MD Simulation of Phonon Transport in Single-Walled Carbon Nanotubes

Shigeo Maruyama

Department of Mechanical Engineering, The University of Tokyo,
7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan
Tel: +81-3-5841-6421 Fax: +81-3-5800-6983
E-mail: maruyama@photon.t.u-tokyo.ac.jp

We have simulated the heat conduction characteristics of finite length single walled carbon nanotubes (SWNTs) with the molecular dynamics method [1-3] with Tersoff-Brenner bond order potential. Temperature at each end of a SWNT was controlled by the phantom technique, and the thermal conductivity was calculated with Fourier's law from the measured temperature gradient and the energy budgets in phantom molecules. Hence, without the use of periodic boundary conditions in the nanotube axis direction, thermal conductivity of finite length nanotube was calculated. The thermal conductivity was diverging [2,3] with the power-law characteristics with nanotube length at least up to the 0.4 μm long nanotube for (5, 5). This feature can be compared with the theoretical 1 dimensional heat conduction calculations. The temperature dependency of measured thermal conductivity behaved as 1/T in high temperature range. The limitation of classical molecular dynamics in low temperature calculation was also discussed [3].

As the first step for exploration the basic heat conduction mechanism, phonon density of states and phonon dispersion relations were directly extracted from the molecular dynamics trajectories as in Fig. 1. The phonon dispersion relations and density of states were calculated from each components of displacement vector (r, θ, z) or velocity components (v_r, v_θ, v_z). It can be seen that all 36 distinguishable branches of dispersion relations are reproduced in Fig. 1. The dispersion relations calculated from eigen values and eigen vectors of dynamical matrix made with the force-constant tensor scaled from 2 D graphite [4] is also shown in Fig.

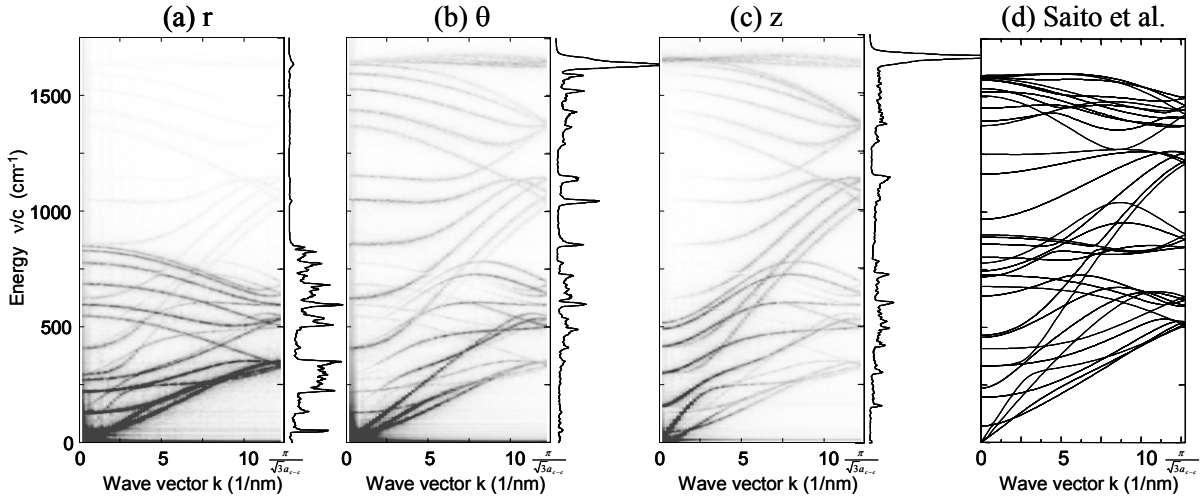

Fig. 1 Phonon dispersion relation and phonon density of states for 101 nm long (5, 5) SWNT. Dispersion relations from r, θ and z components of displacement are shown in (a), (b) and (c) respectively. The phonon density of states calculated as power spectra of v_r, v_θ, v_z are shown as the right hand side of dispersion relations. (d) The dispersion relations solved from the dynamical matrix using the force-constant tensor scaled from those for 2D graphite [4].

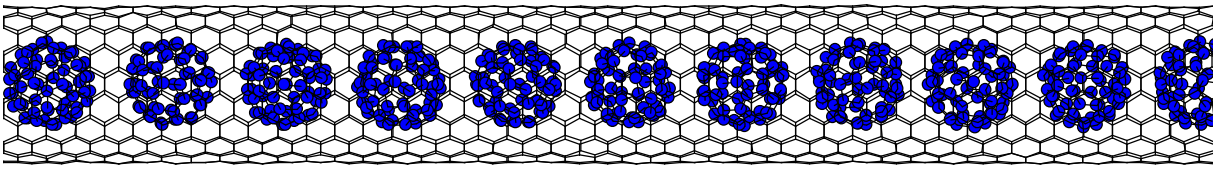

Fig. 2 A peapod structure with C_{60} molecules in (10,10) SWNTs.

1(d) as comparison. The group velocities of four acoustic phonons were estimated as longitudinal acoustic mode: 17 km/s (z-direction), transverse acoustic mode (degenerate): 7 km/s (r-direction), twisting acoustic mode: 10 km/s (θ-direction), in good agreement with the dynamical matrix result in Fig. 1(d).

The alternation of phonon dispersion relations and phonon density of states, for example, by defects in structures or by inserting other molecules into the tube were simulated. An example of such modification was the peapod structure with fullerene molecules filled inside a SWNT as shown in Fig. 2. In order to simulate the structure in Fig. 2, in addition to the Brenner potential, van der Waals force were assumed as the Lennard-Jones potential between two carbon atoms that were not part of a molecule. A macroscopic experiment showed that by filling C_{60} into SWNTs a higher thermal conductivity was obtained [5]. The prediction of the alternation of phonon dispersion relations by filling C_{60} is also important to predict the Raman assignments of peapods.

References

[1] S. Maruyama and S.-H. Choi, “Molecular Dynamics of Heat Conduction through Carbon Nanotube,” Therm. Sci. Eng., (2001), vol. 9, no. 3, pp. 17-24.

[2] S. Maruyama, "A Molecular Dynamics Simulation of Heat Conduction of Finite Length SWNTs," Physica B, (2002), in print.

[3] S. Maruyama, "A Molecular Dynamics Simulation of Heat Conduction of a Finite Length Single-Walled Carbon Nanotube," Micro. Thermophys. Eng., (2002), submitted.

[4] R. Saito et al., “Raman Intensity of Single-Walled Carbon Nanotubes,” Phys. Rev. B, (1998), vol. 57, pp. 4145-4153.

[5] J. Vavro et al., "Electrical and thermal properties of C60-filled sigle-wall carbon nanotubes," Appl. Phys. Lett., (2002), vol 80, no. 8, pp. 1450-1452.