Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Thermal boundary resistance between carbon nanotubes in nanocomposites with Monte Carlo simulations[1] KHOA BUI, BRIAN GRADY, DIMITRIOS PAPAVASSILIOU, The University of Oklahoma — Enhancing the thermal conductivity of composites by incorporating carbon nanotubes (CNTs) has been an area of vigorous research recently. Measurements of the effective thermal conductivity (keff) for CNT-polystyrene composites at high CNT %wt found that the ratio (keff/kpolymer) at high concentration of CNTs is not as good as that at low CNT concentration [1]. It appears that the CNT dispersion pattern becomes worse, resulting in the formation of CNT bundles. In this work, we apply Monte Carlo simulations to investigate the keff at different weight fractions taking into account the bundle size and orientation, as well as the thermal boundary resistance. By validating with the experiment data, we found that the phonon transmission probability at the interface decreases by temperature. In addition, the poor enhancement of keff at high CNT concentration is because of the CNT-CNT contact resistance and because of the bundle geometry itself, which is equivalent to the presence of one low aspect ratio nanotube. References [1] Peters J. E.; Papavassiliou D.V; Grady B. P., Macromolecules 2008, 41, 7274-7277.

[1]DoE ER64239 0012293; DoD FA9550-10-1-0031

Dimitrios Papavassiliou
The University of Oklahoma

Date submitted: 29 Nov 2010 Electronic form version 1.4