2D composites with rod-like fillers: Computer simulation of electrical conductivities

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By means of computer simulation, we examine electrical conductivity of two-dimensional composites with rod-like fillers [1–3]. We use a lattice approach. A host matrix (a substrate) is treated as a square lattice; rod-like fillers are represented as linear k-mers, i.e., particles occupying k adjacent adsorption sites of the lattice. The k-mers are deposited onto the lattice by the random sequential adsorption. Overlapping with predeposited k-mers, hence, a monolayer is formed. Detachment of the deposited k-mers from the surface is forbidden. We consider two different models, viz., an insulating host matrix and conducting fillers and a conducting host matrix and insulating fillers. A high electrical contrast between a host matrix and fillers is assumed. We examine both the isotropic and anisotropic systems. We transform the monolayer into a random resistor network to calculate its effective electrical conductivity. The electrical conductivity of such a monolayer in both the x and y directions for different lengths and concentrations of the k-mers is calculated [1], and its behavior in the vicinity of insulator-to-conductor phase transition is analyzed. An insulator-conductor phase transition is observed near the percolation threshold. For large values of k (k=64,128), the electrical conductivity increases rapidly with the initial increase of concentration of fillers from 0 to 0.1

Additionally, we examine the effect of defects on the behavior of electrical conductivity in such composites [2]. In our study, the defects in the host matrix are distributed randomly and these lattice sites are forbidden for the deposition of k-mers. The k-mers are deposited onto the substrate until a jammed state. The defective sites are distributed randomly on the deposited k-mers. The lattice sites filled with k-mers have a high electrical conductivity, whereas the empty sites, and the sites filled by either types of defect have a low electrical conductivity. The effect of the concentrations of defects on the electrical conductive is studied.

We also study effect of diffusional relaxation of deposited particles on electrical conductivity of the 2D composite [3]. In this study, after deposition of k-mers up to a given concentration, the random walk (translational diffusion) of deposited k-mers is allowed. When the concentration of fillers exceeds the percolation threshold, the system in its initial state is a conductor. Diffusional reorganization leads to a decrease in the electrical conductivity. The conductor–insulator phase transition occurs when the concentration of fillers is slightly above the percolation threshold.

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