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SIMULATING FIELD-INDUCED PERCOLATION IN A THREE-DIMENSIONAL ARRAY OF STRAIGHT NANOTUBES

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An examination of the percolation phenomenon in a system of straight nanotubes has been conducted, and a tailored model for the process has been proposed. A computational algorithm has been devised to determine the likelihood of nanotube percolation, employing three-dimensional graphics visualization tools. The investigation delves into the impact of geometric dimensions and nanotube concentration on percolation probability. Through an exploration of the relationship between percolation probability and dispersion angle values dictating nanotube orientation, fundamental patterns in the formation of conductive clusters under the influence of an electric field are identified. The optimum parameters for a nanotube system exhibiting field-controlled percolation have been ascertained through this analysis.

Key words: nanotubes, percolation, percolation probability, 3D visualization

Introduction. The widespread adoption of percolation theory for modeling and analyzing diverse systems stems from the significant impact of geometric characteristics on the underlying processes within these systems [1,2]. A critical challenge lies in developing innovative algorithms, grounded in the principles of geometry and discrete mathematics, essential for the effective application of percolation theory in intricate systems boasting a large number of elements.

Percolation theory, at its core, examines the connectivity of numerous elements, assuming that connections between adjacent elements occur entirely at random [3,4]. Examples of such systems range from crystalline semiconductors with impurities to composites comprising both conductor and dielectric components or security systems within computer networks.

A noteworthy application of percolation theory lies in unraveling the electrical properties of disordered systems, where various components possess distinct electrical characteristics, such as insulators and conducting elements [5]. Nanocomposites, specifically those featuring metallic nanotubes dispersed in a dielectric matrix, present an intriguing avenue for exploration due to their advantages over conventional electronic materials [6-8]. Theoretical and experimental investigations into these composites, including computer simulations of charge transfer processes within the percolation theory framework, are of paramount practical significance [9-11].

Exploring percolation phenomena at the nanoscale within systems based on carbon nanotubes reveals a profound influence of material anisotropy on the percolation threshold [12,13]. Notably, the controlled manipulation of carbon nanotubes to create a conductive path is of particular practical importance. For instance, in a groundbreaking study, thin film composites comprising carbon nanotubes suspended in liquid crystal exhibited morphological changes under the influence of an electric field. The nanotubes formed a conductive network within the liquid crystal, allowing for rearrangement under voltage and adopting a prevailing orientation aligned with the electric field.

Consequently, investigating the impact of the predominant orientation of nanotubes on percolation network formation through computer modeling assumes significance as it sheds light on the macroscopic electrical parameters of nanocomposites [14,15]. This study focuses on the analysis of percolation phenomena within a three-dimensional nanotube system, emphasizing the exploration of geometric sizes and spatial orientation's influence on the probability of percolation cluster formation.

Approach and methodology. In the devised model, the nanotube system is conceptualized as a volumetric element taking the form of a rectangular parallelepiped, with nanotubes distributed in a random fashion (Fig. 1). To streamline the system's description, nanotubes are treated as hollow cylinders possessing a length denoted as L and a diameter denoted as D. Each individual nanotube is constructed from three fundamental constituent elements: two hemispheres situated at the tube's ends and a cylindrical section connecting these hemispheres. The spatial placement of each nanotube is defined by the coordinates of two boundary points located at opposite ends of the tube. During the generation process of the nanotube system, the volume's element count is computed based on the specified concentration and geometric dimensions. Nanotubes within the system can exist either in isolation or in direct contact with one another.

The simulation of the percolation of the tube system is executed by systematically evaluating the distances between all nanotubes. The determination of contact between two tubes relies on the condition that the distance between them does not exceed the diameter of the nanotubes. Given the random positioning of the nanotubes, the existence or absence of a connection between any two specific tubes is inherently a stochastic event. Nevertheless, as the number of objects in the system increases, the system parameters cease to be random variables and become contingent on both the concentration and geometric dimensions of the nanotubes.

In simulating the electrical properties of the system, solving the percolation problem involves identifying current pathways through the electrically conductive nanotubes connecting the two opposing sides of the rectangular parallelepiped (Fig. 1). The current flow between these electrodes is contingent upon various parameters of the system under examination, including the filling density, the ratio of conducting to non-conducting nanotubes, their orientation, length, and diameter (or aspect ratio).

