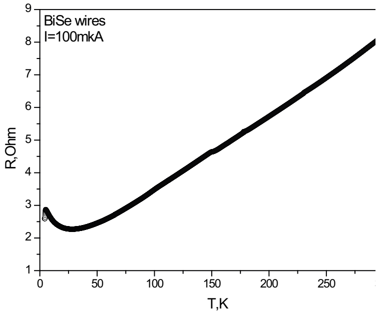
Magnetotransport properties of BiSe nanostructures are very interesting from the physical point of view. Firstly, the weak anti-localization (WAL) effect was observed in the magnetoresistance measurement of BiSe microcrystals, showing the presence of topological surface states at low temperatures [1]. Secondly, the positive magneto-resistance value of Bi_2Se_3 films measured at low temperatures (2–100 K) confirmed the gapless topological surface states in Bi_2Se_3 thin films [2].

Transverse magnetoresistance of BiSe whiskers with doping concentration $1x10^{19}$ cm^{-3} was studied in the temperature range 4.2 – 77 K and in magnetic fields up to 10 T. Temperature dependence of resistance for heavily doped n-type BiSe whisker at a zero magnetic field is shown in Fig.1.

A sharp drop at temperature below 4.2 K and minimum at temperature about 30 K are found on the temperature dependence of resistance in BiSe whiskers. The revealed sharp drop of resistance below 4.2 K indicates in a possible partial superconductivity in the whiskers. The observed minimum on the temperature dependence of resistance for n-type BiSe whiskers is likely resulted from a contribution of Kondo effect in the whisker conductivity. The practical application of BiSe whiskers was also proposed as result of the studied low temperature properties.



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Dimensionality and anisotropy of upper critical fields in nanometer-thin superconducting NbN films

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Superconducting niobium nitride (NbN) was recognized as the material of choice in developing future generation quantum devices, largely due to its advantageous superconducting properties and wide applications in superconducting electronics. The combination of a large penetration depth (> 180 nm), a short coherence length (~5 nm), a sufficiently high transition temperature T_c and upper critical fields H_{c2} makes it possible to use such films where the dimensions of device elements are on the nano- and mesoscales. In addition, it is one of three model materials that are intensively used to study the superconductor-insulator quantum transition, accompanied by the formation of flat two-dimensional (2D) regions known as nanoscale superconducting puddles.

In our work, we have studied comparatively clean NbN layers of the thicknesses of 10, 50, and 100 nm with T_c's ranged from 9 to 16 K, respectively. Transport properties were measured in a Quantum Design physical properties measurement system close to T_c and at different angles by sweeping the magnetic field up to 6 T. In all samples, the in-plane field was larger than outside the plane. This finding can be explained by the weakening of the orbital pair breaking impact on the parallel component of the critical field due to the reduced dimensionality. Effects caused by the crowding of vortices in dissimilar orientations of the current along the sample and the in-plane magnetic field were revealed. Unexpectedly, we have detected the evidence of the 2D behavior even in the thickest samples and at sufficiently low temperatures, probably due to the emergence of nm-thin superconducting puddles inside the films studied. Surprisingly, this phenomenon manifests itself quite far from the superconductor-insulator transition.

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Strongly nonlinear excitation of short-wavelength exchange spin waves in magnetic nanowaveguides

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Spin waves, the collective excitations of the magnetic orders, provide a scalable wavelength and exhibit a variety of distinct nonlinear phenomena that make spin waves promising for data processing at the nanoscale [1]. To the date, many spin-wave processing elements, both analog and digital, have been proposed and verified [2]. However, several problems hinder the construction of integrated spin-wave circuits, one of which is a lack of an efficient mechanism to excite long-running exchange spin waves with normalized amplitudes.

Here, we report a possible solution of this challenge. We study excitation of forward-volume spin waves in 200 nm wide nanoscale waveguides by a micron-wide microstrip antenna with microfocused Brillouin light scattering spectroscopy. Nanoscale width allows to achieve an unprecedented nonlinear frequency shift above 2 GHz, corresponding to a quasi-uniform magnetization precession with the angle of 55° under the antenna, which transforms into exchange spin waves with a wavelength of down to ten nanometres outside the antenna with an efficiency of more than 80%. Even more intriguing is that the amplitude of the excited spin waves is constant and independent of the input microwave power due to the self-locking nonlinear shift, enabling robust adjustment of the spin wave amplitudes in future on-chip magnonic integrated circuits.

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Acoustoelectronic effect in semiconductor quantum dots with a multilayer shell

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An important factor that affects the spectral characteristics of radiation of the quantum dots (QDs) is elastic deformation. The source of elastic deformations can be both internal factors (the mismatch of lattice parameters, the point defects) and external factors. In particular, the cause of periodic deformation can be an acoustic wave. Such deformation can occur during electromagnetic irradiation of QDs. In this case, the thermo-deformation mechanism of sound generation is used [1]. Also, the QDs are widely used in medicine and can be exposed to ultrasound.

QDs with a multi-layer shell also undergo significant deformations due to the mismatch of lattice parameters of the contacting layers. Therefore, there is a need to develop a model of the core-multilayer shell QD, that is exposed to an acoustic wave.

As a result of the interaction of the acoustic wave with the electronic subsystem of the QD, the following effects can be observed:

1) the periodic deformation due to self-consistent electron-deformation coupling leads to a local periodic displacement of the bottom of the conduction band and the top of the valence band and, accordingly, to the modulation of the energy of electron and hole and the width of the band gap;

2) the emergence of a gradient of the refractive index under the influence of ultrasound leads to a periodic change in the direction of QD radiation;

3) the propagation of an acoustic wave in a certain direction leads to an increase in the size of QDs in this direction, and, accordingly, to a distortion of their shape and a change in the energy of electron and hole.

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Magnetism of highly doped CdTe:Cr crystals with self-assembled doping-induced nanoprecipitates

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In the heavily doped CdTe:Cr single crystals, grown by the modified PVT method, the doping-induced crystallographic phase separation was revealed due to the exceeding of Cr solubility limit in this compound. The separation resulted in the formation of the array of nano-thick monoclinic Cr_3Te_4 crystalline lamellas, which are crystallographically oriented with respect to the CdTe matrix. The ferromagnetism of such heterogeneous material was proved in the range from liquid nitrogen temperature to above room temperature by magnetization measurements using a vibrating sample magnetometer. Off-axis electron holography experiments proved that the observed ferromagnetic behavior is mainly governed by the embedded Cr_3Te_4 particles, although a weak contribution of the $Cd_{1-x}Cr_xTe$ matrix itself to the overall ferromagnetism can be also supposed. Electron holography revealed anisotropy of the precipitates, their easy magnetic axis is perpendicular to the [101] crystallographic direction. The EMR spectra consisted of multiple lines found to originate from both Cr atoms dissolved in the CdTe crystalline lattice and from Cr-related extrinsic phases. The lines coming from Cr_3Te_4 lamellas were distinguished in the spectra at a high magnetic field, and the shape anisotropy of the precipitates was calculated from the angular dependence of the resonance field for these lines.

Theory of electric field effect on the optical properties of elliptical quantum wires

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Modern technologies allow the growth of semiconductor quantum wires with various cross-sectional shapes. Theoretical studies are mainly carried out for cylindrical quantum wires, as exact solutions of the Schrödinger equation exist in this case. Wave functions are obtained analytically using Bessel functions, enabling their use in constructing solutions for more complex problems.

Elliptical nanowires, due to the anisotropy of their shape, possess unique physical properties that can be utilized to create new electronic nanostructures with pronounced anisotropy of intensity and polarization of emitted light.

In this study, the effect of a perpendicular electric field on the energy spectrum and wave functions of quasiparticles in an elliptical quantum wire is investigated. For this, solutions of the Schrödinger equation were calculated by the matrix method on the base exact wave functions for the case of an absent electrical field. The angular and radial parts of the exact quasiparticle wave function are expressed in terms of even and odd angular and radial Mathieu functions of the first kind.

It is shown that the spectra of electrons consisting of energy subbands correspond to the even and odd states of quasiparticle, which depend differently on the ellipticity of the nanosystem. In the case of a cylindrical quantum wire, the energy levels are degenerate. Only the quasiparticle ground state, which is an even state, is nondegenerate.

The selection rules were established and the dependences of the oscillator strength of the electron intersubband quantum transitions in the dipole approximation on the ellipticity of the nanosystem and the electric field strength were obtained.

As a result of the calculations, it is shown that the ground state of the electron undergoes the largest shift under the action of the electric field. Its wave function is the most deformed. This is reflected in the electric field dependencies of the elliptical quantum wire's optical properties.

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Peculiarities of magnetoresistance in GaAs whiskers at low temperatures

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The studies of magnetoresistance of nanostructures give an opportunity to deeper understanding of exotic nanosize effects. In particular in such structure WL exists in low (up to 1T) magnetic fields and low temperatures, which is explained by free electron spin relaxation in n-type GaAs [1]. Besides, heavily doped with S and Te n-GaAs layers reveales positive magnetoconductance in the temperature range of 3–80 K, which is attributed to the magnetic field suppressed weak localization [2]. A 2D electron system (2DES) exposed to a magnetic field at low temperatures provides an excellent platform for observing physical phenomena such as weak localization and weak anti-localization, giant negative/positive magnetoresistance [3],

The present paper concerns to investigation of temperature and magnetoresistance of GaAs whiskers at low temperatures. The magnetoresistance measurements were conducted in the magnetic fields up to 14 T in the temperature range 4.2-77 K. For measurements the current passing through the samples was about 1 mA. By investigation of I-U characteristics we haven't observed any deviation from Ohm law. So the current was suitable for the sample and don't call their heating. The magnetic field induction was applied to the sample in perpendicular to the current direction. The correspondent field dependencies reveal a jump-like change in the transverse magnetoresistance, which is observed in magnetic fields up to 0.2T. The further enlargement of magnetic field induction leads to transition to a linear change of magnetoresistance with magnetic field that can be used in sensors of magnetic field based on the investigated whiskers.

