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Simulation of the conductive network formation in nanotubes composites

Karbovnyk I.[1], Chalyy D.[2], Lukashevych D.[2], Stelmashchuk A.[1], Klym H.[3]
[1]*Department of Electronics and Computer Technologies, Ivan Franko National University of Lviv, 107, Tarnavskogo str., Lviv, Ukraine*
[2] *Lviv State University of Life Safety, 35 Kleparivska str., Lviv, Ukraine*
[3]*Lviv Polytechnic National University, 12, S. Bandery str., Lviv, Ukraine*

Nanocomposites obtained by filling the insulating host matrix with nanotubes (*e.g.* carbon) exhibit noticeably improved mechanical and electrical properties with respect to the host material [1]. This type of materials has a significant potential for photonics and sensors applications [2]. Another remarkable effect is the influence of conductive nanotubes on the electrical properties of the matrix [3]. Nanotubes have large length-to-diameter ratio, which plays an important role in the formation of long-range conductive path inside the composite (percolation). The percolation threshold depends on variety of factors and a number of approaches were developed in order to simulate the process using numerical calculations. Such modeling is important as it allows to optimize parameters of the system prior to designing the real structure, thus making the tailored nanocomposite design process more efficient.

In this work we describe three-dimensional model of the dielectric composite with random distribution of nanotubes and discuss calculation of the percolation threshold. The results of complex simulations are presented, in which the possibility of nanotube bending is considered and the conductivity between neighboring nanotubes can be due to either direct geometric overlapping or caused by tunneling effect.

In the presented simulations, the tunneling range value is introduced. If the shortest distance between two tubes does not exceed the tunneling range, it is assumed that these two tubes make a tunneling contact. The minimum distance between the axes of two nanotubes where tunnel effect is occurring is evaluated as [4]:

$$D_{tunnel} = \hbar / \sqrt{8 m_e \Delta E} \qquad (1)$$

where m_e is the electron mass, ΔE is the height of the barrier between the nanotube and the polymer filler and $\hbar$ is the Planck constant.

Typical 3D view of the randomly generated network of bent nanotubes is shown in Fig. 1. For the study of electrical conductivity, the opposite edges of the simulated 3D box serve as electrodes between which the current is flowing.

Mathematically the system is represented as a graph and the percolation search is the search of the connected component of the graph, which contains elements that touch opposite edges of the box ('electrodes'). 'Electrodes' are simulated as pseudo-tubes (having zero dimensions).

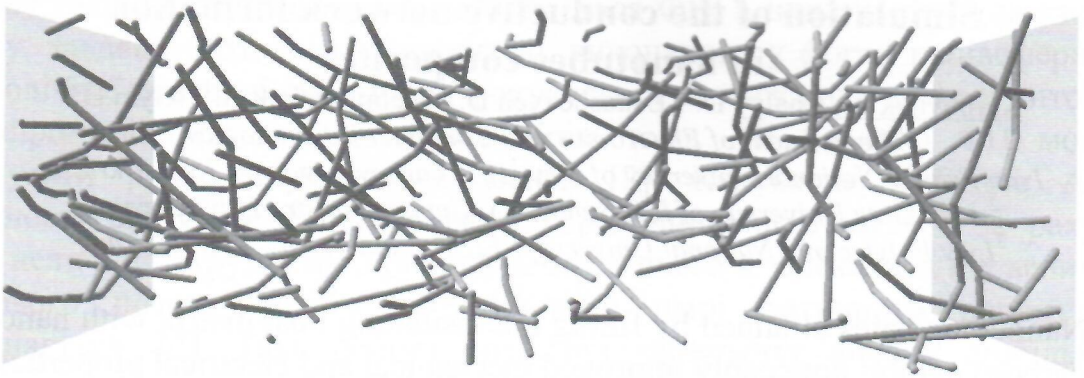

Fig. 1. Computer-generated 3D view of the simulated system of bent nanotubes in insulating medium.

In order to find the conducting cluster we have implemented weighted quick union algorithm with path compression. Around 20 simulations have been performed for each system with the same parameters. Percolation threshold value was retrieved as an average value from obtained results.

Thus, a viable three-dimensional model describing the percolation phenomenon in the nanocomposite "conductive nanotubes/insulating medium" system was developed. The process of nanotube network formation was described mathematically. Numerical calculations were performed taking into account tunneling mechanism of electrical conductivity and the obtained values of the percolation threshold are in a satisfactory agreement with experiments reported up to date. Increasing the size of the simulated system (*i. e.* the number of nanotubes in the box) and/or number of computer experiments lead to more accurate results, which correlates better with experimental data. It was also demonstrated that direct contact 'soft-core' model that does not allow for tunneling can not produce reliable results. It was shown that increasing the alignment angle generally lowers the percolation threshold. The influence of the alignment is more pronounced for 30 to 50 degrees angle range.

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