128b Heat Transfer in Carbon Nanotube Composites

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The superior physical properties of carbon nanotubes are promising the development of new applications and the synthesis of new materials. Possible applications of carbon nanotubes (CN) include the facilitation of heat transfer in microchannels and in composite materials. Since CNs are excellent heat conductors (for multi-wall, thermal conductivity is about 3000 W/(K.m), for single wall it is about 6000 W/(K.m)), it can be advantageous to utilize them by making heat sinks with composites with CN fillers, capitalizing on CN's high thermal conductivity. An unexpected problem for the development of this idea further is the heat resistance (Kapitza, P.L., J. Phys. USSR, 4, 181, 1941) that exists at the interfaces between different solids and between solid and liquid in contact. Since heat is transferred by phonons in insulator solids, mismatch of phonon frequencies (acoustic mismatch) causes this additional resistance that could be large even at room temperatures. It is, thus, important to resolve this problem before a heat removal design can be achieved.

The focus of this study is to predict the thermal properties of new materials that can be synthesized with carbon nanotubes (e.g., thin nanotube composite layers to be used as thermal shields). Random walk simulations of thermal walkers are used to study the effect of interfacial resistance on heat flow in dispersed carbon nanotube composites. Effective heat conductivity through CN composites, as a function of nanotube length, orientation and percent composition was also calculated. The work has generated a parallelizable off-lattice Monte Carlo code of a large number of random walkers traveling in the computational cell for a relatively long time. The off-lattice Monte Carlo simulation successfully shows how the system can be replaced with an effective medium approximation, as well as the role of the thermal boundary resistance at the CN surface in diminishing the impact of the CN's effect on the heat conduction. The adopted algorithm effectively makes the thermal conductivity of the nanotubes themselves infinite. Our algorithm is more efficient than a typical random walk algorithm, and much faster than a Molecular Dynamics algorithm. Even though it cannot provide results at the fundamental molecular level as Molecular Dynamics can, it can be used to model physico-chemical properties of randomly-dispersed nanotube materials quite successfully.

In addition to the development of the numerical algorithm, the paper will discuss the effects of carbon nanotube orientation, aspect ratio, volume fraction, and Kapitza resistance on the composite effective conductivity. We find that orientation is crucial in maximizing the impact of the CNs on heat conduction. It was found that the effective thermal conductivities of nanotube composites are much lower than those calculated from the modified Maxwell theory. The effect of the Kapitza resistance becomes important when the surface area of the CNs and their aspect ratios are small.