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Electric field effect on the absorption coefficient of hemispherical quantum dots

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The increased interest in hemispherical quantum dots [1-2] is caused by the outstanding properties and potential applications of such nanostructures in optoelectronic devices such as photodetectors, solar cells, and others.

This study presents a simple model within the effective mass approximation to describe the effect of an external electric field on the energy structure and wave functions of electrons and holes in type II hemispherical quantum dots. The case of a uniform electric field perpendicular to the surface on which a hemispherical quantum dot is grown is considered.

The solutions of the Schrödinger equation were obtained by the matrix method on the orthogonal basis of the exact wave functions of quasiparticles in this nanostructure without the influence of an electric field.

It is shown that the shift of the energy levels of the electron localized in the core of the nanostructure depends linearly on the electric field. And the shift of energy levels of the hole is non-linear.

The values of the wave functions expansion coefficients show that new states of quasiparticles are formed from several old neighboring states, the number of which increases with increasing electric field intensity.

At the same time, the basic state, which makes the greatest contribution to the formation of a new state, can change. Such a change in the symmetry of the quasiparticle state occurs in the case of energy levels anticrossing. As a result, the oscillators strength of quantum transitions, which are forbidden in the absence of an electric field, increase significantly.

The optical transition energies and the absorption coefficient dependences on external electric field are investigated.

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Frequency response of nanoscale core-shell of silicon wires doped by boron and nickel

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In the paper, a study of the p-type silicon wires doped with boron impurity and modified with nickel was carried out. The object of the study was silicon crystals with a concentration of boron charge carriers of 5.5×10^{18} cm^{-3}. The research was carried out in the temperature range from 4.2 K to 77 K. The alternating current passing through the sample was 10 - 250 kHz.

The use of frequency spectroscopy allows us to analyze the electrical response of the sample under study to the alternating current that passes through the sample and causes the transfer of charge carriers. In this case, the frequency response of the sample will be determined by the superposition of microscopic charge transfer processes, which cause a change in the macroscopic signal, which is recorded by the device, during the transfer of charge carriers. Since charge transfer can be associated with several interrelated processes, each of which can occur at different speeds or through different channels (including charge transfer across phase boundaries, electrode boundaries, and others), frequency spectroscopy allows us to study the mechanisms of electrical conductivity in more detail [1]. For studied samples were obtained the dependencies, which are shown in Nyquist diagrams. The frequency response of the samples was evaluated and the mechanisms of charge carrier flow were proposed depending on the observation conditions.

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Plasmon enhancement of luminescence of cyanine dye J-aggregates

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Supramolecular high-ordered assemblies, known as J-aggregates, exhibit a range of unique spectral properties that are distinct from those of individual molecules. These properties include a narrow absorption band, near-resonant luminescence, high oscillator strength, giant third-order susceptibility, and effective resonant energy migration. The specificity of J-aggregates' optical properties is governed by the electronic excitations delocalized over molecular chains and molecular (Frenkel) excitons formation due to translational symmetry and strong dipole-dipole interaction between molecules in the J-aggregate chain. One of the characteristic features of J-aggregates is the narrow red-shifted exciton band, called J-band, with the width determined by the exciton coherence (or delocalization) length.

J-aggregates are promising candidates for novel photonic materials, particularly in the form of thin films, especially polymer films. While J-aggregates in solutions often possess low photostability, their stability becomes much higher in polymer films. However, J-aggregate formation in polymer films also reveals some drawbacks, such as the low luminescence quantum yield of formed J-aggregates. One way to manipulate J-aggregates' optical properties in solid samples is by utilizing the effect of exciton-plasmon coupling via aggregates' interaction with noble metal nanostructures.

Typically, J-aggregates and metal nanostructures interaction is studied in the strong coupling regime, as due to unique J-aggregate spectral properties, giant Rabi splitting can be reached up to several hundreds of meV at room temperatures. Often, the corresponding hybrid exciton-plasmon polariton modes, formed at strong J-aggregate-metal nanostructures interaction, are called plexcitons. In the weak regime of exciton-plasmon coupling, quantum yield enhancement of the J-aggregates luminescence was demonstrated by placing the J-aggregates at the optimal distance from metal nanoparticles.

This report provides an overview of the features of exciton-plasmon interaction of J-aggregates and metal nanostructures, with special attention to the plasmon enhancement of J-aggregate luminescence.

Phonon spectra and electron-phonon interaction in a quantum dot – quantum ring semiconductor nanostructure

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The intensive development of nanotechnology has made it possible to create new nanostructures with clear geometric shapes. In particular, structures containing quantum dots and nanorings have already been created and are being intensively studied [1].

In this work, we investigate a nanostructure consisting of a cylindrical semiconductor quantum dot (quantum well, GaAs medium), which through a finite potential barrier ($Al_xGa_{1-x}As$ medium) is tunnel-connected to a coaxial cylindrical nanoring (quantum well, GaAs medium).

The stationary Schrödinger equation for an electron is solved analytically exactly. Radial wave functions are obtained as a linear combination of Bessel, Neumann, and modified Bessel functions.

As for phonon spectra, the energies of bounded and interface phonons, as well as the corresponding polarization field potentials, are found in the dielectric continuum model. In this case, the potential of the polarization field of bounded phonons is sought in the form of an expansion in terms of the complete system of cylindrically symmetric Bessel and Neumann functions. To calculate the potential of the polarization field and the energies of the interface phonons, the Laplace equation is solved in each of the regions of the multilayer nanostructure using the limiting conditions for the continuity of the tangential component of the electric field strength and the normal component of the electric bias vector.

It has been found that the energies of bounded phonons in a nanostructure coincide with the energies of longitudinal optical phonons of the corresponding massive three-dimensional analogues of nanocrystals.

The energies of interface phonons are obtained from the solution of the corresponding dispersion equations, and their value depends on the geometrical parameters of the nanostructure.

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Molecular dynamics simulations of the adsorption processes of H_2 molecules on the surface of ZnO nanoclusters

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In this study, we conducted a comprehensive analysis of the mechanisms involved in the adsorption of H_2 gas on ZnO nanoclusters using the Molecular Dynamics (MD) method. To accurately capture the nature of these nanostructures, we employed the Reactive Force Field (ReaxFF) interatomic potential. This potential has been specifically developed to encompass a wide range of chemical compounds, including ZnO, and has been successfully applied in our previous research [1, 2].

To investigate the adsorption process, we systematically varied the gas pressure, size of the ZnO nanoparticles, and system temperature as the main parameters of interest. It was observed that at elevated temperatures, the smaller nanoclusters began to melt during the initial stages of the simulation. Conversely, when excessively large nanoclusters were employed, the simulation times significantly increased, hindering a comprehensive analysis of the system's evolution until the final moments of the modeling process. Consequently, meticulous selection of optimal initial conditions was crucial.

To characterize the adsorption processes, we employed the total energy of the system, radial distribution functions (RDF) and Centro-symmetry parameter (CSP) as key descriptors. These metrics allowed us to gain insights into the intermolecular interactions and spatial arrangements of the adsorbed H_2 molecules on the ZnO nanocluster surface. Overall, our study provides valuable insights into the intricate processes underlying H_2 gas adsorption on ZnO nanoclusters, and it contributes to the broader understanding of nanomaterials adsorption capabilities.

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Deformation-induced band gap variation in phosphorene: tight-binding model vs first-principles simulations

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We study the effects of the uniaxial tensile strain and shear deformation as well as their combinations on the electronic properties of single-layer black phosphorene. The evolutions of the strain-dependent band gap are obtained using the numerical calculations within the tight-binding (TB) model (with the distant-dependent hopping parameters) as well as the first-principles simulations based on the density functional theory (DFT) and compared with previous findings. TB model allows to carry out calculations for the systems containing millions of atoms (as the real experimental samples contain), and thus is substantially less computationally demanding in comparison with any ab initio simulations, restricted to periodic supercells or lattice fragments with a relatively small number of atoms due to the computational expensiveness. The TB-model-based findings show that the band gap of the strain-free phosphorene agrees with experimental value and linearly depends on the both stretching and shearing: increases (decreases) as the stretching increases (decreases), whereas gradually decreases with increasing the shear. A linear dependence is less or more similar as compared to that obtained from the ab initio simulations for shear strain, however disagrees with a non-monotonic behaviour from the DFT-based calculations for the single-axis tensile strain. Possible reasons of the discrepancy are discussed. As the parameter defining the bond-length dependence of the hopping integrals in the TB model enhances, the linear dependence of the band gap on the uniaxial tensile strain becomes the non-monotonic one and similar to that obtained from the DFT calculations. In case of a combined deformation, when both strain types (tensile/compression + shear) are loaded simultaneously, their mutual influence extends the realizable band gap range: from zero up to the values respective to the wide-band-gap semiconductors. At a switched-on combined strain, the semiconductor-to-semimetal phase transition in the phosphorene is reachable at a weaker (strictly non-destructive) strain, which contributes to progress in fundamental and breakthroughs.

Composite Abrikosov vortices dissociation in 2-band superconductors and their nonlinear rf current response

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Multiband superconductors such as MgB_2, Fe-based pnictides, etc., have several superconducting gaps, which means there are several superconducting condensates that can exist. It is predicted that each condensate supports vortex excitation with fractional quantized flux [1]. Vortex formed from fractional vortices is called a composite vortex, and it turns out that under certain conditions, composite vortices in multiband superconductors can dissociate [2,3].

In the present work, we consider the possibility of composite vortex dissociation in two-band superconductor under the action of strong rf current which breaks the coupling of fractional vortices. For the case of dc current flow, such kind of dissociation of composite vortices in two-band superconductors and its manifestation on dc current-voltage characteristics were considered in [3]. Here we extend this type of consideration for the case of ac currents action on composite vortices in two-band superconductors, calculate the threshold value of the ac current amplitude for the onset of dissociation of composite vortices into the fractional ones, and also investigate how this dissociation should manifest itself in the microwave properties of two-band superconductors, in particular – through the amplitude and frequency dependencies of the nonlinear surface resistance.

