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MODELING OF PERCOLATION PHENOMENA IN 3D NANOTUBE SYSTEM

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In this paper, the analysis of percolation phenomena in the system of straight nanotubes is carried out and appropriate model is proposed. The algorithm for finding the probability of nanotubes percolation is implemented using a three-dimensional graphics visualization tools. The influence of geometric sizes of nanotubes and their spatial orientation on the probability of a percolation cluster formation is studied. Based on the analysis of the dependence of percolation probability on the limiting values of the dispersion of the polar and azimuthal angles determining the nanotubes orientation in the 3D space, the basic regularities of the conductive cluster formation in isotropic and anisotropic nanotubes systems are established. The optimum values of the investigated system parameters for discovering percolation are found.

Keywords: percolation system, nanotubes, percolation probability, 3D visualization.

Widespread use of the percolation theory in the modeling and analysis of various phenomena is due to the influence of geometric characteristics on the physical properties of materials or physical processes course. The development of new algorithms that combine ideas on geometry and discrete mathematics is an important task for the practical application of the percolation theory in various fields.

The theory of percolation considers the connectivity of a large number of elements, provided that the connection between adjacent elements is completely random in nature [1-3]. Such systems are the crystalline semiconductor with impurities, composites consisting of two materials: conductor and dielectric, models of the spread of fires and epidemics, and security systems of computer networks.

The most widespread application of percolation theory is the study of electrical properties of disordered systems, which are a mixture of substances with different electrical properties, in particular, dielectric and conductor [4, 5]. Such systems include nanocomposites based on conducting nanotubes in a dielectric matrix [6, 7]. Composites have a number of advantages over traditional electronic materials and today are intensively investigated experimentally and theoretically [8-10]. In particular, computer simulation of charge transfer processes into such functional materials within the percolation theory is of great practical importance.

The study of percolation phenomena in the nanosystems based on carbon nanotubes shows a significant influence of the anisotropy level of the material on the threshold value of

percolation [11]. Therefore, the study of the influence of the nanotubes predominant orientation on the percolation network formation by computer modeling is an important task of studying the electrophysical parameters of a nanocomposite. In this work, an analysis of percolation phenomena in a three-dimensional system of nanotubes is carried out. Particular attention was paid to exploring the influence of geometric sizes of nanotubes and their spatial orientation on the probability of percolation cluster formation.

In the proposed model, the nanotube system was represented as a volume element in the form of a parallelepiped, in which nanotubes are located chaotically (Fig. 1). Nanotubes are considered as hollow cylinders with length L and diameter D to simplify the description of the system. In the graphic representation, the nanotube is constructed of three primitive constituent elements two hemispheres at the ends of the tube, connected by a cylinder. The position of each nanotube in space is given by the coordinates of two boundary points on the opposite ends of the tube. During the process of generation of the nanotubes system, their number in this volume is calculated according to the given concentration and geometric sizes. Nanotubes can be isolated or in contact with each other. The simulation of percolation of the tube system is provided by alternating checking of distances between all nanotubes. The contact of two tubes is determined by the condition that the distance between them does not exceed the diameter of the nanotubes. Since the position of the nanotubes is random, the presence or absence of a connection between two specific tubes is also an accidental event. However, for a large number of objects, the system parameters are no longer random variables but depend on the concentration and geometric dimensions of the nanotubes.

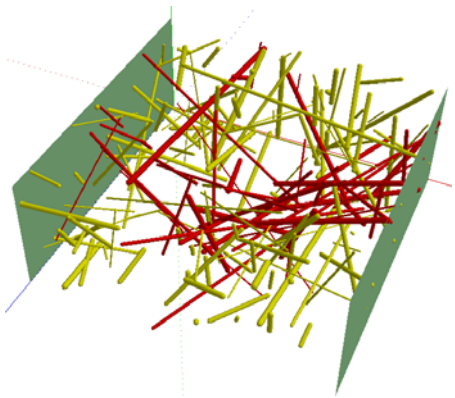


Fig. 1. Model of nanotubes system with a highlighted conductive path between two opposite sides of parallelepiped.

In the simulation of the electrical properties of the system, the solution of the percolation problem is aimed at finding the paths of current passing through the connected electrically conductive nanotubes between the two opposing sides of the parallelepiped (see Fig. 1). The passage of current between these electrodes depends on such parameters of the investigated system as the density of parallelepiped filling with nanotubes, the ratio of conducting and non-conducting nanotubes, their orientation, length and diameter.

