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Monte Carlo Simulation of Thermal Conductivity in Randomly Distributed Nanowire Composites W. TIAN, R. YANG, Dept. of Mech. Engr., Univ. of Colorado, Boulder — In this paper, we investigated the thermal conductivity of composites made of two types of randomly stacked nanowires with high contrast ratio of bulk thermal conductivity. Thermal conductivity predictions based on solving the phonon Boltzmann transport equation by using the Monte Carlo method are presented for different contrast ratios of thermal conductivity, sizes of nanowires and the volumetric fractions in the composites. For composites made of nanowires with high contrast ratio thermal conductivity, the thermal conductivity of the nanocomposites increase dramatically when the volumetric fraction of high thermal conductivity nanowire is higher than the geometry percolation threshold, although existing correlations in percolation theory do not fit the results due to the phonon interface scattering. On the other hand, when the the size of nanowires is small and the volumetric fraction of high thermal conductivity nanowire is less than percolation threshold, the thermal conductivity of the nanocomposites decreases with increasing the volumetric fraction of the high thermal conductivity nanowires. The results of this study may help the development of nanoscale thermoelectric materials in which the figure of merit is optimized by choosing appropriate nanowire size, property contrast and composition. RY acknowledges the funding support for this work by DoD/AFOSR MURI grant FA9550-06-1-0326. The simulation was conducted on a 24-node cluster supported by Intel Corporation and managed by Prof. Gang Chen and Mr. Lu Hu at MIT.

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