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Mechanism and Limitation of Heat Conduction in Three-Phase Polymer Composites Having Carbon Nanotubes and Inorganic Nanoparticles HAI DUONG, FENG GONG, National University of Singapore, DIMITRIOS PAPAVASSILIOU, University of Oklahoma — For the first time, an Off-Lattice Monte Carlo method is developed successfully to predict thermal conductivities (K_{eff}) of three-phase composites having carbon nanotubes (CNTs) and tungsten disulfide (WS_2) nanoparticles more accurately and faster than previous methods such as effective medium theories, molecular dynamics and finite element methods. The K_{eff} predicted by our model using a random walk algorithm and taking into account various thermal boundary resistances at each interface and inter-CNT contact has an excellent agreement with experimental data. Our model can comprehensively explain the mechanism of heat conduction in complex composite structures. Effects of WS_2 and CNT morphologies (diameter, length, inter-contact, bundle), CNT concentrations, CNT orientations (parallel, random and perpendicular to heat flux) and thermal boundary resistances of CNT-polymer, WS_2-polymer, CNT-CNT, CNT-WS_2 on heat conduction limitation of the three-phase composites are also investigated systematically. Our model can be also applied to the biological and nanofluid systems.

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