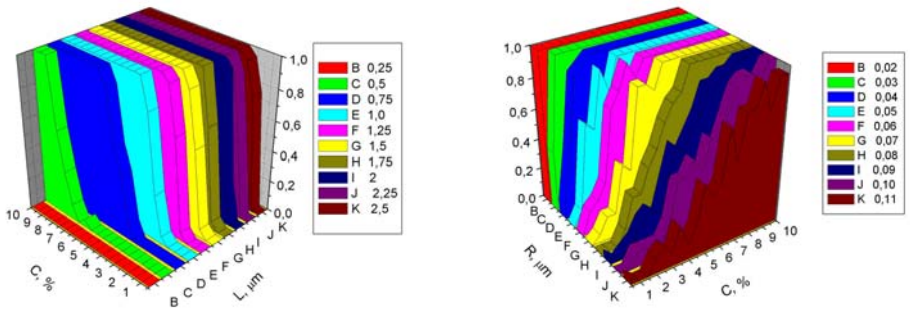
To find the conductive cluster in nanotube system between two electrodes and to calculate the probability of percolation, an algorithm based on graph theory is used. According to the algorithm, all tubes of the system are represented as vertices of a simple graph whose edges

correspond to the connections between the tubes. Nanotubes that come in contact with the opposite sides of the parallelepiped form two subsets corresponding to the electrode. At the next stage, a component that combines these subsets is sought by means of the union-find algorithm. Thus, a conductive path in the nanotubes system is formed.

For the implementation of the algorithm for modeling percolation phenomena in the nanotubes system, a high-level programming language C++ and a Qt cross-platform toolkit were used [12]. In order to reduce computing time, multithreaded implementation of algorithms is used. The 3D visualization of the model of a nanotubes system was performed by means of OpenGL using a virtual camera that generates a raster image of an object on a flat surface using special procedures for drawing graphics [13]. As a result, for each image pixel, the color and intensity reflected from the object of light are determined for each image pixel. These visualization tools were used for model testing and displaying of the conductive path between two electrodes.

The analysis of percolation phenomena in the nanotubes system was carried out with the help of the developed program for finding the percolation probability. The program interface allows changing the model parameters that affect the percolation threshold value. As a result of multiple numerical experiments, dependencies of the probability of percolation cluster formation on the concentration and geometric sizes of nanotubes and their spatial orientation were found. The nanotubes percolation probability is the percentage of positive results of the calculation that is when a conductive path is established.

The dependence of the percolation probability on the concentration and geometric dimensions of nanotubes in the conditions of their uniform and isotropic distribution in 3D space is shown in Fig. 2. Analysis of the obtained dependences indicates a reduction of the percolation threshold due to an increase in the length of nanotubes from 0.5 to 2.5 microns. The minimal concentration of nanotubes for forming of the conductive cluster decreases from 9 to 2.5%. An increase in the radius of nanotubes from 20 to 110 nm leads to an increase in the percolation threshold. It may be related to decreasing in the number of nanotubes in a given volume at increasing in their diameter for constant volumetric concentrations.



a) *b*)

Fig. 2. Dependence of the percolation probability on the concentration and length of nanotubes (*a*), on the concentration and radius of nanotubes (*b*).

Anisotropy was introduced by limiting the angles α and β between the nanotube axis and the normal to the electrodes as shown in Fig. 3 to study the influence of nanotubes orientation on the percolation probability in the 3D model of the system. For a completely anisotropic system, all nanotubes are oriented along the normal and $\alpha = \beta = 0$. The isotropic distribution of nanotubes corresponds to a limit of $-90^o < \alpha < 90^o$, $-90^o < \beta < 90^o$. In the case where $\alpha = 0$ or $\beta = 0$ and an arbitrary dispersion of another angle, a 2D model of the percolation system can be obtained. Fig. 3 illustrates the isotropic and anisotropic distribution of nanotubes with different angular dispersion.