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Interface influence on the structure of ion lattice subsystem of semi-infinite metals

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Modern experimentally obtained and studied metallic nanosystems are characterized by ~10 nm. Due to the "quantum-size effect" [1, 2], the physical and mechanical properties of such nanosystems are significantly different from bulk ones. The presence near the "metal–vacuum" interface of a near-surface electron layer, the thickness of which reaches the order of two lattice periods of an ideal metal (without "metal–vacuum" interface), leads to a change in the lattice structure of the ion subsystem. This, in turn, leads to a change in the mechanical characteristics (Young's modulus, Poisson's ratios, force constants, etc.) of such nanosystems. The works [3, 4] consider models for describing such changes within the framework of solid media mechanics, which doesn't take into account the discreteness of the ion subsystem and therefore requires some unreasonable assumptions (in particular, the presence of a mass flow).

In this paper, a quantum-statistical model for the influence of "metal-vacuum" interface on the structure of the lattice ion subsystem is proposed. Using as a "reference system" a subsystem of interacting conduction electrons in the field of positive "jellium" [1, 2] in the adiabatic approximation, taking into account pairwise "ion-ion" interactions, an effective Hamiltonian of the ion subsystem was obtained. The free energy of the proposed model was calculated. The equations for the displacements that minimize the free energy were obtained and solved.

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Shallow impurities in delta-doped Si quantum well under a transversal electric field

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This work presents the results of our theoretical studies of the effect of a transverse electric field on the properties of silicon quantum wells (QWs) delta-doped in the center or at the edge with a shallow n-type impurity at various temperatures.

In our earlier papers [1], we reported on the possibility of adjusting the energy distance between spatially quantized levels in a quantum well using temperature. The reason for this effect is the change in the shape of the bottom of the QW–with increasing temperature, the half-width of the V-shaped bottom decreases. This leads to an increase in the energy distance between the first spatially quantized QW levels, which are important in intersubband optical transitions.

The results of our calculations show that the application of a transverse electric field makes it possible to more easily tune the energy gaps between the spatially quantized levels. In addition, an increase in the transverse electric field can give a much larger range of energy gap tuning.

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About possible Quantum Bits on Q1D-SE vibration levels over Helium film

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The concept work [1] considers for QC a hydrogen-like levels of the surface electrons (SEs) over microelectrodes under helium using the Stark's shift of Ridberg's levels into resonance with mkm-radiation. Here proposed possible realization quantum bits using a Q1D-SE vibration levels over helium film. Considered a set of micro-channels or dielectric threads (δ in thickness) arranged as coaxial rings with R and r radius which is coupling each other same radial lines equidistant situated. The system of channels is situated in a mkm-cavity with H_{11} mode working at super-low temperature, T. Over nodes of the large radius ring in pressing electric field is formed Q1D-SEs. The two vibration states corresponding UHF is considered as a qubit basis |0> and |1>. The vibration spectrum vs film thickness d is $\omega d^2 = e^2 / [(1 + \varepsilon_s) m d^3]$ (here e and m are the charge and mass of electron correspondently and ε_s is the dielectric constant). The Q1D-SEs states superposition is defined by the Rabbi frequency pulses both either the UHF or the pressing electric field pulse. The SEs can move between rings at changing the radial electric field. The entanglement of states is possible at SEs Wigner crystallization in space between rings. The temperature T_c and electron density ns connected as $T_c < 0.226\times 10^{-6}\, n_s^{1/2}$. Read out of the Q1D-SE state after reverse electric field can be perfomed with some probability at node both either the micro-capacity or the SET (single electron transistor).

Estimates: R~1mm; r~0.1mm; δ~10μm; UHF-cavity H_{011} resonance is 10^{10} Hz, ΔE=0.5K and T~20mK. The linear electron density over nodes can be ~ 5×10^4m^{-1}. Near ring of small diameter the electron crystal goes to melt at 20 mK [2].

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Simulation of the optical characteristics of organic solar cells with the addition of noble metals of different spherical shapes

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Investigating changes in the optical characteristics of solar cells, we are looking for parameters that will help increase the efficiency of these cells. We investigated the optical characteristics of solar cells with the addition of spherical particles of noble metals (Ag, Au). The main changes in the particles were a change in shape from elongated to flattened. We marked the vertical radius as R_v, and the horizontal radius as R_h.

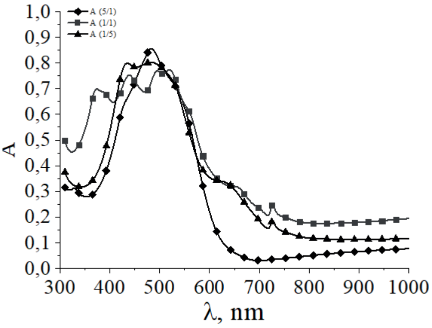

***Fig.1**. Ag, R_v/ R_h:5/1; 1/1; 1/5*

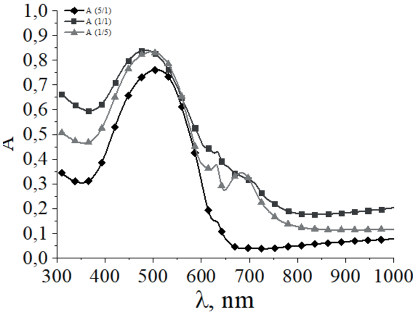

***Fig.2.** Au, R_v/ R_h:5/1; 1/1; 1/5*

On figures show the scattering of light with the addition of silver and gold particles Fig. 1. and Fig.2. in accordance, with different values of the ratios of the radii of the metal spheres.

First principle calculations of intrinsic Hall effect in $Sr_2FeMoO_{6-\delta}$ with oxygen nonstoichiometry

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$Sr_2FeMoO_{6-\delta}$ is a multifunctional double perovskite [1] with transport properties depending on both material processing and atomic scale structure.

Here, an interplay between electronic band structure and anomalous Hall conductivity in $Sr_2FeMoO_{6-\delta}$ has been studied. The band structure for minority and majority spin bands was obtained by DFT method and effect of oxygen nonstoichiometry on Fermi energy was determined. Calculations of intrinsic Hall effect was performed using maximally localized Wannier functions and based on Berry curvature correction to the electron dynamics, which manifests as transverse Hall current. The results have shown that intrinsic mechanism makes dominant contribution into anomalous Hall effect in $Sr_2FeMoO_{6-\delta}$ due to topological anomalies in band structure strengthening Berry curvature.

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Influence of impurity field and perpendicularly applied electric field on absorption in spherical nanoheterosystems

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Recently, nanoheterosystems with quantum dots (QDs) have been widely used. The most actual task of modern nanotechnologies is the development of new high-performance devices with improved parameters. It is very significant to control mentioned properties with high accuracy. Ways to solve this range of problems are the change QD size, doping and applying external fields. Also important is the case when we can control the properties of the system without changing the shape and size of the quantum dot. In this case, the physical properties of the spherical QD, such as an optical absorption coefficient can significantly depend on the presence of impurities in QDs and applied electric field. And it is also important to note that the impurity can be located anywhere in the quantum dot. We have already considered the case of a parallel applied electric field. We also study the case when the electric field is applied perpendicularly and in an arbitrary direction.

The linear optical absorption coefficient which is caused by the interlevel optical transition from the ground state to the first excited state has been determined.

The electron density in the QDs is chosen on the assumption that the QD has only one electron (impurity's electron). That is why $\sigma = 3 / (\pi a^3)$

As a result of research optical properties of GaAs/AlAs heterosystem is determined. The QD optical absorption coefficient with the off-central impurity shows that the displacement of the impurity from the QD center causes the shift of absorption bands into the low energy range. It is also proved that some obtained results are qualitatively similar to the results of the off-central donor impurity.

The dependence of the absorption coefficient on the radius of the quantum dot, the location of the impurity from the center of the quantum dot, and the magnitude of the perpendicularly applied electric field is shown.

Self-Ordering in the dynamics of forming Periodic 1D-structures controlled by external irradiation

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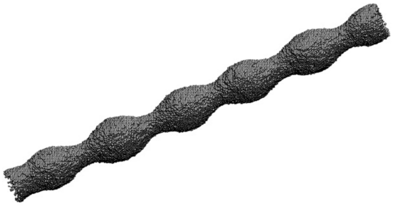
The spontaneous formation of transversely modulated 1D structures occurs either during the disintegration of nanowires into separate fragments or during the diffusion deposition of atoms onto their surface. In both versions, the main mechanism providing a fairly strict periodicity in the arrangement of the forming nanoclusters is surface diffusion of atoms. At a given temperature, T, the dynamics of the process corresponds to a decrease in the free energy, F, of the system: $dF=dU-TdS$. In our work, physical mechanisms are shown that can be controlled both in cases where the decrease in free energy is associated with a decrease in internal energy, U, and cases when this is achieved due to the dominant increase in entropy, S, despite the accompanying increase in U. The results obtained by us on the basis of the kinetic Monte Carlo model show that the indicated diversity in the dynamics of the system corresponds to the same diversity in their morphology at the final stage of evolution. We have demonstrated, for example, that for a given orientation of a nanowire relative to its internal crystal structure (variants of FCC, BCC and diamond-like crystal structures are considered), the period of its breakup can be significantly changed both upward and downward, up to the formation of super-short-wavelength "frozen in time" surface perturbations (unduloids-see the figures above), the occurrence of which corresponds to overcoming the threshold of the so-called energy instability of the surface. The variety of morphologies in the synthesis of one-dimensional systems and methods for controlling their parameters are demonstrated in the case of diffusion deposition of germanium or silicon atoms onto a silicon/germanium nanowire.



Cadmium iodide nanostructures and their dielectric properties

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Crystals of CdX_2 cadmium halide compounds (X = F, Cl, Br, J) are layered materials of class $A^{II}\,B_2^{VII}$, which by their structure occupy an intermediate place between ionic and molecular compounds, between three-dimensional and two-dimensional structures. As the size of the halogen (X = F, Cl, Br, J) increases, the degree of CdX_2 anisotropy increases, reaching its maximum value for cadmium iodide crystals. Their C_6 structural type is based on a tight hexagonal packing of J-Cd-J layers, within which the interactions are strong ion-covalent, and between the layers - weak van der Waals one. This causes a strong anisotropy of many physical properties of CdJ_2 and allows in some cases to use them as models of two-dimensional crystals. Both crystals and films of cadmium iodide are promising from a scientific and practical point of view. They are optically and radiation stable. The indirect edge of their fundamental absorption at 290 K lies in the region of 3.2 eV and shifts as the temperature decreases, reaching a value of about 3.5 eV at 80 K.

