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Radial Heat Transfer Dynamics in Multiwall Carbon Nanotubes

MOHAMED OSMAN, TAEJIN KIM, Washington State University — The dynamics of radial heat transfer in zigzag and armchair double wall carbon nanotubes (DWCNT) have been examined using molecular dynamic (MD) simulations with the goal of understanding the role of radial phonon modes in heat transfer. The MD model uses Tersof-Brenner potential for bonded C-C interactions within each shell and non-bended van der Wall interaction between inner and outer shells. The simulation procedure involves, (1) quenching the DWNT to 0 K, (2) minimization of the potential energy and (3) raising the temperature of the outer shell to the desired steady state temperature while maintaining the inner tube at 0.1 K. The heat baths are removed from the outer and inner shell and their energies are examined. The energies of inner and outer exhibit an out of phase oscillatory behavior due the exchange of the energies between the two shells. The energy of the inner tube shows a weak gradual increase due to the temperature gradient. The beat frequencies determined from the Fourier transform of the energy oscillations of the inner and outer nanotubes were found to be in the tera Herz range. We will also discuss the temperature and length dependence of oscillatory energy exchange between the nanotube shells.

Mohamed Osman
Washington State University

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