The Percolation Model of the Structure of the Polymer Nanocomposite, Containing the Carbon Nanotubes, with the Orient Factor Availability

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Abstract. The percolation lattice model of the structure of the polymer thin film, containing the carbon nanotubes, with the orient factor availability is proposed in this paper. From the model: the polymer matrix is the square lattice with linear size L; the carbon nanotubes are k-meres (k consecutive occupied nodes of the lattice); the interphase regions are nodes of the bond between k-meres. Also where is the orient factor for the carbon nanotubes in the form of the electric current, flowing in one direct during the structure formation of the nanocomposite. For the modeling the periodic boundary conditions are used. For the model the percolation threshold values are obtained for two cases: for the uniform distribution of the k-meres on the square lattice and for the unidirectional k-meres on the square lattice. According to the made natural experiments [1], the linear orientation in the field of electric current force is possible at the small concentration of nanotubes. In the model it is supposed, during the consolidation all nanotubes manage to be developed and get the identical direction.

1. Introduction

It is known, that polymer nanocomposites properties can be operated by the addition of the various concentration of nanomodifiers and the presence of some, for example, the ordering factors. In the work [1] the electrical conductivity of the epoxy, modified by the carbon nanotubes, is researched for two cases of the curing epoxy whit electrical current through the nanocomposite and without current. The significant increase of the electrical conductivity value of the baked nanocomposite with electrical current through it is revealed. By the authors it is assumed that at current influence during the nanocomposite consolidation the carbon nanotubes get the direction, parallel to the current, and thereof, the value of the electrical conductivity of baked nanocomposite much more, than the baked nanocomposite with the disordered distribution of nanotubes. The purpose of the work is the modeling of the polymer nanocomposite structure, containing carbon nanotubes and taking into account the orient factor and the existence of the interphase regions.

2. The problem and modelling methods

For the research of the structure and properties of the polymer nanocomposite, containing the carbon nanotubes, the percolation model of the k-meres on the square lattice is offered, which mathematically looks as follows

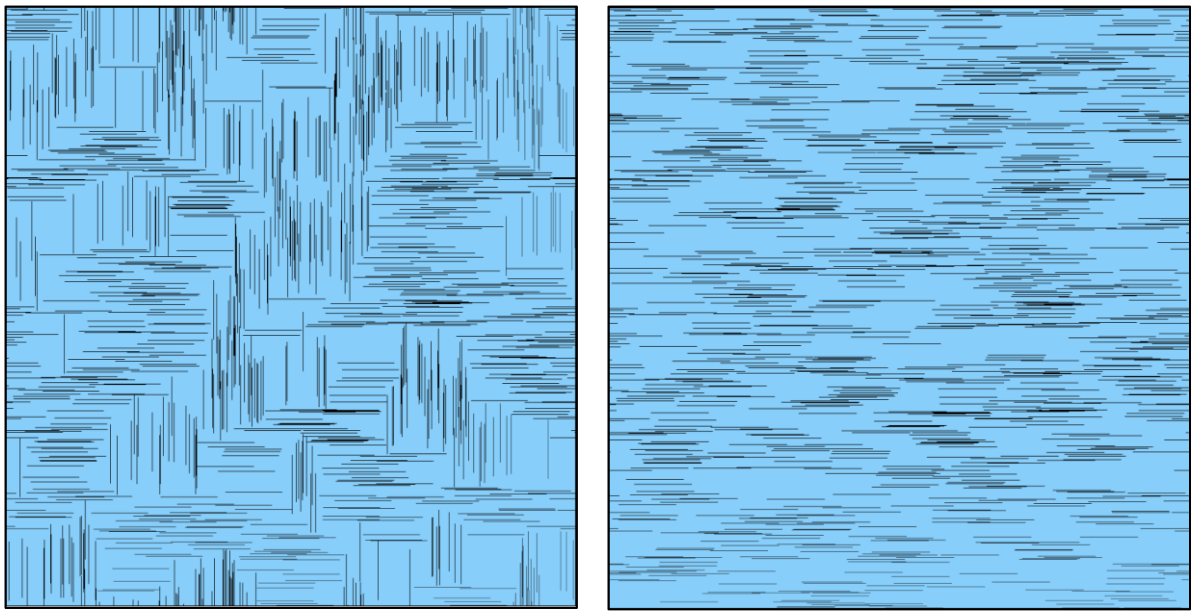
$$M = \langle L, Z_n, k, bl, p, K \rangle$$