The paper examines the influence of the dimensionality of the crystal structure on the calculations of the frequency and dispersion dependence of the components of the dielectric function (or absorption coefficient and refractive index) for crystals of different dimensions in the random phase approximation.

The influence of the anisotropic environment on the dynamic and static components of the z-th component of the dielectric constant ε_{zz} is studied through the non-parabolic law of electron dispersion. It is shown that in one-dimensional systems ($\alpha=0$) in the static case ($\Omega=0$), the behavior of $\varepsilon_1(q)$, $\varepsilon_2(q)$ dependence and extrema on the corresponding curves are related to singularities in the real component of the polarization loop at $q=2k_F$ and $q=2(\pi - k_F)$. In the dynamic case ($\Omega\neq0$), with increasing frequency, the dielectric function $\varepsilon_1(q,\Omega)$, decreases in magnitude, while in the frequency interval $\Omega<2t$ it has a sign-changing character, and at $\Omega>2t$ - oscillating, but without singularities, and a $\varepsilon_2(q,\Omega)$, decreasing function, which at $\Omega>2t$ becomes zero because then $\mathrm{Im}\Pi(q,\Omega)=0$.

Numerical calculations of the quasi-two-dimensional and three-dimensional cases ε_1, ε_2 were carried out for the following positions of the Fermi energy level:

i) $\varepsilon_F<2t$, ii) $\varepsilon_F>2t$. The frequency dependence of $\varepsilon_1(\Omega)$ and $\varepsilon_2(\Omega)$ was calculated for small ($q_x=q_y=0$, $q_z=0.01$), and ($q_x=q_y=q_z=0.01$), $\alpha=0.10$eV, $t=0.01$eV.

In the two-dimensional case ($t=0$), the sharp minimum of *ReП* ($Re\Pi=-7.42^*10^{-2}$) is realized at $\Omega=1.5^*10^{-3}$eV. When we talk about the "anisotropy" of a chemical bond, it follows from the comparison of the dispersion curve in different directions of the inverse space.

The optical characteristics were also analyzed, namely the frequency dependence of the absorption coefficient (χ) and refractive index (n) for different values of the position of the Fermi level. They were obtained with the help of the found real and imaginary components of the dielectric constant due to the validity of the Kramers-Kroning relation in the entire frequency range. The obtained results were compared with experimental measurements of optical spectra of both crystals and films cadmium iodide at low temperatures.

Dynamic modes maps of incommensurate superstructures with elementary cell multiplication

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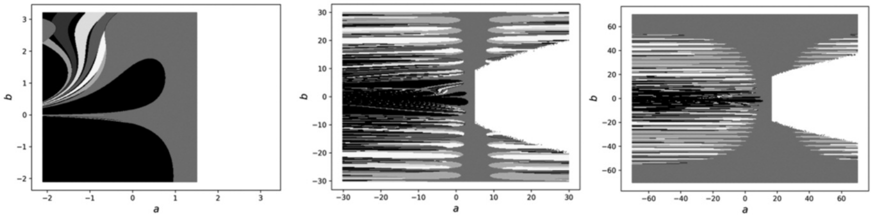
The crystals of the $[N(CH_3)_4]_2MeCl_4$ group (where Me = Zn, Cu, Co, Fe) are characterized by a complex sequence of phase transitions, including the transition to the incommensurate phase with nano-periodicity (with a period of ~ 100÷160 nm). Fig. 1 shows the maps of dynamic modes for systems characterized by different multiplication of the elementary cell.



n=3 *n=4* *n=5*

Fig.1. *Dynamic modes map in the a and b axes, where a=K is the value of the anisotropic interaction parameter described by the Dzialoszynski invariant, and b=T is the value of the long-range interaction parameter of the given system.*

In our case, the two-dimensional mappings were defined by recurrence equations as follows: *xn*+1=*f(xn,yn)*; *yn*+1=*g(xn,yn)*. A function describing the amplitude (R) of the incommensurability wave or its change *(R')* was used as a function *f(xn,yn)*. The function *g(xn,yn)* acted as a function describing the phase (φ) of the incommensurability wave or its change (φ'). Fig. 1 shows a two-dimensional mapping, where *R'* and φ' were used as functions *f()* i *g()*, respectively. The obtained maps of dynamic modes are characterized by an increase in the number of periodicities, with an increase in the multiplication value of the elementary cell. At *n*=3, when *K* and T change (*K, T*=0÷1), the existence of two disproportionately modulated phases is traced, which is observed in $[N(CH_3)_4]_2CuCl_4$ crystals.

Dynamic modes maps of incommensurate superstructures within the surface energy field

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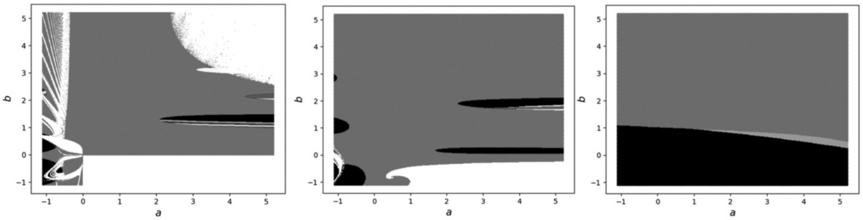
Dynamic mode maps are informative tools for studying the modes of complex systems. Examples of such systems include crystals of the A_2BX_4 group with the chemical formula $[N(CH_3)_4]_2MeCl_4$, where Me=Co; Zn; Mn; Fe; Ni; Cu. In these crystals, the incommensurate superstructure undergoes several modes upon cooling, including sinusoidal, solitonic, and stochastic modes. The influence of surface energy on the incommensurate superstructure leads to a transition from an inhomogeneous state to a homogeneous state, accompanied by the appearance of commensurate long-periodic phases.



n=3 *n=4* *n=5*

Fig.1. *Dynamic modes map in the a and b axes, where a = K is the anisotropic interaction parameter described by the Dzialoszynski invariant, b = T is the long-range interaction parameter of the system on the surface energy at n = 4.*

From the dynamic mode maps (Fig. 1.), it can be observed that the system exhibits a broad spectrum of possible periodicities in the absence of surface energy influence on the incommensurate superstructure. The influence of surface energy on the incommensurate superstructure leads to a narrowing and further contraction of the range of some observed periodicities while expanding the scope of others. The obtained results confirm the existence of the aforementioned dynamics of the incommensurate superstructure under the surface energy influence.

X-Ray diagnostics of nanoscale defects in single-crystals by deformation dependencies method for total integrated intensity of dynamical diffraction

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The interconnection between parameters of deformation dependencies of diffuse component of total integrated intensity of dynamical diffraction (TIIDD) and parameters of imperfect structure of single-crystalline materials is determined empirically. The case of presence of several types of defects in single-crystal, including nanoscale defects, namely clusters-precipitates SiO_2 and ‘small’ dislocation loops (size is about dozens nm) is considered. It is shown that deformation dependencies of diffuse component of TIIDD are different qualitatively for various type defects (see Fig.1). As a result, deformation dependencies of TIIDD are selectively sensitive to every of defect types for monocrystal with several types of microdefects at different values of effective deformation. The multiparametrical diagnostics of single-crystal defect structure by using only one deformation dependencies of TIIDD, which is obtained by approximation of dynamical ‘thin’ crystal is carried out.

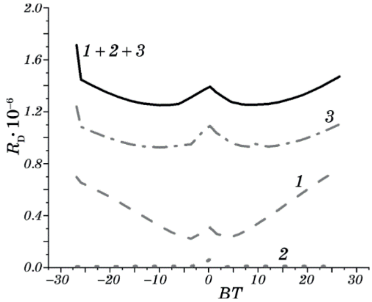

***Fig.1.** The deformation dependencies of diffuse component of TIIDD R_D: 1 — presence in single-crystal clusters-precipitates SiO_2 only, 2 — presence in single-crystal ‘large’ dislocation loops only, 3 — presence in single-crystal ‘small’ dislocation loops only, 1 + 2 + 3 — total deformation dependency of TIIDD taking into account all mentioned defect types in single-crystal (single-crystal Si, reflex (880) radiation MoK).*

Spin crossover phenomena in mixed rare-earth cobaltites

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The rare earth cobaltites are widely examined as thermoelectric, catalytic and gas sensor materials. A main feature of such materials is the presence of spin transitions in Co^{3+} ions from low spin (LS, t^6e^0) to immediate (IS, t^5e^1) or high (HS, t^4e^2) states, which are accompanied by magnetic and isolator-metal (IM) transitions, temperatures of which strongly depend on the size of rare earth element.

More than 60 polycrystalline single phase mixed solid solutions with nominal composition $R_{1-x}R`_xCO_3$ (R, R` – rare-earth element) were obtained by solid-state reaction or sol-gel method. Phase purity at the ambient environment of the investigated samples was confirmed by X-ray powder diffraction technique. The La-contained solid solutions are crystallized in two types of symmetry – rhombohedral (space group *R-3c*) or orthorhombic (space group *Pbnm*), while the rest powders have an orthorhombic structure. A multiphase region in the

$R_{1-x}R`_xCO_3$ systems localised within the average ionic radii of R between 1.197 Å and 1.205 Å. Calculated from structural data, the values of average bond lengths reduce with reducing average ionic radii of rare earth elements, while deformation of the perovskite cell increase. Evaluated bandwidth of Co-O-Co overlapping allowed predicting the temperature of diamagnetic-to-paramagnetic phase transition in investigated systems. The thermal expansion of more than 30 selected solid solutions was studied by X-ray synchrotron powder diffraction technique in the temperature range of 293-1173 K. The structure symmetry remains during a heating in the temperature range investigated, however abnormal thermal expansion behavior was revealed in $R_{1-x}R`_xCO_3$ solid solutions, similar to the "pure" rare earth cobaltites studied early. Additional analysis of valence bond lengths, octahedral tilt angles and perovskite deformation confirm the absence of structural phase transition and the presence of abnormal thermal expansion caused by the spin state transition of Co^{3+} ions. The magnetic and isolator-metal transition impacts in abnormal thermal expansion manifested in extra maxima on the temperature dependence of the thermal expansion coefficients (TEC). The values of the high-temperature TEC maxima agree well with the temperature of the isolator-metal transition obtained from electro-physical measurements.