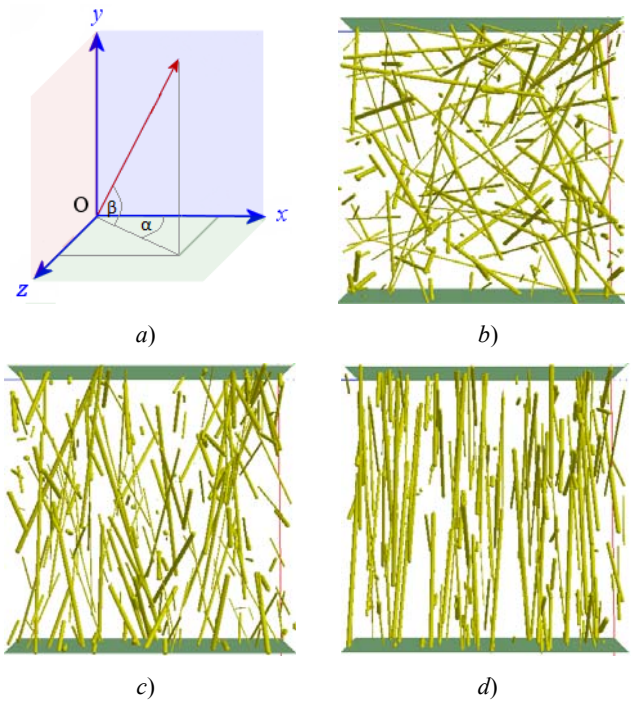


Fig. 3. Determination of the nanotube orientation in 3D space (*a*) and the isotropic (*b*) and anisotropic (*c*), (*d*) nanotubes distribution with angular dispersion limitation:
$-90^o < \alpha < 90^o$, $-90^o < \beta < 90^o$ (*b*); $-30^o < \alpha < 30^o$, $-30^o < \beta < 30^o$ (*c*); $-5^o < \alpha < 5^o$, $-5^o < \beta < 5^o$ (*d*).

The simulation results of the system show that the percolation probability significantly depends not only on the concentration and geometric sizes of nanotubes but also on their orientation. Thus, with a fixed angle $\alpha = 90°$, the greatest probability of formation of a percolation cluster is observed for a 2D system corresponding to the angle $\beta = 0$ (Fig. 4). Such result may be related to the placing of all nanotubes in the plane (i.e. in a thin layer of the composite). An increase in the angle β corresponds to decrease in the anisotropy of the system and reduces the formation probability of percolation cluster. In addition, with a high mass concentration of nanotubes a maximum percolation probability for nanotubes in the 2–3 microns length is observed, which may be related to an increase in their number at a fixed mass.

