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THERMAL BOUNDARY RESISTANCE EFFECTS IN NANOCOMPOSITES

Dimitrios V. Papavassiliou[*1], Khoa Bui[2] and Huong Nguyen[3]

[1] Division of Chemical Bioengineering and Environmental Transport, National Science Foundation, Arlington, VA 22230, USA, dvpapava@ou.edu
[2] School of Chemical, Biological and Materials Engineering, The University of Oklahoma Norman, OK 73072, USA,
[3] School of Chemical, Biological and Materials Engineering, The University of Oklahoma Norman, OK 73072, USA

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Carbon nanotubes (CNTs) have been suggested as fillers in composite materials due to their exceptional electrical, thermal and mechanical properties. In terms of thermal properties, incorporating CNTs into a polymer matrix increases the effective thermal conductivity (Keff) of the resulting composite [1,2], but not as much as one would expect based on the effective medium theory. The effective thermal conductivity of the composites is dominated by the thermal boundary resistance (TBR) between the CNTs and the matrix material, and by the dispersion pattern and geometry of the CNTs. While the value of the TBR can be roughly estimated by the acoustic mismatch theory [3], in the case of CNTs in epoxy resins or in suspension, molecular dynamics studies are more accurate. To model the effects of the CNT length and dispersion pattern at the mesoscale, methods like Monte Carlo (MC) simulations are more appropriate [4,5,6].

In this work, we report on recent developments from our group, both in terms of new algorithms for generating CNTs with worm-like geometry in 3D, and in terms of molecular dynamics simulations for the effects of CNT length and CNT configuration on the Keff of composites. The composite configuration is obtained from microscopic images that provide information on the length and dispersion pattern of the CNTs, and then models of curved CNTs are randomly placed in a periodic computational box that represents a realistic case. We will present the methodology and the validation of the method, which is used to study the effects of CNT length and curvature, dispersion and volume fraction on the effective thermal conductivity of the CNT composites. The discussion will include a comparison between theoretical predictions of the value of the thermal resistance at the CNT-polymer interface for cases where the CNTs are coated with silica relative to the case when the CNT-polymer interface is not coated, as well as comparisons between the effective medium theory and the MC results. The effects of silica coating on the thermal conductivity will also be discussed with the use of molecular dynamics methods.

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