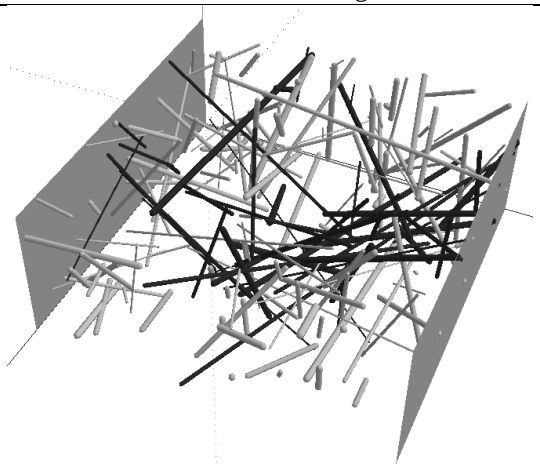


Fig. 1. Nanotube system model: highlighting the conductive pathway across opposite sides of a parallelepiped.

To discern the conductive cluster within a nanotube system between two electrodes and calculate the percolation probability, an algorithm rooted in graph theory is employed. In this algorithm, all tubes within the system are represented as vertices of a simple graph, with edges corresponding to the connections between the tubes. Nanotubes in contact with the opposite sides of the parallelepiped form two subsets representing the electrodes. Subsequently, a component combining these subsets is sought through the application of the union-find algorithm, thereby forming a conductive path in the nanotube system.

For the practical implementation of the algorithm modeling percolation phenomena in the nanotube system, a high-level programming language, C++, and the Qt cross-platform toolkit were utilized. To optimize computational efficiency, a multithreaded implementation of the algorithms was employed. The 3D visualization of the nanotube system model was accomplished through OpenGL, employing a virtual camera that generates a raster image of the object on a flat surface using specialized procedures for graphic rendering. Consequently, for each image pixel, color and intensity, reflected from the object under light, are determined. These visualization tools served the dual purpose of model testing and displaying the conductive path between the two electrodes [16].

Results and discussion. The investigation into percolation phenomena within a nanotube system was conducted utilizing a bespoke program designed to determine percolation probability. The program interface offers the flexibility to manipulate model parameters influencing the percolation threshold value. Through numerous numerical experiments, dependencies of percolation probability on the concentration, geometric dimensions of nanotubes, and their spatial orientation were established. The nanotubes' percolation probability denotes the percentage of successful calculations, where a conductive path is established. The calculations also delved into examining the impact of applied voltage on the probability of forming a conductive network from straight nanotubes.

Fig. 2 illustrates the dependency of percolation probability on the concentration and geometric dimensions of nanotubes, considering their uniform and isotropic distribution in 3D space. Analysis of these dependencies reveals a reduction in the percolation threshold with an

increase in the length of nanotubes, ranging from 0.5 to 2.5 microns. The minimal concentration of nanotubes required for forming a conductive cluster decreases from 9 to 2.5%. Conversely, an increase in the radius of nanotubes from 20 to 110 nm results in a corresponding elevation of the percolation threshold. This observation may be attributed to the decreased number of nanotubes within a given volume and the increase in their diameter, maintaining constant volumetric concentrations.

These findings offer valuable insights into the intricate relationship between nanotube characteristics and percolation behavior, providing a foundation for understanding the system's response to changes in concentration, length, and diameter. Furthermore, the study sheds light on the dynamic interplay of these factors in the presence of an applied voltage, contributing to a comprehensive understanding of nanotube system behavior under varied conditions.

