The Modeling of the Polymer’s Thin Film, Modified by Carbon Nanotubes, this Using of the percolation theory’s methods

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Abstract. The polymer nanocomposites, containing the carbon nanotubes and owing to the unusual properties, are interest. For the research of the structure and properties of the polymer nanocomposite, containing carbon nanotubes, the percolation lattice model is proposed. From the model the polymeric matrix is presented by the square lattice with the linear size L, nanotubes – k-meres. For the modeling the periodic boundary conditions are used. For the uniform distribution of k-meres on the lattice and for their distribution on the clusters and the search of the percolation cluster the efficient algorithms are developed. The percolation problems of k-meres of the identical length on the square lattice, k-meres of the varied length on the square lattice; non-linear k-meres on the square lattice are investigated.

Keywords: polymer, carbon nanotubes, computer and mathematical modeling, percolation theory.

1. Introduction
Now the creation technologies of the nanomaterials develop. The polymer nanocomposites, containing the carbon nanotubes and owing to the unusual properties, are interest. It is known, that the addition of carbon nanotubes in the polymer is possible to the regulating its properties. For example, can to increase the nanocomposite durability or to make the polymer by the conductor etc. The creation of the new nanomaterals represents hi-tech, laborious and financially expensive process. Therefore, there is the need for the laboratory and computer experiments. The percolation theory often use by the computer modeling of the structure and properties change of the polymer nanocomposites [for example, 1].

The research problem is the computer modeling of the structure of the polymer’s thin film, modified by carbon nanotubes. By the authors the following tasks are solved:

1) the analysis of the researches (laboratory experiments, mathematical and computer modeling) of the structures and properties of the polymer nanocomposites, containing carbon nanotubes, is carried out;

2) the percolation model of the polymer’s thin film structure, modified by carbon nanotubes is offered;

3) the computer program and efficient algorithms are developed for the computer modeling of the structuring process of the polymer’s thin film, containing carbon nanotubes;

the theoretical analysis of the computer modeling results is carried out.

The results of the computer modeling can be used for the prediction of the concentration’s value of the carbon nanotubes in the polymer for the change of any property of the nanomaterial.
2. The problem and modeling’ methods
For the research of the structure and properties of the polymer nanocomposite, containing carbon nanotubes, the percolation lattice model is proposed. From the model the polymeric matrix is presented by the square lattice with the linear size $L$, nanotubes – $k$-meres ($k$ of in the row busy lattice sites). The $k$-mers cannot be crossed. The horizontal and vertical orientations of $k$-mer’s are appeared with the equal probability. The $k$-meres are evenly distributed on the lattice. The model is described mathematically

$$M = \{L, Z_n, k, p, K\},$$

there $L$ – the linear size of the square lattice, $Z_n = \{x_i, y_i\}$, $i = 1, n$ – the set of coordinates pairs of the $k$-mer’s began, $k$ – the $k$-mer’s length, $p$ – the $k$-mer’s concentration, $K$ – the test’s number at each level of the concentration.

For the modeling the periodic boundary conditions are used. For the uniform distribution of $k$-meres on the lattice and for their distribution on the clusters and the search of the percolation cluster the efficient algorithms are developed, which are described in [2]. The main question of the percolation problem is the percolation threshold value. The percolation threshold corresponds to the critical concentration of the carbon nanotubes in the polymer, in which the nanocomposite is changed their properties.

The following percolation problems are investigated:

a) the percolation of $k$-meres of the identical length on the square lattice;

b) the percolation of $k$-meres of the varied length on the square lattice;

c) the percolation of non-linear $k$-meres on the square lattice.

3. The results
The results of the modeling for the wide range of $k$-mer’s length are received. $k$-meres of the variable length and the various form are investigated.

3.1. The percolation of $k$-meres of the identical length on the square lattice
The values of the percolation threshold $p_c$ for the various values of $k$-meres length are present on the Figure 1. For $k = 1$-10 the results of the modeling coincide with results of other researchers [3-6].

