Molecular Dynamics Simulation of Heat Conduction through a SWNT

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The heat conduction along a single walled carbon nanotube (SWNT) was simulated by the molecular dynamics method with the Tersoff-Brenner bond order potential [1]. The thermal conductivity of SWNTs, which was speculated to be higher than any other materials along the cylindrical axis, was measured from the simulations for SWNTs with several different chiralities and lengths. Temperature at each end of a SWNT was controlled by the phantom technique [2], and no periodic boundary condition was applied to minimize the boundary scattering of phonons. The thermal conductivity was calculated from the measured temperature gradient as in Fig. 1 and the heat flux obtained by the integration of the additional force by the phantom molecules. The preliminary result showed that the thermal conductivity was about 200 ~ 300 W/mK. The temperature jump near the heating and cooling region was explained by assuming the thermal boundary resistance due to the miss-match of the phantom technique to the structured phonon density distribution.

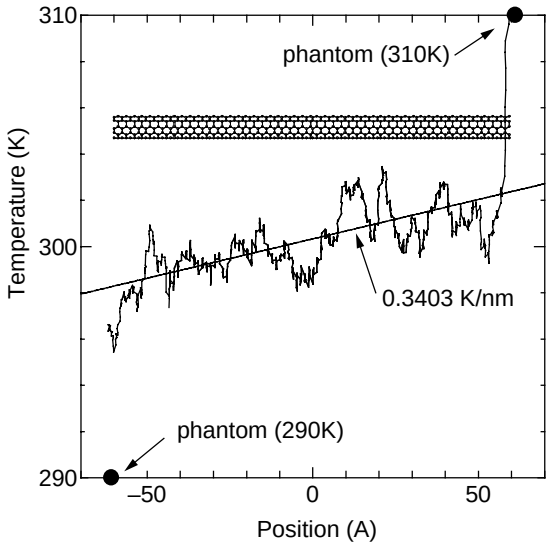

Fig. 1 Temperature distribution along (5,5).

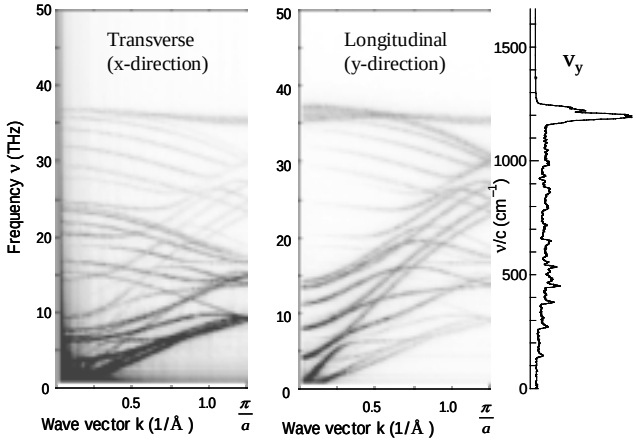

Fig. 2 Phonon dispersion relation for (5,5).

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. The theoretical 36 lines were reproduced, but the group velocities were about 30 % smaller compared with theoretical calculations with tuned force constants for (10,10) [3]. Simulations with different potential parameter sets [1] would be also discussed.

[1] Brenner, D. W., Phys. Rev. B, 42-15 (1990), 9458.
[2] Maruyama, S. and Kimura, T., Therm. Sci. Eng., 7-1 (1999), 63.
[3] Saito, R. et al., Phys. Rev. B, 57-7 (1998), 4145.

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