where L – the linear size of square lattice, $Z_n = \{x_i, y_i\}$ ($i = 1, 2,\ldots, n$) – the set of coordinates pairs of the k-mer's began, k – the length of the k-mer's, bl – the length of the bond between k-meres, p – the concentration of the k-meres on the lattice, K – the number of tests.

The algorithm of the uniform distribution of the k-meres on the lattice and the further ordering in the one direction is developed for model. The algorithm of packing works as follows:

1. The k-mer direction is generated (the horizontal or the vertical).
2. The coordinates of k-mer began are generated (the pair of integer i and j, where $1 \le i \le L$ and $1 \le j \le L$).
3. The attempt to pack generated k-mer is made: if when checking nodes, they are appeared the free, then they are marked as occupied, and the k-mer it is considered packed; otherwise the k-mer is rejected, and new coordinates for a k-mer placement are generated. The packing of k-meres happens until necessary concentration of p is reached (figure 1 (a)).

After the packing the ordering algorithm comes into force: the all vertical k-meres on the lattice are developed concerning the middle by k/2. The example of finish structure is shown on the figure 1(b).



(a) **(b)**

Figure 1. Example of the uniform packing of the k-meres on the square lattice (a) and the further ordering of the k-meres in the one direction (b), $k = 100$, $L = 1000$

The k-meres can form in the clusters. The percolation cluster is the cluster, which connect the top and the bottom or the left or the right sides of the lattice. The percolation threshold corresponds to the concentration of k-meres in the system, at which the probability of the percolation cluster emergence is equal to 50 %.

In the model the interphase regions (the regions of the nanocomposite, which don't belong to either polymer, or the nanomodifier and are on the border of interaction of the polymer with the nanoparticles) are bond nodes between k-meres. The bond between k-meres characterizes their accessory to one cluster (from the model the length of bonds is the number of the nodes, belonging to the so-called interphase region). That is, if any k-mer gets to the region of bonds length of other k-mer, then the k-meres are belong to one cluster (figure 2).

The modeling is carried out with use of Monte-Carlo methods. For the computer calculation of the model the program in the C# programming language is written. The technique of the percolation threshold definition is described in the work [2].

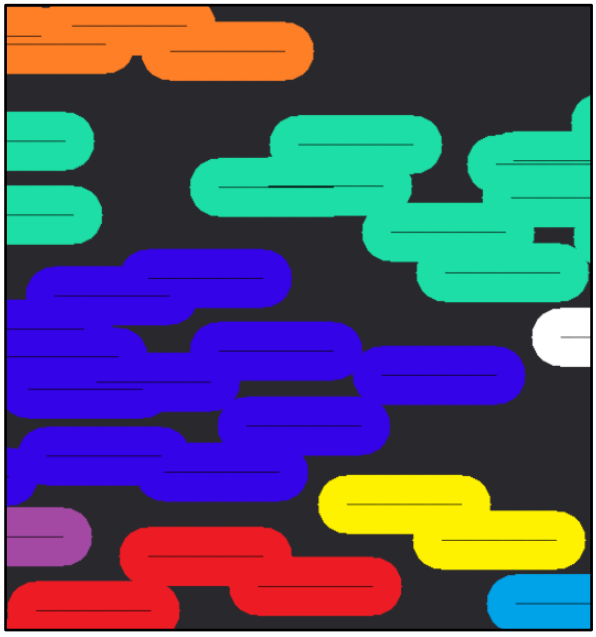


Figure 2. The part of structure, *k* = 100, *bl* = 25

3. The results

The result of computer program is text file with data: the probability of the percolation cluster emergence for the *k*-meres' concentration, *k* = 100 (100 is the aspect ratio of simple carbon nanotube), *bl* = 0, 1, 2, 5, 10, 15, 20, 25, 40, 50, 75, 100. For each set of the data-ins of the model the percolation threshold values are obtained (table 1, figure 3, 4), which are approximated by the function

$$p_c(bl) = A + B1 \times \exp(-bl/C1) + B2 \times \exp(-bl/C2) \quad (1)$$

where $A = 0{,}472 \pm 0{,}117; B1 = 44{,}677 \pm 1{,}213; C1 = 1{,}447 \pm 0{,}045; B2 = 13{,}948 \pm 1{,}18;\ C2 = 8{,}281 \pm 0{,}692.$

