Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Theoretical and Experimental Studies of Functionalized Carbon Nanotubes for Improved Thermal Conductivity[1] ALEXANDER KERR, TIMOTHY BURT, KIERAN MULLEN, Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, DANIEL GLATZHOFER, MATTHEW HOUCK, Department of Chemistry and Biochemistry, University of Oklahoma, PAUL HUANG, School of Chemical, Biological and Materials Engineering, University of Oklahoma — The use of carbon nanotubes (CNTs) to improve the thermal conductivity of composite materials is thwarted by their large thermal boundary resistance. We study how to overcome this Kapitza resistance by functionalizing CNTs with mixed molecular chains. Certain configurations of chains improve the transmission of thermal vibrations through our systems by decreasing phonon mismatch between the CNTs and their surrounding matrix. Through the calculation of vibrational normal modes and Green's functions, we develop a variety of computational metrics to compare the thermal conductivity (κ) of our systems. We show how different configurations of attached chains affect the samples' κ values by varying chain identity, chain length, number of chains, and heat driver behavior. We vary the parameters to maximize κ. To validate and optimize these metrics, we perform molecular dynamics simulations for comparison. We also present experimental results of composites enhanced with CNTs and make comparisons to the theory. We observe that some composites are thermally improved with the inclusion of CNTs, while others are scarcely changed, in agreement with theoretical models.

[1]This work was supported by NSF grant DMR-1310407.

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Date submitted: 11 Nov 2016 Electronic form version 1.4