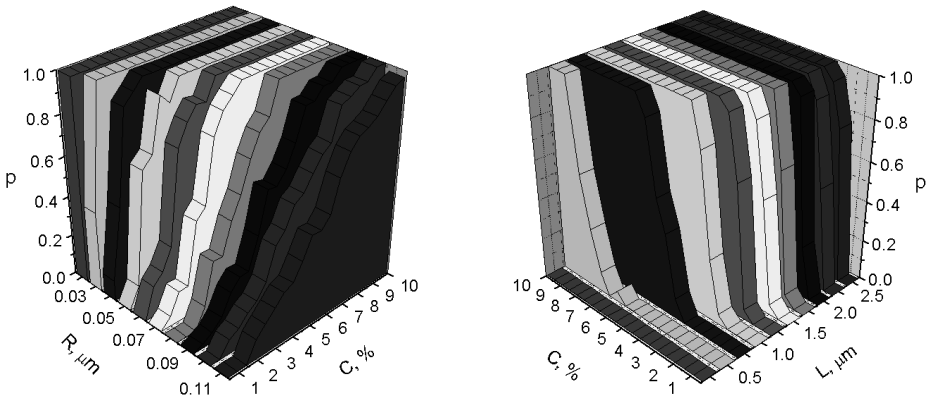
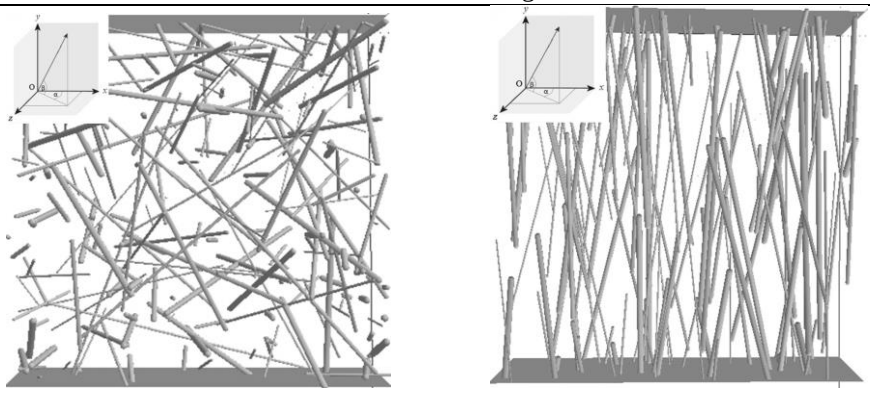


Fig. 2. Variation in percolation probability on the nanotube concentration and length (a), and nanotube concentration and radius (b).

The introduction of anisotropy in the system involved imposing constraints on the angles α and β between the nanotube axis and the normal to the electrodes, as illustrated in Fig. 3. The primary objective was to explore the impact of nanotube orientation on percolation probability within the 3D model of the system. In a fully anisotropic system, all nanotubes align exclusively along the normal, leading to $\alpha = \beta = 0$. On the other hand, an isotropic distribution of nanotubes spans the range of $-90° < \alpha < 90°$ and $-90° < \beta < 90°$. The absence of restrictions on nanotube orientation corresponds to the scenario where the applied voltage is 0. Furthermore, in cases where $\alpha = 0$ or $\beta = 0$, with an arbitrary dispersion of the other angle, a 2D model of the percolation system can be derived.

This deliberate introduction of anisotropy adds a nuanced layer to the investigation, allowing for a comprehensive examination of how nanotube orientation, characterized by α and β angles, influences the percolation behavior within the 3D framework. The defined constraints offer a spectrum of scenarios, ranging from complete alignment to unrestricted orientations, facilitating a nuanced understanding of the system's response under varying degrees of anisotropy. This approach enhances the study's capability to uncover the intricate interplay between nanotube orientation and percolation probability in the broader context of the 3D nanotube system.



a b

Fig. 3. Determining the orientation of nanotubes in 3D space analyzing the isotropic (a) and anisotropic (b) distribution of nanotubes with specific angular dispersion constraints: -90 degrees < α < 90 degrees, -90 degrees < β < 90 degrees (a); -15 degrees < α < 15 degrees, -15 degrees < β < 15 degrees (b).

To investigate field-controlled percolation within a 3D system of straight carbon nanotubes, the relationship between the orientation limitation angle and the applied voltage U was examined, as illustrated in Fig. 4. The initial distribution of nanotubes in the disordered system at $U = 0$ adheres to an angular dispersion limitation of $-90° < \alpha < 90°$ and $-90° < \beta < 90°$. As the voltage applied to the percolation system increases, the orientation limitation angle nonlinearly decreases. At $U = 10$ V, the nanotube orientation is restricted by an angle of approximately 15°. The formulation of the dependence of the orientation limitation angle on the applied voltage is informed by experimental findings related to field-controlled nanocomposite morphology changes [16]. Fig. 3,b provides visual representations of both isotropic and anisotropic nanotube distributions with an angular dispersion of 15°.

