Percolation in a Random Network of Conducting Nanotubes: a Computer Simulation Study

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Abstract – **present paper reports the algorithms and the results of the conductivity percolation effect in 3D network of conducting nanotubes.**

Keywords - **Nanotubes, Percolation, Conductivity.**

I. Introduction

Nanotube/dielectric composites [1] exhibit some desirable features that aren't found in the individual components. A wide range of dielectric media can be reinforced with carbon nanotubes providing significant enhancement of specific properties in a controlled way. As far as the electric conductivity of such materials is considered, computer simulations can be effectively used in order to investigate percolation threshold.

II. Modeling the Network of Nanotubes

A model system is considered as the 3D box filled with 'nanotubes', i. e. conducting cylindrical open-ended tubes of random lengths and thickness [2]. Tubes lengths are much smaller than the size of the box. In such a system there may (as depicted in Fig. 1), or may not, exist the conductive path between the opposite edges of the box.

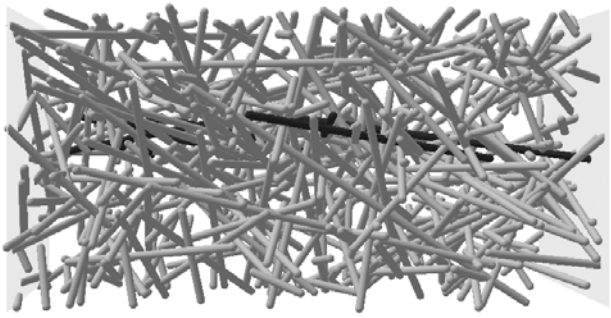

Fig.1 3D box randomly filled with nanotubes

In the framework of the model described above the percolation threshold is investigated as a function of various parameters of the system. For these purpose the volume fraction of the nanotubes is gradually increased until the box becomes conductive.

III. Software Implementation

Conductive path search algorithm and 3D visualization of the statistical network model have been implemented in a C# program. The program can be run in two modes: threshold calculation or conductive path existence verification. The parameters of the simulated system as well as the results of the calculation session can be saved to MySQL database. In order to increase the calculation efficiency the modeled network is divided into subsystem and multithread computing approach is exploited.

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III. Results

The principal result of the simulation is the dependence of the percolation threshold on the volume fraction of the nanotubes which is shown in Fig. 2 for nanotubes with different length-to-diameter ratio.

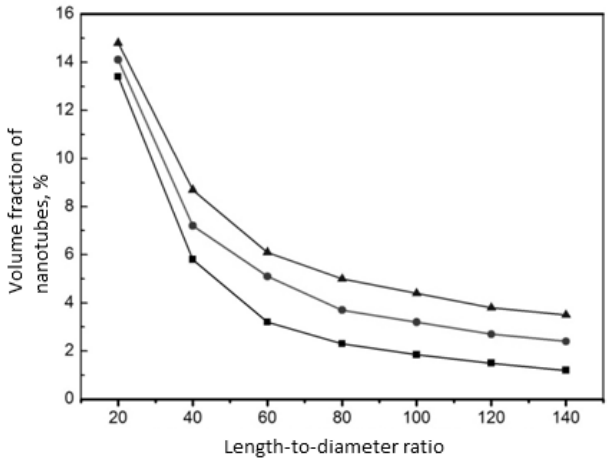

Fig.2 Results of percolation threshold modeling: squares – 100% of conductive tubes, circles – 80% of conductive tubes, triangles – 60% of conductive tubes

Simulations were performed using two different computing systems: Intel Core 2 Duo (dual core) machine and Intel Core i5 (quad core) machine. It has been shown that using of multithread approach allows to perform the overall calculations almost twice as fast.

III. Conclusion

Computer simulations of conductivity in the framework of the statistical 3D model of nanotubes/insulator composite have been carried out. Percolation threshold has been investigated as a function of model parameters. Parallel computing algorithms were successfully exploited in order to decrease the calculation time.

References

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