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Application of clusters formed in a supersonic jet of noble gases as cryomatrices

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The use of clusters formed in a supersonic jet of inert gases as cryomatrices is a powerful and versatile tool for studying the properties of both the matrix and the embedded molecules or atoms and has applications in a wide range of fields.

The two-component Ar-N_2, Ar-CH_4, Xe-CH_4 and N_2-CH_4 clusters are formed in a supersonic gas jet exiting into the vacuum. Clusters are excited by electrons with an energy of 1 keV and 20 mA current. The range of the cathodoluminescence spectra is between 100 and 200 nm [1].

The high efficiency of VUV spectroscopy for studying the processes of heteroatomic cluster formation depending on the initial concentration of an impurity in a gas mixture is demonstrated. The concentrations of mixture components and conditions of supersonic jet outflow at which the formation of mixed clusters takes place were determined. The mechanisms of electron beam energy conversion and excitation energy transfer in clusters of different compositions are investigated.

In mixed Ar-CH_4 clusters, a full radiation quenching of Ar_2^* and $(Ar_4^+)^*$ centres accompanied by the appearance of an atomic hydrogen Ly-α (121.6 nm) line was detected. This indicates the presence of cryochemical reactions of CH_4 dissociation in the clusters occurring after the interaction of impurity methane and the matrix's hole carriers. The desorption mechanisms of electronically excited H^* atoms from clusters are proposed based on the analysis of energy transfer pathways from the matrix to the impurity.

It is shown that the directions of physicochemical reactions in clusters can change, and new processes can be initiated, which are not possible in the gas phase under single collisions.

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Stagnant layer contribution to the electrical conductivity of concentrated suspensions

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It is widely recognized that interface regions, such as the electrical double layers (EDLs), can significantly affect the electrical properties–say, the electrical conductivity σ_{eff} – of dispersed systems. At the same time, the actual nature, morphology and properties of interface regions, as well as the physico-chemical mechanisms through which these regions and their structural units contribute to σeff at different volume filler concentration c, remain, in many cases, unknown.

Recently [1], we suggested, formalized it into a many-particle theory, and scrutinized the following physical picture for the formation of σeff in suspensions. At low c, σeff is mainly a result of ion transport along conducting paths occurring beyond the slip plane. For given ion concentrations and mobilities, the conductivities of these paths are governed by the electric potential distribution in the outer (mobile) parts of the diffuse EDLs, that is, by the ζ-potential at and the location of the slip plane. For a hard particle, due to an ionic-size of the Stern layer, the distance between its surface and slip plane actually represents the thickness of the stagnant layer (immobile part of the diffuse EDL in between the Stern layer and the slip plane) or an analogue of the latter. These considerations should remain valid for high c provided the mobile parts of the diffuse EDLs are suppressed.

We present the elaboration of theory [1] for the latter situation. Under reasonable assumptions, σeff is obtained in the form of simple analytic expressions applicable for all available *c*. Processing with them data [2] for concentrated suspensions of ghost particles (fabricated by lysis from human erythrocytes and, in our opinion, covered with a 'repaired' layer before the slip plane) gives a better agreement with experiment than Maxwell's theory [2]. These results indicate the significance of incorporating the stagnant layer or its analog into the theory for σ_{eff}.

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A systematic analysis of rheological properties of nanofluids

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Suspensions of nanoparticles (nanofluids, NFs) possess unique physical properties like low drag due to the velocity slip boundary conditions at solid surfaces [1], high heat capacity and heat conductivity [2], dielectric and magnetic properties. Therefore, different types of NFs are used as efficient coolants for fluid flow based coolers for micromotors and microchips or heaters for the lab-on-a-chip applications. Microfluidic systems are used for homogeneous fluid mixing or fluid separation [2]. Efficiency of the NF-based microsystems is determined by rheology, phase transitions and aging processes. Despite many experimental and theoretical studies on rheology of NFs, many essential problems remain unclear.

In this study a review of experimental measurements, theoretical models and numerical simulations on rheological properties of NFs prepared on different base fluids (water, oil, ethylene glycol) and the nanoparticles of different shape, size and nature (crystals, metals, rods, fibers, ribbons, fullerenes, etc.) is given. A comparative analysis of different techniques for viscosity measurements for nanofluids with their positive and negative features is done.

A mathematical problem of the steady laminar flow of a NF with a base fluid with given density (ρ_{bf}), thermal conductivity and capacity (λ_{bf}, c_{bf}) and viscosity (μ_{bf}), and the concentration (C_{NP}) of nanoparticles with different size, shape and material properties (d,χ_j,ς_j) in a circular tube with known radius R and length L is considered for different inlet velocity, inlet and wall temperatures. The second order velocity slip and temperature jump boundary conditions have been considered. The hydraulic resistance Z_h and thermal resistance Z_{th} of the system have been computed with AnSys2023R1 software. An optimal value of C_{NP} providing the highest thermal conductivity at the lowest NF viscosity has been determined for any flow regime.

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Ab initio modelling of the $In_{4/3}P_2S_6/CuInP_2S_6$ heterojunction structure and electronic properties

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Metal thiophosphates have attracted increasing researchers' interest due to the vast range of their functional properties, originating from various occupations and complex interactions of metal cations in the P-S structure. In particular, ferroelectric materials are attractive for information storage applications due to their spontaneous polarization, which can be switched by an applied electric field. Guided by the requirements of device miniaturization and lowering energy consumption, the ferroelectric tunnel junction (FTJ) was proposed to be one of the most promising types of memory. In turn, 2D Van der Waals (vdW) ferroelectrics are attractive due to their uniform atomic thickness, absence of dangling bonds, and ability to integrate with other vdW materials providing their useful functionality. Thus, the search for new combinations of vdW materials to create artificial functional materials currently is an important challenge for scientific groups. In the presented work, we propose to consider selected promising vdW crystals to build functional heterostructures with peculiar electron and mechanical properties applicable in optoelectronics. We propose to focus on $In_{4/3}P_2S_6$, and $CuInP_2S_6$ crystals for their further use in functional electronics.

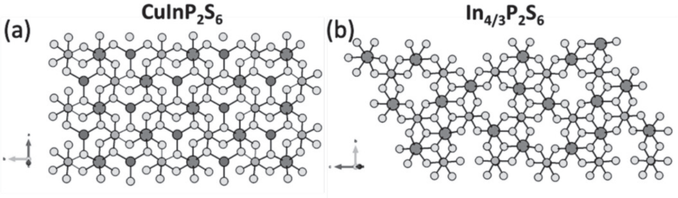

Fig 1. *Crystal structure of* $CuInP_2S_6$ *(a) and* $In_{4/3}P_2S_6$ *(top and lateral views [1]).*

First of all, structural modeling of heterostructures based on $In_{4/3}P_2S_6$ and $CuInP_2S_6$ crystals was carried out. After obtaining the most energetically advantageous artificial structure, first-principle calculations to study electronic and optical properties were conducted.

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Quantum capacitance of quasi-2D crystals dependent on parameters

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There are about half a thousand crystals in nature that can be classified as so-called quasi 2D-crystals. Such structures are of interest due to the specifics of their physical characteristics, namely, sharp anisotropy, diversity of electrical characteristics, specific mechanical properties. Such structures have been (and still are) the objects of intensive scientific research. Moreover, they are particularly promising in solving the actual scientific and technical problem of creating high-capacity electric energy storage devices.

The following abstract presents an analysis of the quantum capacitance of quasi-2D structures.

In the general case, the total capacitance C is determined by the equation for capacitances in series - the classical C_{el} being of an electrostatic nature and the quantum C_q being caused by a change in the chemical potential during charging [1].

Typically, $C_q >> C_{el}$ and therefore, in the case of in-serious connected C_{el}, C_q the latter C_q is ineffective. But in the case of low-dimensional structures, the situation may be reversed.

In the present work, a quasi-2D crystal is modelled by a Kronig-Penney potential in which neighbouring barriers corresponding to the crystal layers are located at a distance *a.* The smallness of a is the cause of dimensional quantization, namely, discrete states in the case of a single well are blurred into mini zones by the tunneling effect. The 2D zone of the electron in the plane of the layers is superimposed on each of them. It determines the resulting stepped character C_q, depending on the filling of the zone E_F The width of the shelves depends on the interlayer distance *a*, which can be changed by intercalation, hydrostatic or axial compression, etc. The width of the shelves depends on the temperature: the lower the temperature, the wider the shelves.

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Nonlinear localized waves and their stability near a combined linear and nonlinear metasurface

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The study of nonlinear waves in structured anharmonic media is one of the main problems of the dynamics of nonlinear waves and solitons. Considerable attention is paid to the theoretical and experimental investigations of spatial localization of high power electromagnetic beams in structured media with metasurfaces.

In the present work, we study both analytically and numerically the localized states of nonlinear waves propagating along a combined linear and nonlinear metasurface (defect layer). In the framework of the nonlinear Schrödinger equation with δ-functional potential containing both linear and nonlinear spatial perturbations, we describe all possible soliton states localized near such a metasurface in the linear medium, and investigate their stability. Via the wave localization mainly at the metasurface, there nonlinear properties appear; consequently, we take into account the Kerr nonlinearity only in the defect layer. It is demonstrated that the soliton states localized near the metasurface can exist at any sign of anharmonicity inside the defect layer in the case of attraction of elementary excitations to the metasurface. However, for the mutual repulsion between the excitations inside the layer, the localized states can exist only in the case of attraction of elementary excitations to the metasurface. For all possible localized states, the total number of elementary excitations and total energy of the system were found.

We performed the analysis of stability of all localized states and found that only soliton states with attraction of elementary excitations to the metasurface will be stable.