Table 1. The percolation threshold values for different values *bl* with an error ± 0,001, %

bl	*Pc*	*bl*	*Pc*
0	59,129	20	1,870
1	35,118	25	1,419
2	22,698	40	0,761
5	9,673	50	0,565
10	4,387	75	0,319
15	2,667	100	0,206

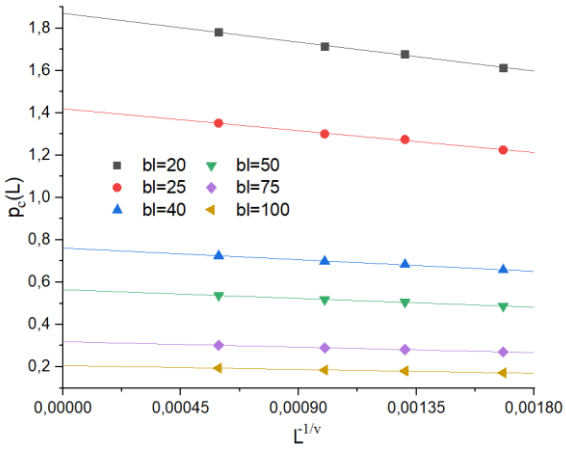


Figure 3. The definition of the percolation threshold values for values *bl* = 20…100

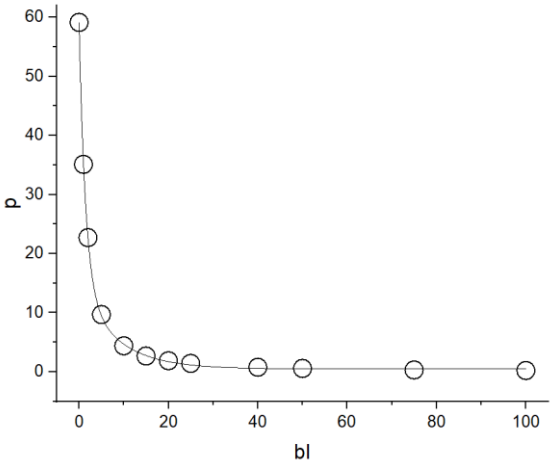


Figure 4. The percolation threshold values for different values *bl* and approximation by the function (1)

It was also revealed, that the structures with ordered *k*-meres along one direction have distinctiveness – the possibility of the several percolation clusters emergence in the system – the figures 5, 6 (on them the percolation clusters are white color, and all others are blue). The several percolation clusters emergence depends on the linear size of the lattice, the length *k*-mer and also bond length between *k*-meres. Examples of the ratio of the formed percolation clusters average quantity from the linear length of the lattice, and also of the most received number (average) of the percolation clusters from the bond length can be seen in figures 7, 8.

