Computational Study of Electrical Processes in Nanotubes/Dielectric Composite

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Filling the insulating polymer matrix with nanotubes (e.g. carbon nanotubes, CNTs) improves noticeably the electrical and mechanical properties of the resulting composite [1]. Usually, very low concentration of nanofiller is needed to transform nanocomposite into conductor as the aspect ratio for nanotubes is very high [2]. Electrical conductivity of nanocomposite is to a large extent determined by the configuration of CNTs.

Since the electrical conductivity of nanocomposite is dependent on many factors, significant efforts are required to explore study it experimentally. Therefore, a number of approaches were developed in order to simulate the process using numerical calculations.

In this work, nanocomposite is modelled as 3D volume box also known as representative volume element (RVE) randomly filled with high aspect ratio conductive nanotubes. Electrodes are attached to the opposite sides of nanocomposite in order to test its's electrical properties. CNTs can potentially create connections between each other and, therefore, form long chains of connected tubes between the opposite sides of RVE [2].

In this model, we consider solid CNTs, that means they cannot overlap each other by volume. An electric contact between nanotubes is ensured by tunneling effect.

The simulation process starts with generating a set of CNTs inside the RVE. Start point and the direction in space of each CNTs is randomly chosen. Before adding newly generated CNTs into the system we have to perform additional check to be sure that this CNT doesn't overlap the existing ones. To perform such check, the shortest distance between generated tube and all other CNTs is calculated. Only in case when all these distances are larger than CNT diameter ***d***, the newly generated CNT is going to be added to the system.

If the shortest distance between CNTs is less than tunneling cut-of distance, then we assume that these CNTs are in electrical contact. Several bunches of mutually connected nanotubes form clusters. The cluster is called conductive if it contains CNTs connected to both electrodes. For finding conductive clusters in RVE we utilize the union find algorithm.

Set of connected CNTs can be interpreted as a random network of resistors. After applying the combination of Kirchhoff's current law and Ohm's law the system of linear equations is created. After applying potential boundary conditions and solving the system we obtain the values of potentials V_i at all network nodes then all currents flowing through resistor elements are calculated. Finally, we calculate the total equivalent electrical conductivity of random resistor network using Ohm's law and total current flowing through system and applied potential values.

We have developed software for the simulation of nanotube-dielectric composite conductivity using the method described above. Model nanocomposite sample is characterized by the following parameters. Dimensions of the nanocomposite are 1000 nm, 1000 nm and 100 nm respectively. The CNT diameter is 2 nm and the length is 20 nm, intrinsic conductivity is 10^4 S/m. The tunnel cut-off distance is set to 1.8 nm. Simulation results are in agreement with experimental measurements reported in [2].

[1] R. Khare, S. Bose, Carbon Nanotube Based Composites - A Review, *J. Minerals & Materials Characterization & Engineering* **4**(1) (2005) 31-46.

[2] N. Hu, Z. Masuda, C. Yan, G. Yamamoto, The electrical properties of polymer nanocomposites with carbon nanotube fillers, *Nanotechnology* **19**(21) (2008) 215701.