The results of the present study can be useful for the description of relevant systems in optics, in nonlinear dynamics of solids, structured media with metasurfaces, in Bose–Einstein condensation, etc.

Atomic and electronic structure of structurally modified graphene

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It is known, that at any finite temperature the thermal fluctuations in low-dimensional crystalline systems should lead to a displacement of atoms by a distance that is close to the interatomic distance [1,2]. This means, that two-dimensional crystals are to be thermodynamically unstable. Experimentally, it has been shown that graphene corrugation results from the thermal fluctuations with waves of 50–100 Å size [3]. All these means, that the corrugation effect can stabilize the structural modifications of graphene. This is an idea that the present work is based on. The ab-initio modeling method (*Quantum*-ESPRESSO program package) was used to demonstrate the possibility of the formation of a structural modification of graphene (M-graphene). The process of M-graphene formation from graphene sheets and added carbon atoms is simulated. The energetics of the interaction of added atoms with graphene has been studied in detail. The energy of formation of possible configurations with added atoms on a graphene sheet are calculated. The processes of transition of these atoms from one configuration to another have been studied. It has been established that hydrogen atoms destabilize the "bridge" configuration and act as a kind of catalyst for the "bridge" - "pair" transformation. Conditions are determined under which an increase in the number of added atoms leads to the energetic advantage of only the "pair" configuration. This configuration consists of two atoms stabilizing a vacancy in graphene. It is shown that such pairs of atoms can be ordered in different ways, forming several crystalline phases of graphene. The unit cell of M-graphene contains 10 atoms (symmetry group No. 191 P6/mmm). The enthalpy of formation and the phonon spectrum of this crystalline phase predict the possibility of its existence. With a less dense packing of "pairs", atoms with sp2 and sp3 bonds are located at the graphene plane. This phase of M-graphene is a conducting system.

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Electronic and magnetic properties of oxygen-terminated zigzag BeO nanoribbons

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The potential applications of honeycomb monolayer structures, including graphene, silicene, plumbene, and others, have garnered significant interest in recent years within the field of modern nanotechnology. These structures have attracted attention due to their unique properties and the exciting possibilities they offer for various technological advances. Recently, the hexagonal BeO monolayer has been experimentally obtained on the Mo(112) and Ag(111) surfaces [1-3]. Moreover, polar and non-polar zigzag-edged BeO nanoribbons (NRs) with different widths have been grown on the Mo(112) surface [2].

In this work, the width-dependent electronic and magnetic properties of oxygen-terminated zigzag BeO nanoribbons and polar zigzag BeO nanoribbons, have been investigated using density functional theory. We used both standard and hybrid exchange-correlation functionals. The energetics of the formation of one-dimensional hexagonal BeO nanostructures with different widths have been analysed. The structures of non-polar oxygen-terminated zigzag-edged BeO NRs are less energetically favourable than polar zigzag-edged BeO NRs. Edge metallization and ferromagnetism of the free-standing BeO nanoribbons are compared and discussed.

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Influence of low-power optical irradiation on alcohols Droplets evaporation processes

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The acceleration of heat and mass transfer during the evaporation of various liquids under external influence is a fundamental scientific problem that is widespread in various fields of application. The nature of droplet evaporation in different media depends on a number of parameters: droplet shape, size, and parameter of the gaseous medium in which evaporation occurs. In the presented work, the influence of external factors (pressure, wavelength 390, 565 and 625 nm) on the characteristics of the evaporation process of representatives of the homologous series of monohydric alcohols (propanol, butanol, pentanol, heptanol, octanol and decanol) in a nitrogen atmosphere at a constant temperature of 293 K was studied.

The studies were carried out using the technique presented in [1]. On the basis of the studied experimental data, the systems can be divided into two groups. The first group consists of systems containing alcohols with a relatively low molar mass (propanol, butanol, pentanol), the second – with heptanol, octanol and decanol. It has been found that when systems containing alcohols of the first group are irradiated and at different pressures, no change in their evaporation velocity is observed. In turn, for systems containing alcohols of the second group, an increase in the evaporation rate of alcohols (heptanol (37%), octanol (36%) and decanol (85%)) under the influence of irradiation with a wavelength of 390 nm at a pressure value of buffer gas 100 mm Hg. In its turn, under irradiation with lengths min λ=5565 and λ=625 nm, no increase in the evaporation rate of heptanol droplets is observed, and the behavior of octanol and decanol is similar to irradiation with lengths min λ= 390 nm.

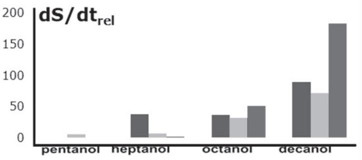

Fig. 1. *Visible increase in the velocity of vaporization of alcohols under the infusion of prominence pressures of 390 (■), 565 (■) ma 625(■) nm for a pressure value of the gaseous medium of 50 mm Hg.*

An analysis of the income of the results showed that the heating of drop alcohol under a dose of alcohol cannot produce such an increase in the rapidity of alcohol evaporation.

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Effect of PbO polymorphism and UV irradiation on the electrical properties of $PbMoO_4$ single crystals

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$PbMoO_4$ crystals are widely used in modern electronics as multifunctional materials. The main areas of applications are acousto-optics, laser technology and cryogenic scintillation systems for detecting rare events in physics of elementary particles. These applications require large-sized crystals of good quality. However, $PbMoO_4$ crystals grown from a melt on a seed, as a rule, contain characteristic structural imperfections. Among them there are nanometer-sized clusters, including intrinsic point defects and impurities, photoinduced complexes based on anionic MoO4 groups with trapped photoelectrons, inclusions of foreign phases. Such defects have a strong effect on the electrical and optical properties of crystals. In this work, we study the effect of variations of the initial mixture composition and UV irradiation on polarization and charge transfer processes in $PbMoO_4$ single crystals.

$PbMoO_4$ crystals were grown by conventional Czochralski technique in air from the charges of stoichiometric composition and with deviations from stoichiometry towards an excess of molybdenum oxide. The charge was prepared by using α- and β-crystalline modifications of PbO. According to our knowledge, the question of the effect of PbO polymorphism on the properties of $PbMoO_4$ has not been considered previously.

Electrical properties of the grown crystals were studied in the temperature interval 300 – 700 K and frequency range 10^2-10^6 Hz. It was shown that deviation from the stoichiometry of the composition and using the α-modification of PbO for the crystal growth strongly affected the processes of polarization and charge transfer, including phenomena induced by preliminary UV irradiation of the crystals. The observed effects are discussed within the framework of the hopping conduction model. It is assumed that they are associated with a redistribution of the density of localized states in the band gap of $PbMoO_4$ crystals, caused by the appearance of structural and photoinduced nanometer-sized defects in the crystal lattice.

Electric-controlled remagnetization of magnetic tunnel junctions

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The effect of electric-induced transitions between local magnetic states underlies the operation of magnetic tunnel junctions (MTJs), leading devices for field sensing, non-volatile magnetic random access memories and spin logic applications. It realizes through the internal effective magnetic field affecting localized magnetic moments with forming corresponding magnetic configuration of MTLs that realizes magnetic recording. Corresponding frequency, recording density and energy losses of the MTJ under applied electric field depends on the character of the transformation of the electric field into the internal effective magnetic field and the corresponding torque exerting on magnetic order of the active free layer of the MTJ [1]. To the greatest extent, the specified characteristics are provided by the direct transformation of the applied electric field into the perpendicular effective internal magnetic field via the voltage-current anisotropy effect related to the change of the occupancy of atomic orbitals and the Rashba spin-orbit coupling at the interface [2]. At the same time, the ultra-speed remagnetization of the MTJs in subnano-second region occurs under the ultra-short pulses of the applied electric field [3]. The phenomenological description of the electric-field control of the remagnetization is based on the Landau-Lifshitz-Gilbert model. However, the description of its dependence on an atomic and electron structure involves the microscopic approach based on the non-equilibrium Green functions.

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Electro-thermo-mechanical coupling in isotropic polarized structures

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This study aims to highlight some specific features of the local gradient theory of electro-thermo-elasticity which is employed to analyze the coupled mechanical and electric fields induced by non-uniform temperature distribution (thermal inclusion) in structures made of centrosymmetric materials with cubic symmetry. This higher-grade theory takes into consideration the effect of changes in material structure on coupled fields in dielectrics [1]. Under the plane strain assumption, we used the governing system of equation of local gradient theory of dielectrics in order to study the effect of thin thermal inclusion on the coupled fields in a polarized elastic medium and a thin plate. We showed that the plane thermal inclusion in non-piezoelectric structures induces the electric field and polarization localized close to the thermal inclusion interfaces. Hence, in the polarized layered structures, a part of the thermal energy induced by the inhomogeneous distribution of temperature is spent on the solid polarization. Due to the layer interfaces polarization, the bound electric charges are induced on its surface. Thus, the local gradient theory covers the thermopolarization effect. This effect is more pronounced for small-scale structures. Explorations of thermo-electric effect in elastic structures made of non-piezoelectric materials may have notable implications in both academia and industry.

Acknowledgement. Financial support from the Slovak Research and Development Agency and Ministry of Education and Science of the Ukraine under the bilateral grant Nos. SK-UA-21-0010 and 0122U002392 is gratefully acknowledged.

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Spectroscopic and microscopic studies of $BiSmFeO_3$multiferroics

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Bismuth samarium iron oxide (BSFO from $BiSmFeO_3$) belongs to novel ceramics combining ferroelectric and magnetic properties. It is a derivative of either bismuth ferrite ($BiFeO_3$) alone or bismuth ferrite – lead titanate ($BiFeO_3$-$PbTiO_3$) solid solution via substitution of a fraction of A-sites in BFO by the Sm ions in order to enhance the ferroelectric and ferromagnetic ordering and magneto-electric effect. For example, Maurya *et al.* [1] demonstrated that doping of BFO at levels of 10 at.% leads to increased magnetization and a sharp magnetic transition at 380 °C.