![Figure 1](image-url)  
**Figure 1.** The values of the percolation threshold $p_c$ for the various values of $k$-meres length.

In the figure 1 it is visible that at the increase in the $k$-mer’s length the percolation threshold decreases, and having reached the minimum value at the $k = 13$, further increase in $k$-mer’s length the
percolation threshold begins to increase. It means that the more long $k$-meres are more ability to agglomeration.

3.2. The percolation of $k$-meres of the varied length on the square lattice
It is known that the nanotubes have various lengths. In this regard, the various values of $k$-mer’s length on the square lattice are investigated. The small nanotube has aspect ratio 100 (the nanotube length relation to radius). $k$-mer’s lengths are distributed according to the normal distribution law with the expectation equal 100, and various values of the dispersion. That is, it is supposed that all nanotubes in the system have approximately identical length with the some deviation. In the figure 2 the change of percolation threshold value at the various values of the distribution’s dispersion of the length is shown. Than more the dispersion, that a threshold of a percolation is less. That is, the more distribution dispersion of the nanotubes lengths in the polymer, the less them it is necessary to the change properties of the nanomaterial.

![Figure 2](image)

**Figure 2.** The values of the percolation threshold $p_c$ for the various values of the distribution’s dispersion of the $k$-mer’s length: $\nabla: \sigma=3$, $\triangle: \sigma=2$, $\bullet: \sigma=1$, $\square: \sigma=0$

3.3. The percolation of non-linear $k$-meres on the square lattice
It is known that the nanotube can have bends. In this regard, the percolation problem of the non-linear $k$-meres is investigated. From the model $k$-meres can have one bend in the one of the ends or in the middle of the $k$-mer. It is supposed that in the percolation system there are the linear and non-linear $k$-mees. The values of the percolation threshold at the various values of the non-linear $k$-mer’s number are obtained. The results for $k = 7$ and the various values of the non-linear $k$-mer’s number are presented in the figure 3. It is revealed that at the increase of the number of the non-linear $k$-meres the percolation threshold decreases.
4. Summary
By the authors the percolation model of the structure of the thin film of polymer, modified by carbon nanotubes was offered and investigated. From the model the authors developed the efficient algorithm of the distribution of the \( k \)-mers on the square lattice, of the splittings \( k \)-mers into the clusters and of the searching of the percolation cluster among them.

The computer program for the computing modeling experiment on the carbon nanotubes’ dispersion in the thin film of the polymer and to calculation of the percolation threshold values was developed.

The main result of the modeling is the values of percolation threshold at various parameters of the model were experimentally received. The three percolation problems are investigated: the percolation of \( k \)-mers of the identical length on the square lattice; the percolation of \( k \)-mers of the varied length on the square lattice; the percolation of non-linear \( k \)-mers on the square lattice.

The further research of the polymer structure, modified by the carbon nanotube, by the combination of all three modifications is supposed. Also it is supposed for the model to consider the interaction between nanotubes (interparticle interaction) and the interaction between the polymer and the nanotube (interfacial interaction). Besides the consideration of the three-dimensional percolation systems is planned.

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References
[1] Mikitaev A K, Kozlov G V 2015 Materials Physics and Mechanics 22 101-106
[2] Bokov K A, Buzmakova M M 2018 Vestnik Perskogo universiteta. Matematika. Mekhanika. Informatika 1 (40) 51-55
[3] Ziff R M 1986 Test of scaling exponents for percolation-cluster perimeters Phys. Rev. Lett. 56 545-548
[4] Cherkasova V A, Tarasevich Y Y, Lebovka N I, Vygornitskii N V 2010 Percolation of aligned
dimers on a square lattice *Eur. Phys. J. B.* 74 (2) 205-209

[5] Vandewalle N, Galam S, Kramer M 2000 A new universality for random sequential deposition of needles *Eur. Phys. J., B* 14 407–410

[6] Tarasevich Y Y, Lebovka N I, Laptev V V 2012 Percolation of linear k-mers on a square lattice: From isotropic through partially ordered to completely aligned states *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics* 86 061116