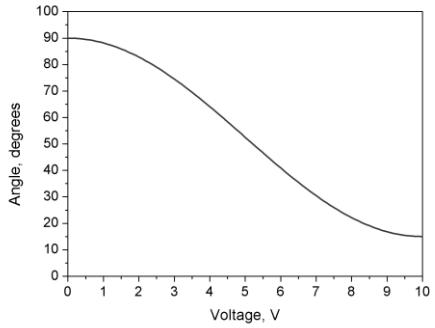


Fig. 4. The relationship between the limitation angle of nanotube orientation and the applied voltage

Simulation results underscore that percolation probability is significantly influenced not only by the concentration and geometric dimensions of nanotubes but also by their predominant orientation, a characteristic that can be manipulated through the application of an electric field. Fig. 5 depicts the dependencies of percolation probability on the applied voltage for different nanotube lengths, with calculations conducted at a fixed concentration of 3% in

the composite. These findings illuminate the intricate interplay between applied voltage, nanotube length, and percolation probability, providing valuable insights into the dynamic behavior of the system under varying conditions.

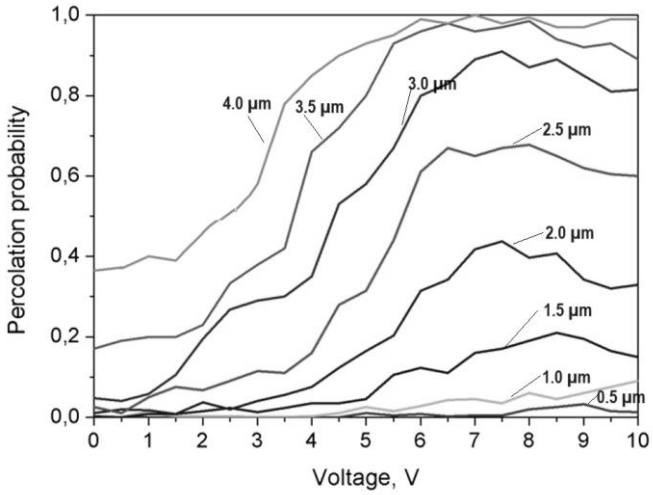


Fig. 5. Variations in percolation probability with applied voltage across distinct nanotube lengths (with a constant nanotube concentration, C, set at 3%).

In scenarios where no electric field is applied ($\alpha = \beta = 90°$), the percolation probability for nanotubes with lengths up to 3 nm approaches zero. However, an increase in the applied voltage results in a reduction of the orientation limitation angles (α and β), consequently leading to an increase in the percolation probability. These findings align well with the results from studies conducted on carbon nanotube systems in 2D models [17]. Specifically, for nanotubes ranging from 3 to 4 nm in length, the percolation probability reaches high values, ranging between 0.8 and 1.0, under a voltage of 5 V. It is noteworthy that even without an applied electric field, at a 3% concentration, nanotubes longer than 3 nm can form a conductive network.

Conversely, for nanotubes in the 0.5–1.5 nm length range, the efficiency of conductive cluster formation is low when oriented randomly (Fig. 5). Therefore, the optimal length for nanotubes in an electrically controlled percolating system appears to be around 3 nm. Fig. 6 illustrates the results of calculations depicting the dependence of percolation probability on voltage for different concentrations of nanotubes, all with a fixed length of 3 nm.

The analysis of these results reveals a weak dependence of percolation in the system of straight nanotubes on the level of distribution anisotropy within the concentration range of 0.5–1.5%. Notably, efficient switching to a conductive regime under applied voltages exceeding 5 V is achievable in nanocomposites with nanotube loadings of approximately 3–4%. These findings provide valuable insights into the conditions favoring the electrically controlled percolation behavior of nanotube systems.

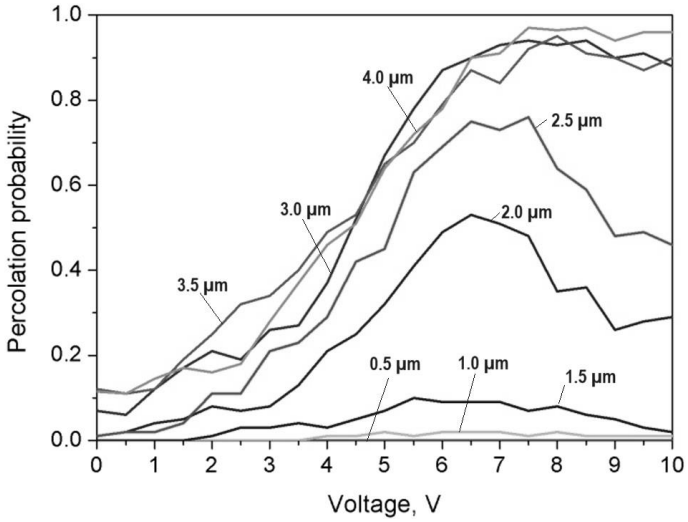


Fig. 6. Percolation probability plotted against applied voltage for various nanotube concentrations, with a fixed nanotube length of 3 nm.