Sharma *et al.* [2] studied the structural and multiferroic properties of $Bi_{0.885}Sm_{0.115}FeO_3$ in comparison to pristine BFO. They used a solid-state reaction route to form ceramics: the powders were calcined in two steps of 650 °C for 1 h and 830 °C for 1.5 h with grinding in between. Then powders were mechanically pressed into circular pellets and sintered at 830 °C for 1.5 h. The micro-Raman measurements ($\lambda_{exc} = 632.8$ nm) were carried out to identify the optical-phonon active modes. There are 9 such modes were observed for pure BFO out of 13 (4A1+9E) predicted for the rhombohedral *R3c* symmetry. Instead, 3 A1 modes and 5 E phonon modes were observed for BSFO. The lattice distortion caused due to lower ionic radii of Sm ion (0.96 Å) substituted at higher ionic radii Bi ion (1.03 Å) essentially leads to a blue shift and decremental broadening of the active phonon modes.

Recently we reported on the influence of the sintering pressure on the structural and magnetic properties of the nanocrystalline manganites doped with different alkali ions and chromium [3]. For this study we synthesized a set of nanostructured BSFO nanotubes using the sol-gel membrane-assisted method. Their vibrational signatures were studied with complimentary Raman and FTIR spectroscopies. Morphology was assessed with scanning electron microscopy. A correlation between structural features and characteristic spectral manifestations has been found. These observations provide important experimental data for further theoretical analysis establishing relation between the nanostructural arrangement and vibrational pattern of novel BSFO materials.

Acknowledgement. This study was funded under the Marie Skłodowska-Curie grant agreement No 778070 – TransFerr – H2020-MSCA-RISE-2017 from the European Union Horizon 2020 research and innovation programme.

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Positron trapping reduction as non-destructive probe of photo-luminescence efficiency in rare-earth doped chalcogenide glasses

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The method of PAS (positron annihilation spectroscopy) in lifetime measuring mode is employed to track free-volume deviations in chalcogenide glass-forming networks under the incorporation of photoluminescence-efficient rare-earth (RE) ions. The most efficient positron traps in undoped chalcogenide glasses such as As_2Se_3 represent free-volume voids within the arrangement of corner-sharing polyhedrons (trigonal pyramids), composed of atomic-accessible geometrical holes arrested by surrounding atomic-inaccessible Se-chain-based bond free solid angles (BFSA). Positron trapping is depressed in Ga- or In- co-doped chalcogenide glasses due to agglomeration of intrinsic free-volume voids, thus resulting in a gradual decrease in positron trapping rate and a fraction of trapped positrons.

The effect of successful RE-doping in the glass-forming network is explained in terms of competitive occupancy of negatively-charged vacancy-type sites available for both RE ions (RE^{3+}) and annihilating positrons. Under doping, these ions are stabilized in the network due to $(RE)^{3+}$-Se-Ga(In) linkages, eliminating neighboring voids as potential positron-trapping sites. Therefore, the effect of successful RE-doping in chalcogenide glass results in a notably reduced positron trapping rate in free-volume defects originated from their decreased content and slightly altered atomic-deficient free volume. Numerous examples of this positron-trapping reduction model are analyzed for different types of mixed-cation and mixed-anion glasses and RE activators.

Temperature and magnetic field dependences of transport properties of $Bi_2(Te_{1-x}Se_x)_3$ thin films

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V_2VI_3 - based materials (including $Bi_2(Te_{1\ x}Se_x)_3$ alloys) are among the best materials for thermoelectric cooling devices, and they are increasingly used in thin-film converters. Interest in studying the transport properties of V_2VI_3 thin films has increased after it became known that V_2VI_3 compounds belong to the new class of quantum objects – topological insulators with unique properties of the surface layer. Previously [1], we studied the dependences of the transport properties of p-$Bi_2(Te_{1-x}Se_x)_3$ crystal on temperature and magnetic field and found that the films prepared from this crystal by thermal evaporation in vacuum onto glass substrates, had a sufficiently high degree of structural perfection [2].

The goal of this work was to compare the transport properties of p-$Bi_2(Te_{0.9}Se_{0.1})_3$ in the thin-film and bulk states and establish the effect of substitution Te→Se on the transport properties of Bi_2Te_3 films. The dependences of electrical conductivity σ, the Hall coefficient RH, magnetoresistance $\Delta\rho/\rho$ of $Bi_2(Te_{0.9}Se_{0.1})_3$ thin films with thicknesses d=50-130 nm on magnetic field B= (0.01–1) T and temperature T= (77-300) K were measured. All films exhibited n-type conductivity over the entire range of B and T, which we attributed to a complex defect structure at x=0.1 and a change in thermodynamic equilibrium conditions in the thin-film state compared to a bulk crystal. Using the RH(B) and $\Delta\rho/\rho(B)$ dependences, the boundary between weak and strong magnetic fields was determined. The temperature and magnetic field dependences of the kinetic coefficients for n-$Bi_2(Te_{0.9}Se_{0.1})_3$ and n-Bi_2Te_3 films were compared.

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Effect of thickness on electrical conductivity of Bi_2Se_3 thin films at low temperatures

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Bi_2Se_3 is a narrow-gap thermoelectric (TE) material [1], which also exhibits the topological insulator properties. The possibility of increasing the TE figure of merit in low-dimensional structures based on V_2VI_3 compounds stimulates the investigations of properties of Bi_2Se_3 thin films. In thin films, when the film thickness d is of the order of the mean free path of charge carriers, the classical size effect (CSE) can be observed. For film applications, it is important to take this effect into account.

For Bi_2Se_3 films, an increase in electrical conductivity σ with increasing d was observed at room temperature in [2] and attributed to the manifestation of CSE and satisfactorily described in terms of the Fuchs-Sondheimer theory. The high structural quality of the films studied in [2] was confirmed in [3]. At lower temperatures, the d-dependences of the TE properties of Bi_2Se_3 thin films have not been studied.

The goal of the work is to establish the influence of the film thickness d on electrical conductivity in Bi_2Se_3 thin films at lower temperatures (77-300K).

The methods of the preparation of Bi_2Se_3 films (d = 15-365 nm) and the measurement of electrical conductivity are described in [2].

It was established that Bi_2Se_3 thin films exhibit n-type conductivity like the initial crystal. σ changes slowly with temperature in the range 77-300K for films with different d, which can be explained by the degeneracy of electron gas. It was shown that the behavior of the σ(d) dependence for thin films at low temperatures is similar to that obtained in [2]: σ increases with increasing d. The observed character of the σ(d) the dependence is explained by the manifestation of CSE associated with an increase in the contribution of diffuse scattering of electrons at the thin film interfaces as its thickness decreases.

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Electric-field-driven spin waves in magnetic nanostructures

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The coherent electric-field-controlled excitation of spin waves in magnetic nanostructures involves the control of their parameters playing the role of transmit information in magnetic systems. Such the excitation through the electric current and spin polarized current is related to the large consumption because of heat losses related to the enough large threshold current density for overcome a potential barrier between magnetic states. The low energy alternative is the electric field-induced excitation related to the voltage-controlled magnetic anisotropy (VCMA) effect of the direct transformation of the electric field into an effective internal magnetic field at the interface between the magnetic and nonmagnetic nanolayer of the system [1, 2].

The efficiency of the excitation of the spin waves under the alternating electric field based on the VCMA effect is related to the parametric resonance character of the energy transfer from the alternating internal effective magnetic field to the precessing spins. This means excitation of the spin wave due to resonant energy pumping from its source. The role of the energy pumping sours can play the internal effective magnetic field or the uniform spin-oscillation mode [2]. The frequencies of the electric-field-controlled spin dynamics is determined by the magnetic exchange interaction which is maximum for antiferromagnetic nanostructures [3].

The self-consistent description of the VCMA-controlled spin waves taking into account electronic structure is based on microscopic approach. The latter is realized in tight-binding model and the non-equilibrium Green functions theory.

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On nano-channels of plasticity in mixed auxetics

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The essentially non-linear mechanical properties of real auxetics are increasingly being used in various fields of human activity: medicine, military affairs, space, electronics, spintronics, etc. At the same time, the prediction of their plastic properties belongs to the currently unsolved nonlinear problems [1]. It is especially difficult to study the plastic deformation of materials that have radically different mechanical properties in different crystallographic directions, varying within the same volume from ordinary (Poisson's ratios $\mu>0$) to auxetic ($\mu<0$).

Therefore, we investigated the stress fields around edge dislocations and the concentration C of defects near them in such crystals in auxetic and non-auxetic directions. Crystals with covalent (-quartz and -cristobalite) and metallic (Cu-Mn system) bond types were chosen as objects of study. All the studied objects at a temperature of 300 K are partial auxetics [2].

It was found that regardless of the type of chemical bond, mechanical stresses near dislocations in auxetic directions in these crystals are many times smaller than in non-auxetic ones. The concentration C of point defects in dislocation atmospheres in auxetic directions is lower than in non-auxetic ones and is observed in narrow channels near the dislocation core. For example, in the -quartz C at a distance of $r = 10^{-8}$m in the auxetic <100> direction with the Poisson ratio $\mu_{min} = -0.08$, it is 0.3% less than in the non-auxetic one; in -cristobalite ($\mu_{min} = -0.55$) – by 2.2%, and in Cu-82 at. % Mn crystals – by 400%. At a distance of $r = 10^{-6}$m, this difference becomes significantly smaller (0.006%, 0.03% and 1.9%, respectively). Therefore, dislocations in auxetic directions in crystals can be more mobile and perform plastic displacements many times more efficiently.

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Photoexcited charge carrier transport in solution-processed MoS_2 thin films

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Single-layer or few-layer MoS_2 is widely regarded as one of the most extensively studied two-dimensional transition metal chalcogenides (2D-TMDCs). This is primarily due to its remarkable combination of optical and charge transport properties, along with its favorable mechanical and chemical stability, biocompatibility, and affordability [1-3].

