A Molecular Dynamics Simulation of Heat Conduction of Finite Length SWNTs

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The heat conduction of finite length single walled carbon nanotubes (SWNTs) was simulated by the molecular dynamics method with the Tersoff-Brenner bond order potential (parameter table II) [1]. The thermal conductivity of SWNTs, which was speculated to be higher than any other materials along the cylindrical axis [2,3], was measured from the simulations with several different chiralities and lengths. Here, no periodic boundary condition was applied to the longitudinal direction since the heat transfer characteristic of finite length nanotube is necessary for the applications such as thermal devices. Since the photon mean free path is estimated, as order of 100nm ~ 1μm, heat conduction of nanotubes with about 1μm length should have the nearly 'ballistic' features with much less apparent thermal conductivity than infinitely long nanotubes.

Temperature at each end of a SWNT was controlled by the phantom technique [4], and the thermal conductivity was calculated from the measured temperature gradient and the heat flux obtained by the integration of the additional force by the phantom molecules. The Fourier's law of heat conduction may not be obeyed for these almost one-dimensional materials when rather high heat flux conditions. The basic heat conduction mechanism was explored through the phonon dynamics extracted from the molecular dynamics simulations. The phonon density of states was measured as the power spectra of velocity fluctuations as in Fig. 1. The photon dispersion relations were also directly measured as the time-space 2-D Fourier transforms of the position of each molecule as shown in Fig. 1. The theoretical 36 lines were reproduced, with the group velocities almost the same as the previous estimations [5].

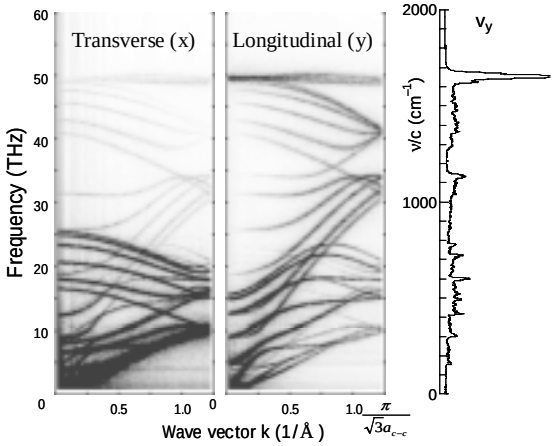

Fig. 1 Phonon dispersion relation and photon density of states for (5,5) SWNT.

References

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