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Physics Procedia 72 (2015) 47 – 50

Physics Procedia

Conference of Physics of Nonequilibrium Atomic Systems and Composites, PNASC 2015, 18-20 February 2015 and the Conference of Heterostructures for microwave, power and optoelectronics: physics, technology and devices (Heterostructures), 19 February 2015

Numerical Simulation of the Percolation Cluster of Carbon Nanotubes in Membranes

P.A. Likhomanova[a*], Yu.S. Eremin[a], I.V. Tronin[a], A.M. Grekhov[a,b]

[a]*National Research Nuclear University MEPhI, Kashirskoye shosse 31, Moscow 115409, Russia*
[b]*A.V.Topchiev Institute of Petrochemical Synthesis RAS, Leninsky prospect 29, Moscow 119991, Russia*

Abstract

The results of Monte-Carlo simulations of the percolation clusters of carbon nanotubes in the two-dimensional finite thickness membranes are presented. Simulations are performed by the Hoshen-Kopelman and modified Newman-Ziff algorithms. The dependence of the particles critical concentration (percolation thresholds) on the membrane aspect ratio are calculated. The critical concentration decreases with increase of the membrane aspect ratio.

Peer-review under responsibility of the National Research Nuclear University MEPhI (Moscow Engineering Physics Institute)

Keywords: Diffusion; nanotubes; percolation threshold; modeling

1. Introduction

In recent years, there has been an increased interest in matrix mixed membranes produced by the embedding of carbon nanotubes (CNTs) into the polymer's matrix [1]. Such a membrane modification leads to significant changes of various membranes properties such as transport properties, selectivity, mechanical strength, etc. Numerical simulations [2] and nature experiments [1] show that a smooth change in the embedded particles concentration leads

* Corresponding author. Tel.: +7-929-571-7691.*E-mail address:* likhomanovapa@gmail.com

Peer-review under responsibility of the National Research Nuclear University MEPhI (Moscow Engineering Physics Institute)
doi:10.1016/j.phpro.2015.09.012

to an abrupt change of the macroscopic properties of the membranes in a narrow range of concentrations. Such a behavior cannot be described using the standard models - the mixture rule [3], the Maxwell model [4], etc. It is considered that the MMM properties depend not only on the type and amount of embedded nanoparticles, but also on the parameters of the structures, which are formed by particles inside the membrane. A significant change of the transport properties and selectivity occurs when the particles concentration inside the membrane above the critical. In this case, a percolation cluster is formed. Such a cluster has a larger size than the membrane thickness. Therefore, experiments and numerical simulations of the formation criteria and definition of characteristics of the percolation cluster is an urgent task for further development of MMM producing technology [1-6].

Usually analysis of the percolation structures parameters is carried out for the square infinite systems, but the membranes have a thickness much less than the length. In this situation particles size can be compared with the membrane thickness. On the other hand, the formation of the percolation cluster in a perpendicular direction toward the surface of the membrane is necessary for the change of the transport characteristics. Thus, characteristics of such a percolation cluster should be different from the anisotropic case in square matrices [7]. In this paper we focus on the rods percolation in a rectangular matrices with the matrix aspect ratios from 16 to 256.

It is shown that the formation of a percolation cluster occurs at concentrations of the rods in the membranes less than in the square matrices. However, the formed cluster may occupy insignificant part of the membrane. This leads to the formation of inhomogeneous composite material structure and to the instability of the material properties near the percolation threshold. Thus, even insignificant changes in the concentration of rods or the matrix sizes can significantly affect the parameters of the percolation structure.

2. Algorithm

The simulation was performed in the framework of a two-dimensional continuum percolation of the rods in rectangular system with the size $L_x \times L_y$. Percolation threshold calculations was performed by using the Newman-Ziff algorithm [8] - the fastest algorithm for determining the percolation threshold nowadays.

Recently the Newman-Ziff algorithm was adapted to the continuum percolation problems [9,10]. This adaption is the following. The simulation area is divided into square cells (Figure 1). Size of one cell equals to the size of object that filling the system. Such a modification reduces the computational time of checking intersection of the rods: we only need to check intersection of the rods inside the one where we place the rod and rods within the eight neighboring cells.

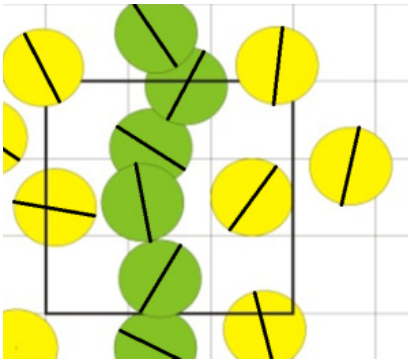

Fig. 1. Cells partition of the plane

The presence of the cluster, connecting the upper and lower edges of the system (percolation cluster) was determined by the following. At the start of each trial the upper and lower edges of the rectangle were filled with clustered rods. A percolation cluster forms when these clusters join together.

If in each trial we stop at the first n where a wrapping cluster appears, then the estimated probability $R_{n,L}$ that a wrapping cluster exists in the microcanonical ensemble with n objects is the fraction of trials that stop on or before the nth step. To obtain the probability R(N,L) of percolation in the grand canonical ensemble, we convolve $R_{n,L}$ with the Poisson distribution [10]:

$$R(N,L) = \sum_{n=0}^{\infty} \frac{\lambda^n e^{-\lambda}}{n!} R_{n,L} \quad (1)$$

This procedure makes it possible to define a continuous function R (N, L) with arbitrary precision. The critical concentration of objects, where percolation transition occurs, is defined by the equation:

$$R(N_c, L) = 0.5 \quad (2)$$

3. Analysis and results

We calculate the percolation thresholds for the five system sizes: 30×16, 30×32, 30×64, 30×128 and 30×256. The rods length is fixed l=1. Periodic boundary conditions are applied for the left and right edges of the rectangle. Figure 2 shows the variation of percolation concentration as a function of aspect ratio of the system.

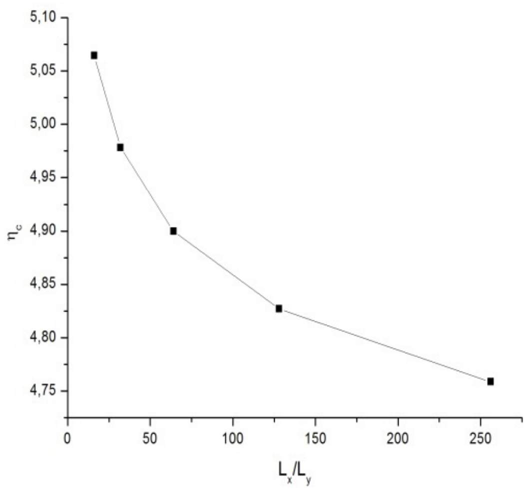

Fig. 2. Percolation threshold as a function of aspect ratio for rectangle

It is seen that the percolation threshold decreases in non-linear manner with increasing aspect ratio. In addition distribution of particles in the membrane can be less uniform. Thereby many clusters consist from free particles which are not belonged in the percolation cluster.

Conclusion

It was shown, that in the membranes the formation of a percolation cluster occurs when the rods concentration is less than in square matrices. However, in this case, the formed cluster is not localized and occupies an insignificant part of the membrane. This leads to the formation of inhomogeneous structure of the composite material and to the instability of the material properties at the percolation threshold. At the high concentrations the probability of agglomeration increases, and that leads to the deterioration of the percolation cluster structure and negatively affects to the properties of the membrane.

Acknowledgments

The work has been performed under support of Ministry of education and science of Russia, Grant No. 3.720.2014/K.

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