MECHANICAL ENGINEERING

John A. Thomas

FINAL PUBLIC ORAL EXAMINATION

Water Flow and Thermal Transport Through Carbon Nanotubes

The atomic-level mechanisms of water flow and thermal transport through carbon nanotubes (CNTs) are examined using molecular dynamics (MD) simulation. To begin, the relationship between water flow rate and pressure gradient for CNTs with diameters between 0.83 nm and 4.98 nm is examined. By calculating the variation of water viscosity and slip length as a function of CNT diameter, it is found that flow through CNTs with diameters greater than 1.4 nm can be understood in the context of continuum fluid mechanics. When the CNT diameter is less than 1.4 nm, water molecules assemble into long-range one-dimensional structures that have neither a well-defined slip length nor a well-defined viscosity. Within this regime, the Poiseuille relation is not applicable and transport is instead related to the CNT diameter-dependent inter-molecular water structure. The thermal conductivities of empty and water-filled CNTs are then predicted using a direct application of the Fourier Law. The transition from ballistic (subcontinuum) to fully-diffusive (continuum) phonon transport is observed with increasing CNT length. A new procedure for calculating phonon properties directly from the velocities of the atoms in a crystal using the spectral energy density is then presented. This procedure, which can be applied to any periodic or non-periodic system, is used to predict the mode-by-mode contributions to the total thermal conductivity of empty and water-filled CNTs.

Monday, February 15, 2010
9:00 AM
Scaife Hall 224

Committee: **Prof. Alan McGaughey (Chair),**
Prof. Shelley Anna (Mechanical Engineering),
Prof. Nadine Aubry (Mechanical Engineering),
Prof. Mohammad Islam (Chemical Engineering)

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John Thomas received his B.S. degree in Mechanical Engineering from Penn State University in December 2005. He joined the Department of Mechanical Engineering at Carnegie Mellon University in January 2006 and works under Prof. Alan McGaughey in the Nanoscale Transport Phenomena Laboratory. He received his M.S. degree in December 2008.

FINAL PUBLIC ORAL EXAMINATION
Doctor of Philosophy