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Improving thermal conductivities of nanotube composites: by end functionalization[1] TIMOTHY BURT, Homer L. Dodge Dept. of Physics and Astronomy, University of Oklahoma, MATTHEW HOUCK, Department of Chemistry and Biochemistry, University of Oklahoma, KIERAN MULLEN, Homer L. Dodge Dept. of Physics and Astronomy, University of Oklahoma, DANIEL GLATZHOFER, Department of Chemistry and Biochemistry, University of Oklahoma — Several computational models of heat transport within functionalized/non-functionalized carbon nanotube-polymer composites were developed. On-lattice random walk simulations were used to predict the effect of interfacial or Kapitza resistance on the heat flow for different orientations of the SWCNTs which were randomly dispersed throughout the polymer. Functionalization, in the sense of adding certain molecules to the ends of a SWCNT which lowers the thermal boundary resistance, increases the thermal conductivity k in the simulations as expected. From our results we find that k $\propto$ N, where N is the number of tubes, for nearly all physically realizable simulations up to $\approx$ 20% volume fraction of SWCNTs with no apparent phase transitions. The effect of changing the aspect ratio of the tubes (L/D) is presented. Results will be compared with measurements of carbon nanotubes functionalized with a variety of polymers and functionalization groups, notably PMMA and amine-terminated SWCNT. Electrophoresis will be used to orient the tubes in a particular direction and k will be directly measured.

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