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 $\lambda$ 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].

The phonon density of states was measured as the power spectra of velocity fluctuations. And, the phonon 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.


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