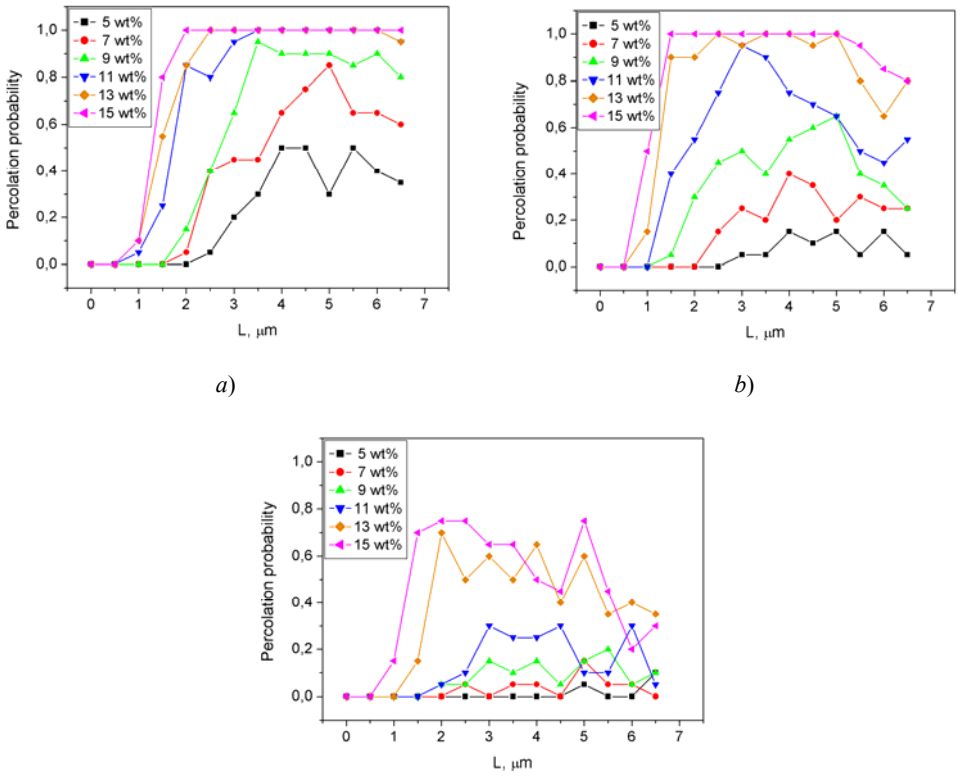


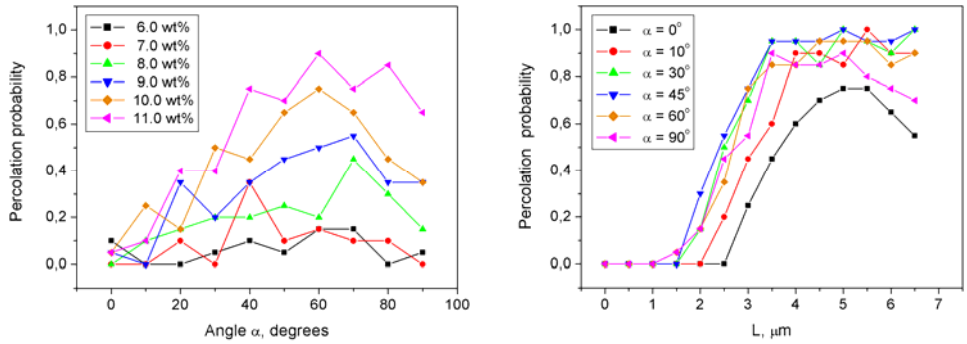
Fig. 4. Dependence of the percolation probability on the nanotubes length for different limitation of the angular dispersion: β=0 (*a*), β=45 (*b*), β=90 (*c*).

Dependence of the probability of indivisible structure formation on the limitation angle of the nanotubes orientation was investigated for a fixed length of nanotubes L = 2.5 microns, which corresponded to a low percolation threshold. Fig. 5*a* shows that the percolation probability increases with the decrease in the anisotropy degree and acquires maximum values at angles of limitation greater than 45° for systems with high nanotubes content. The similar values of the angle of the orientation limitation in the 30–60° range were observed for the maximum probability of nanotubes percolation in the length of 3–6 microns (Fig. 5*b*).

Reducing the anisotropy level increases the probability of contact between randomly oriented nanotubes and as a consequence reduces the effective percolation threshold. The obtained results are in good agreement with the data of studies of the carbon nanotubes system 2D model [14].

Thus, the algorithm for finding the percolation probability in the system of straight nanotubes was implemented. The interface of the developed program provides the possibility of the various parameters changing of the percolation system, in particular, the concentration of nanotubes, their diameter, length and orientation in the given size space. The influence of nanotubes geometric sizes on the percolation threshold was studied on the basis of computer

simulation of the system. It was established that increase in the length of nanotubes from 0.5 to 2.5 microns leads to the decrease in concentration threshold of percolation from 9.0 to 2.5% and increase in their radius causes the increase in the percolation threshold.



a) *b*)

Fig. 5. Dependence of the percolation probability on the angle of the orientation limitation (*a*) and on the nanotubes length (*b*).

The influence of nanotubes spatial orientation on the probability of conductive cluster formation in the model environment by changing polar and azimuthal angles in the spherical coordinate system was investigated. It is shown that 2D percolation systems provide lower values of the percolation threshold compared to the volumetric environment. In addition, the optimal for the percolation cluster formation values of the nanotubes length and boundary angles of the orientation limitation were determined which were 2.5–6 microns and 30–60 degrees, respectively.

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МОДЕЛЮВАННЯ ПЕРКОЛЯЦІЙНИХ ЯВИЩ У 3D СИСТЕМІ НАНОТРУБОК

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Запропоновано модель та виконано аналіз перколяційних явищ у системі прямих нанотрубук. Система розглядається як елемент об'єму у формі паралелепіпеда, хаотично заповненого циліндричними електропровідними трубками. Вільний простір між нанотрубками вважається електрично непровідним. За певних умов між протилежними гранями такого паралелпіпеда існуатимуть провідні шляхи. Для дослідження властивостей системи реалізовано алгоритми генерування випадково розташованих у модельному об'ємі нанотрубок

та знаходження ймовірності перколяції нанотрубок з використанням засобів тривимірної графічної візуалізації. Для пошуку ймовірності перколяції застосовано елементи теорії графів, а імплементація алгоритмів проведена з використанням мови високого рівня C++ and та кросплатформного інструменту розробки Qt. Вивчено вплив геометричних розмірів нанотрубок, зокрема, середнього відношення довжини трубок до їхнього діаметра, і їхньої просторової орієнтації на ймовірність утворення перколяційного кластера. На основі аналізу залежності ймовірності перколяції від граничних значень дисперсії полярного та азимутального кутів, які визначають орієнтацію нанотрубок у тривимірному просторі, визначено основні закономірності утворення провідного кластера в ізотропній та анізотропній системах нанотрубок. Знайдено оптимальні значення параметрів досліджуваної системи для визначення перколяції. Отримані результати щодо значення орієнтаційних кутів є важливими з точки зору подальших досліджень впливу зовнішіх полів на провідність системи «нанотрубки-діелектричний наповнювач», а також вивчення можливостей маніпуляції електричними властивостями цієї системи за допомогою зовнішніх збурень.

Ключові слова: перколяційна система, нанотрубки, ймовірність перколяції, тривимірна візуалізація.