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Modeling the Thermal Conductivity of Nanocomposites Using Monte-Carlo Methods and Realistic Nanotube Configurations[1] KHOA BUI, DIMITRIOS PAPAVASSILIOU, The University of Oklahoma — The effective thermal conductivity (K_{eff}) of carbon nanotube (CNT) composites is affected by the thermal boundary resistance (TBR) and by the dispersion pattern and geometry of the CNTs. We have previously modeled CNTs as straight cylinders and found that the TBR between CNTs ($TBR_{CNT-CNT}$) can suppress K_{eff} at high volume fractions of CNTs [1]. Effective medium theory results assume that the CNTs are in a perfect dispersion state and exclude the $TBR_{CNT-CNT}$[2]. In this work, we report on the development of an algorithm for generating CNTs with worm-like geometry in 3D, and with different persistence lengths. These worm-like CNTs are then randomly placed in a periodic box representing a realistic state, since the persistence length of a CNT can be obtained from microscopic images. The use of these CNT geometries in conjunction with off-lattice Monte Carlo simulations [1] in order to study the effective thermal properties of nanocomposites will be discussed, as well as the effects of the persistence length on K_{eff} and comparisons to straight cylinder models. **References** [1] K. Bui, B.P. Grady, D.V. Papavassiliou, Chem. Phys. Let., 508(4-6), 248-251, 2011 [2] C.W. Nan, G. Liu, Y. Lin, M. Li, App. Phys. Let., 85(16), 3549-3551, 2006

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