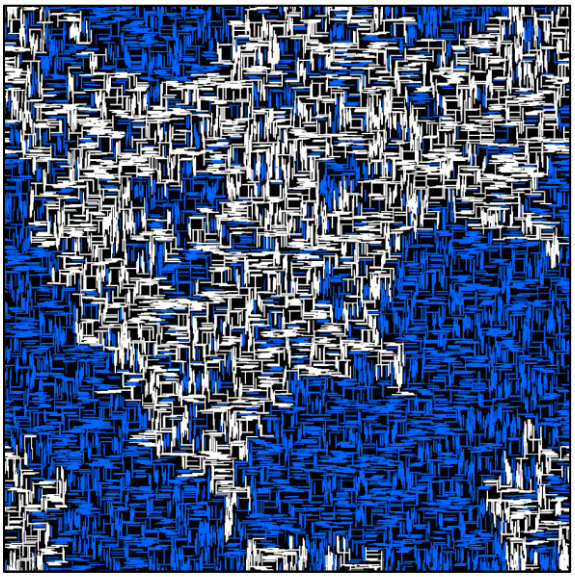


Figure 5. *L* = 5000, *k* = 100, *bl* = 5. One percolation cluster

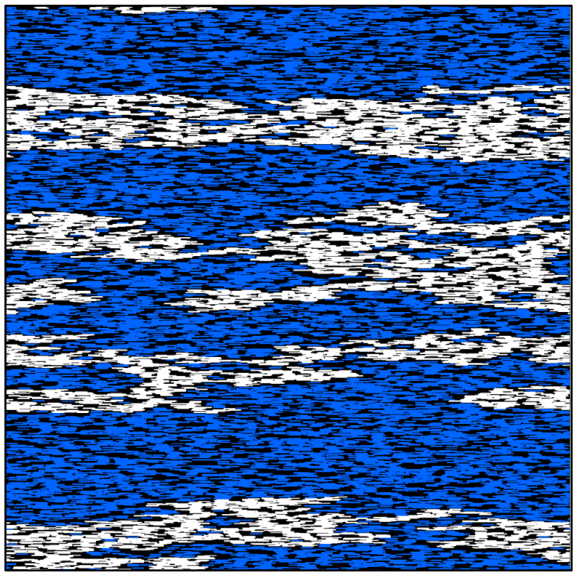


Figure 6. *L* = 5000, *k* = 100, *bl* = 5. Four percolation clusters

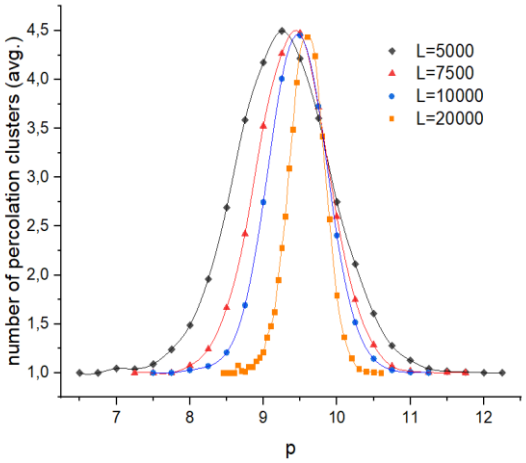


Figure 7. The interpolation of the dependences of the several percolation clusters formation in the structure on the concentration increase for the various lattices, *bl* = 5

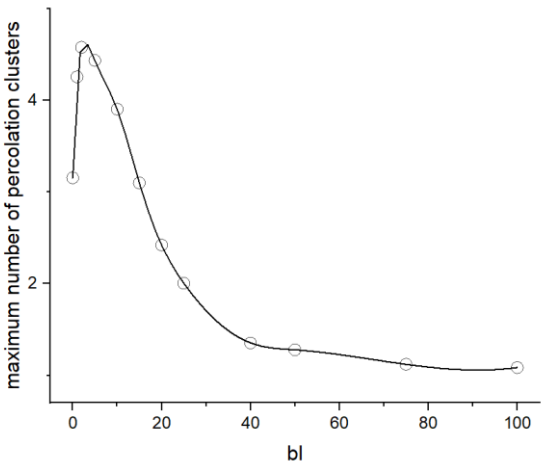


Figure 8. The interpolation of the most received number of the percolation clusters from the bond length *bl* on the lattice with the linear size *L* = 20000

4. Summary

Authors proposed and investigated the percolation model of the structure of the polymer thin film, modified by the carbon nanotubes, with the orient factor availability and the existence of the interphase regions. The main result is the percolation threshold values and the quantity of percolation clusters for the various parameters of the model. The threshold values of the carbon nanotubes concentration in the polymer, at which the accurate anisotropy of the electrical conductivity is observed, are defined in the experiment by authors of the work [1] now. By authors of the present work it is planned, that having compared results of the computer modeling and the natural experiment estimates of the interphase regions size of the polymer nanocomposite, the dependence of emergence of the electric conductance property on the nanotubes concentration and the percolation clusters quantity will be received.

Acknowledgments

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