Solution-exfoliated MoS_2 flakes were formed into SiO_2/Si by spin-coating and thermal annealing at 140°C. To characterize the optical properties of solution-processed MoS_2 thin films, the photoluminescence and Raman spectra of the studied structures were obtained using a micro-Raman system (Renishaw-1000). The photoconductivity measurements were performed in a two-probe configuration under a bias of 100 mV and carried out at temperatures from 10 to 300 K. A 250 W halogen lamp dispersed with a monochromator to excite the photocurrent, which was detected with a current pre-amplifier SR570 (Stanford Research System) and measured under modulated (60 Hz) light excitation by a SR860 lock-in amplifier (Stanford Research System). An enhanced photoresponse due to light absorption in MoS_2 was observed at different temperatures at modulated excitations.

This work was supported by the National Research Foundation of Ukraine [2020.02/134].

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Innovation implementation, digital& green transformation in the energy industry for recovering of Ukraine’s economy

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The world energy sector is going through a fundamental transformation. Therefore it is necessary to develop a new innovative energy security paradigm that will ensure reliability and availability while simultaneously reducing hazardous emissions and widely involving using green energy. It is a convincing global trend in the coming decades. Diversification of the energy supply in Ukraine by investing in renewable energy sources (RES) is one of the promising ways to protect oneself from the risks of energy dependence.

The energy crisis, unfolding amid persistent geopolitical and economic challenges, is dramatically affecting energy markets that remain extremely vulnerable, and the scale of the crisis is a reminder of the fragility and instability of today's global energy system.

According to an analysis of national commitments, financing and infrastructure development, the International Energy Agency [1] stated that only two of the 55 components needed for the planet to reach zero emissions by 2050 can be achieved. Such commitments are the deployment of electric vehicles and the transition to LED lighting. Factors such as the closure of coal-fired power plants and the capture of carbon dioxide from the atmosphere are not yet a priority.

Traditional tenets of energy security, including the importance of diverse energy sources, supplies, and routes, remain as relevant as ever, but at the same time, the issue of the influence of energy on climate change, raising the stake of digitization and the use of "green energy" is gaining importance.

In today‘s ever-evolving energy industry, the twin transition—the path towards greater sustainability and higher digitization– also plays a crucial role [2]. The latest realities indicate the potential synergies between digitalization and sustainability as a main factor in a climate-neutral future too. In this context, for example, almost every fifth company participant of the survey from 13 countries [2] already defines the goal of becoming climate neutral in terms of direct emissions by 2030. Growth in green business areas is important to realizing this goal. More than 50 percent of companies expect annual revenue growth of over 10 percent by the end of 2025 in at least one green and sustainable business area they cover. Innovation implementation and digital transformation are basic enablers to support these ambitions. Every second company aims to increase the share of the IT budget in total costs by 2025. In order to leverage the extensive potential of new green and sustainable products, energy suppliers are facing numerous challenges. While more than 60 percent of utilities already have a digital strategy, 80 percent have not yet defined it along all steps of the value chain. In addition, about half of the companies currently lack a clear vision of the digital capabilities they will need in the future.

Despite all the dramatic challenges currently facing Ukraine, it has a promising future, namely, joining the cohort of innovative world leaders in the field of clean energy. This can happen thanks to the use of advanced technologies and the implementation of positive digitalization experience, which will help both to gain energy independence and to achieve sustainable development, which will lead, in turn, to the recovery of the economy.

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The life time of electrochemically active complexes, -with multi-electron charge transfer in the process of obtaining new nanomaterials at HES

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Earlier [1,2] it was substantiated the possibility of obtaining new nanomaterials by high-temperature electrochemical synthesis (HES). The decisive role in this case belongs to the cationic composition of the melt, an alternative to 6-electron charge transfer (simultaneous and sequential), which was determined by the lifetime of electrons $\Delta\tau$ in intermediate states. In this work, the results of the influence of the lifetime of electrons in intermediate states on the processes of multi-electron sequential charge transfer at HES for obtaining new polymorphic nanomaterials are presented.

According to the Bohr formula, the lifetime $\Delta\tau$:

$$\Delta\tau = \hbar / \Delta E \qquad (1)$$

On the other hand, $\Delta\tau = 1/|\Delta\omega| = 1/(2\pi|\Delta\nu|)$ (calculations of $\Delta\omega$ by the Gamess program). $|\Delta\nu|$- the modulus of the difference in the frequency of oscillations in the transition and final states.

Energy assessment of the advantage of simultaneous 6-electron charge transfer, in comparison with stepwise transfer, which takes into account the lifetime of intermediate intermediates, allows to obtain more complete information when obtaining new nanomaterials.

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Structure of Cr-O-N coatings deposited by PIII&D technique using cathodic arc plasma

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Plasma immersion ion implantation combined with deposition (PIII&D) using cathodic arcs as plasma sources is a technique that has demonstrated to be useful for the fabrication of nanostructured coatings to harden and protect the surface. Three-component Cr-O-N coating systems are of interest due to their high thermal stability, corrosion, and wear resistance. The production of such coatings by the PIII&D method requires the optimization of the parameters of the substrate pulsed bias voltage, which allows for flexible control of the structure of the coatings in order to improve their properties.

The aim of this study is to investigate the effect of pulsed bias voltage parameters on the composition and structure of Cr-O-N coatings deposited by the PIII&D method from a chromium cathode plasma in a gas mixture of N_2+O_2 with a relative oxygen content of 20% at a pressure of 1.8 Pa. The amplitude and frequency of the pulse voltage were varied within the range of 300-700 V and 1-20 kHz, respectively, with duty cycle of 20%.

Using electron microscopy, it was found that in the studied range of potential parameter variations, there are no significant differences in the surface morphology and elemental composition of coatings, which can be characterized as $Cr_{44}O_{42}N_{14}$. X-ray structural analysis of the coatings revealed two textured nanocrystalline phases: cubic NaCl-type CrN and rhombohedral Cr_2O_3. With increasing amplitude of the pulse voltage, the crystallite size of the detected phases decreases from 20 to 5 nm. Variation in the pulse frequency does not have a significant effect on the phase composition. X-ray diffraction patterns of the coatings indicate the presence of a certain amount of amorphous phase. Raman spectra showed that the

Cr_2O_3 phase dominated in the coating structure, identified by narrow and well-separated combination of scattering bands.

The work was financially supported by the NAS of Ukraine and The European Federation of Academies of Sciences and Humanities (ALLEA), within the framework the "European Fund for Displaced Scientists", Grant EFDS-FL2-04.

The Center for High Technologies and Digital Innovations (HTDI) as a platform for the renaissance of the technical and innovation potential of Ukraine

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Sooner or later, armed conflicts are ended. On the one hand, The worldwide experience of overcoming the consequences of disasters, different crises, and wars shows that this is impossible without constant support for the development and use of the fruits of the scientific and technical field. And so that the state does not become only a "resource" country for others, it is important not to forget to support its innovative potential. Therefore, in order to restore the country's economy, support for science and innovation has to occupy a prominent place. It is well-known, investment in science, technology, and innovation (STI) plays an important role in economic development and social progress. Research and development (R&D) contributes to the sustainable development of society [1] Also, the well-known and respected world-stage organization UNESCO highlighted to the countries, the importance of investing in Science, Technology, and Innovation. And strengthening the role of science for a more just, prosperous, and sustainable world requires a long-term commitment from all stakeholders, both private and public, expressed in increased investment along with a corresponding review of investment priorities and in the sharing of scientific knowledge. And also that scientific research and its applications can provide significant returns in terms of economic growth and sustainable human development, including in the fight against poverty, and that the future of humankind depends more than ever before on development and equitable distribution of knowledge is used. [2]

On the other hand, the problem of bridging the gap between science and business is acutely open. Science gives businesses a competitive advantage, which means that businesses turn to it exactly to solve practical problems. In such a system, for applied research is much easier to find funding than for basic research, and this happens all over the world.

Institute of Physics of the National Academy of Science of Ukraine (IoP of the NASU) has International and Innovation cooperation, Technology Transfer, and Intellectual Property Department, which has many-years experience in support innovations, protection IOP and increase cooperation between science and business sphere.

This year IOP launched pilot project, namely, expanded functionality and tools of this Department by creation Innovation Center "High technology and digital innovations" (HTDI). The Center HTDI is dedicated to playing a role as a bridge between business and science. It will create a favorable environment for support developers and implementation of innovations. The latest capabilities of the Center will help accelerate new technology and support developer to implement innovation from scientific ideas to full commercialization at the international level. The development of innovative developments will create a favorable investment climate, which in turn will increase the capabilities and competitiveness of the Institute of Physics of the NAS of Ukraine and other scientific and innovative organizations and universities. This will allow to involve the businesses in cooperation and build new communications that will connect Ukrainian innovations with the world, expanding the scientific network of cooperation. Activity and development in this strategic direction is at the forefront of the international mainstream. Since innovation is central to translating scientific knowledge and technological know-how into useful products, services, and employment, for example, the abovementioned UNESCO is fostering closer linkages between educational entities and industry. This international organization has recently created a network of centers of excellence in the Arab region which are being encouraged to set up innovation centers in converging technologies; it is also encouraging countries to develop innovation hubs also in the form of science and technology parks.[2]

Such centers can be created on the example of a Pilot project is implementing at the Institute of Physics of the NAS of Ukraine. There is a suitable based at the International and Innovation cooperation, Technology Transfer, and Intellectual Property Department, where innovations will be learned, implemented, and tested. In fact, it can play the role also of an "incubator of ideas" (like Torino incubator, etc., guiding from the beginning to the stage of becoming rising, helping to overcome difficulties, and supporting during the process. So, such Centers are very necessary for the circumstances in which the Ukrainian R&D sector is now. It is extremely important for further rapid development, competitive, relevant, and cost-effective research, and development that will be in demand worldwide.

The creation similar of HTDI centers of innovation, under the departments of International cooperation and Innovation, Technology transfer, and Intellectual property protection, will contribute to the expansion of their functional capabilities. This will happen through the creation and development of new modern methods of research, incubation and acceleration, and the application of technological and digital innovations, involving scientists and expanding international cooperation, and establishing contacts with business representatives.

Acknowledgement. The authors express their deep gratitude for the support to the Ministry of Education and Science of Ukraine. This scientific and technical project is implemented at the expense of the External Assistance Instrument of the European Union to fulfill Ukraine's obligations in the Framework Program of the European Union for Scientific Research and Innovation "Horizon 2020".

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