Nanocomposites and nanomaterials

Percolation threshold for polymer filled with particles of different morphology: Monte Carlo simulation

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Hybrid particles can improve the performance and reduce the cost of polymer matrix composites, and thus increasingly used as fillers in multifunctional and structural materials. For these materials, the percolation threshold is of great importance because it determines whether or not the excellent mechanical, electrical and thermal properties of fillers can be fully utilized in the composites.

A three-dimensional (3-D) Monte Carlo model is developed for predicting electrical conductivity of polymer matrix composites filled with conductive graphite nanoplatelets (disks) and/or carbon nanotubes. The conductive fillers are modeled as a 3-D network of finite sites that are randomly positioned. The percolation behavior of the network is studied using the Monte Carlo method, which leads to the determination of the critical filler volume fraction (or the percolation threshold). There are several controlling parameters for different types of filler, namely the nanotubes or nanodisks diameter and their aspect ratio.

Since the production of nanotubes is more expensive than the production of disk-like graphite nanoplatelets, the aim of our study is investigation of the possibility of substitution the nanotubes with nanodisks taking into account losses in percolation threshold. The dependences of the percolation threshold on the aspect ratio of the filler, as well as the effect of the simultaneous presence of the nanoparticles of various morphology with a different aspect ratio are investigated.