Simulation of electrical conductivity of 2D composites with rod-like fillers

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By means of computer simulation, we examined electrical conductivity of two-dimensional (2D) composites with rod-like fillers [1–4]. We investigated the effects of particles length and their alignment on electrical properties of 2D composite with high electrical contrast between a host matrix and fillers. We studied both the isotropic and anisotropic systems. We used both continuous [1,3] and lattice [3,4] approaches.

In the lattice approach [1,2,4], a host matrix (a substrate) was treated as a square lattice; rod-like fillers were represented as linear k-mers, i.e., rectangular particles $1 \times k$ lattice faces. The k-mers were deposited onto the lattice by the random sequential adsorption. Overlapping with predeposited k-mers was forbidden, hence, a monolayer was formed. We transformed the monolayer into a random resistor network (RRN) to calculate its effective electrical conductivity.

The effect of defects on the behavior of electrical conductivity has also been simulated [2]. The defects in the lattice (impurities) and defects in the particles were considered. We examined both isotropic and anisotropic (all particles are aligned along one given direction) composites. We found that even a very small concentration of impurities has strong impact on the electrical conductivity.

For continuous problems, the model with intersections [3] and without intersections [4] rod-like particles were considered. The dependence of percolation thresholds and anisotropy of electrical conductivity versus the order parameter are discussed.

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