A Molecular Dynamics Simulation of Heat Conduction in SWNTs

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The heat conduction in finite length single walled carbon nanotubes (SWNTs) was simulated by the molecular dynamics method with the Tersoff-Brenner bond order potential [1]. Temperature at each end of a SWNT was controlled by the phantom technique, and the thermal conductivity λ was calculated from the measured temperature gradient $\partial T / \partial z$ and the energy budgets in phantom molecules through the Fourier's law $q = -\lambda(\partial T / \partial z)$. The thermal conductivity measured for (5,5) and (10,10) SWNTs with various lengths from 6 nm through 404 nm is shown in Fig. 1 [2]. Measured thermal conductivity for smaller diameter (5,5) nanotube did not converge to a finite value with increase in tube length, but obeyed a striking power law relation similar to the one-dimensional model calculations [3].

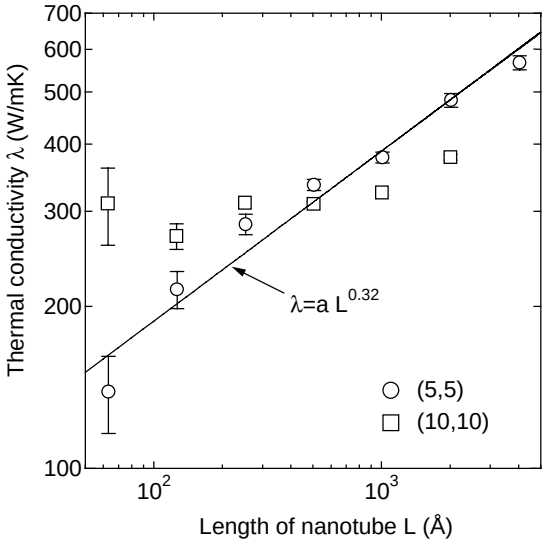

Fig. 1 Dependence of thermal conductivity on length of nanotubes for 300K.

The phonon density of states was measured as the power spectra of velocity fluctuations. And, the photon dispersion relations were also directly measured as the time-space 2-D Fourier transform of the position of each molecule as shown in Fig. 2. This directly measured phonon dispersion relations were compared with the theoretical results [4] and experimental Raman spectra.

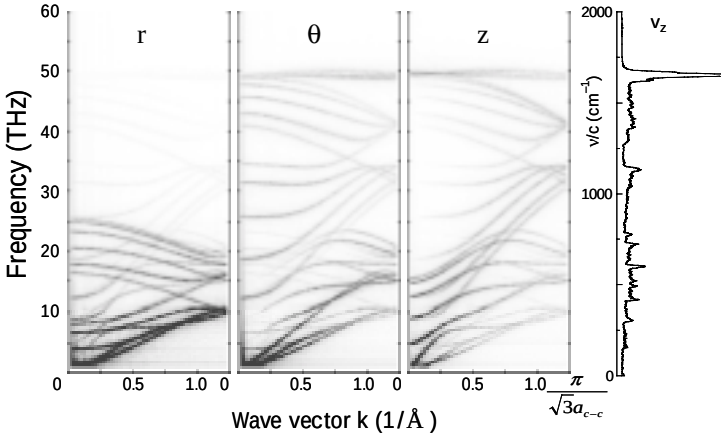

Fig. 2 Phonon dispersion relation and phonon density of states for (5,5) SWNT.

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