Conclusion. This paper presents a comprehensive analysis of percolation phenomena within a three-dimensional system of straight nanotubes. The investigation delves into the impact of geometric dimensions and spatial orientation of nanotubes on the probability of conductive cluster formation, employing a model environment for detailed exploration. Furthermore, the study explores the potential for controlling nanotube orientation through the application of an electric field.

The conducted simulations reveal dynamic variations in the percolation probability of nanotubes, highlighting the sensitivity of the system to parameters such as angular dispersion limits. Notably, the results provide insights into optimal values for nanotube length and concentration, crucial factors for efficiently controlling the states of the percolating system under the influence of an electric field.

In essence, this research contributes to a deeper understanding of the intricate interplay between nanotube characteristics and external influences, offering valuable knowledge for the design and optimization of systems where electrically controlled percolation is a key consideration.

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МОДЕЛЮВАННЯ ІНДУКОВАНОЇ ПОЛЕМ ПЕРКОЛЯЦІЇ У ТРИВИМІРНОМУ МАСИВІ ПРЯМИХ НАНОТРУБОК

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Дослідження явища перколяції в системі прямих нанотрубок і запропоновано адаптовану модель процесу. Розроблено обчислювальний алгоритм для визначення ймовірності перколяції нанотрубок, використовуючи інструменти візуалізації тривимірної графіки. Моделювання перколяції системи трубок виконувалося шляхом систематичної оцінки відстаней між усіма нанотрубками.

Досліджено вплив геометричних розмірів і концентрації нанотрубок на ймовірність перколяції. Аналіз залежностей ймовірності перколяції від концентрації та геометричних розмірів нанотрубок за умов їх рівномірного та ізотропного розподілу в 3D просторі свідчить про зниження порогу перколяції завдяки збільшенню довжини нанотрубок від 0,5 до 2,5 мкм. Мінімальна концентрація нанотрубок, що забезпечують утворення провідного кластера, зменшується з 9 до 2,5%. Збільшення радіуса нанотрубок від 20 до 110 нм призводить до відповідного підвищення порогу перколяції. Це може бути пов'язано зі зменшенням кількості нанотрубок у об'ємі та збільшенням їх діаметра для постійних об'ємних концентрацій.

Показано, що для нанотрубок довжиною 3–4 нм ймовірність перколяції досягає значень (0,8–1,0) під напругою 5 В. При 3% концентрації нанотрубки довжиною понад 3 нм можуть утворювати провідну мережу навіть без прикладеного електричного поля. З іншого боку, ефективність утворення провідних кластерів у системі нанотрубок довжиною 0,5–1,5 нм є низькою для випадкової орієнтації. Тому встановлено, що оптимальна довжина нанотрубок для електрично керованої перколюючої системи становить близько 3 нм.

На основі аналізу результатів розрахунків залежності ймовірності перколяції від напруги для різної концентрації наповнювачів нанотрубок фіксованої довжини (3 нм) встановлено слабку залежність перколяції в системі прямих нанотрубок від рівня анізотропії розподілу для концентрації нанотрубок в діапазоні 0,5–1,5%. Ефективне перемикання перколюючої системи в кондуктивний режим при прикладеній напрузі вище 5 В забезпечується в нанокомпозитах із завантаженням нанотрубок на 3–4%.

Завдяки дослідженню взаємозв'язку між ймовірністю перколяції та значеннями кута дисперсії, що визначають орієнтацію нанотрубок, виявлено фундаментальні закономірності формування провідних кластерів під впливом електричного поля. За допомогою цього аналізу було встановлено оптимальні параметри для системи нанотрубок, що демонструє перколяцію, керовану полем.

Ключові слова: нанотрубки, перколяція, ймовірність перколяції, 3D візуалізація.

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