

# Characterization of Heat Conduction of Carbon Nanotube by Molecular Dynamics Method

Shigeo Maruyama, Yuki Taniguchi and Yasushi Shibuta

*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 been studying the heat conduction along a single-walled carbon nanotube (SWNT) by the molecular dynamics method [1-3] with the simplified form [4] of Tersoff-Brenner bond order potential [5]. Our preliminary results showed that thermal conductivity was strongly dependent on the nanotube length for realistic length scale for device applications [2, 3]. Furthermore, we have reported the direct calculation of phonon dispersion relations and phonon density of states from molecular dynamics trajectories [2, 3]. The calculated thermal conductivity for finite length nanotube was not as high as the previously reported result that it might be as high as 6600 W/mK at 300 K [6]. However, the thermal conductivity was much higher than high-thermal conductivity metals. In order to study the distinctive behavior of heat conduction of carbon nanotubes, several practical molecular dynamics simulations were performed.

One example of the interesting feature is the thermal boundary resistance at the junction of nanotubes with different chiralities. The simulation system is shown in Fig. 1. In this case a (12, 0) zigzag nanotube in the left-hand side and a (6, 6) armchair nanotube were smoothly connected using 5-membered and 7-membered rings at the junction. By applying different temperatures at each end, temperature distribution was measured as in Fig. 3. The temperature jump at the junction is very clear. This thermal boundary resistance is quite realistic and also theoretically accessible by the molecular dynamics simulation. Compared with the junction system, a nanotube with a vacancy of a carbon atom did not have much thermal resistance at the defect point. It can be easily speculated that the difference of phonon structures in both sides was quite

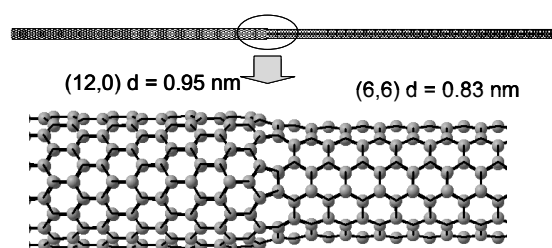


Fig. 1 Junction of 2 different SWNTs.

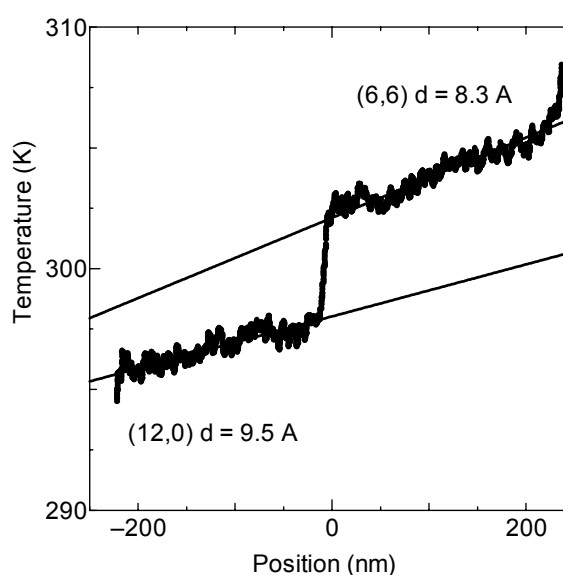


Fig. 2 Temperature jump at the junction by thermal boundary resistance.

important. By comparing several different junction types, we will try to model the mechanism of thermal boundary resistance by the reflection of phonons.

Another example of the molecular dynamics characterization of thermal conductivity is the isotope effect. It is well-known that the inclusion of only 1% of  $^{13}\text{C}$  natural isotope dramatically reduces the thermal conductivity of diamond [7]. However, the previous molecular dynamics result was concluded that the isotope effect was negligible for carbon nanotubes [6]. In order to clarify this point, thermal conductivity of nanotube with randomly distributed  $^{13}\text{C}$  with various ratios was calculated. A preliminary result is shown in Fig. 3. Here, (5,5) nanotube with about 50 nm was used. The dependency of thermal conductivity on isotope ratio was well explained with the following equation as the fit curves in Fig. 3.

$$\lambda = \sqrt{\frac{12}{12(1-x) + 13x}} \cdot \frac{\lambda_{\text{pureC}^{12}}}{C_1 \cdot x(1-x) + 1}$$

where  $x$  is the ratio of  $^{13}\text{C}$ ,  $\lambda_{\text{pureC}^{12}}$  is the thermal conductivity for pure  $^{12}\text{C}$ ,  $C_1$  is the fitting parameter. It is also noted that the thermal conductivity at 100 K is not realistic in Fig. 3 because the classical simulation cannot reproduce the correct change of heat capacity at low temperature [3]. The mechanism of the decrease of thermal conductivity with isotopes is discussed.

We also have studied the difference of the heat conduction among SWNT, peapod and a double-walled carbon nanotubes (DWNTs). The structure of peapod is shown in Fig. 4. In order to represent those models, a Lennard-Jones potential function between carbon atoms was assumed between carbon clusters.

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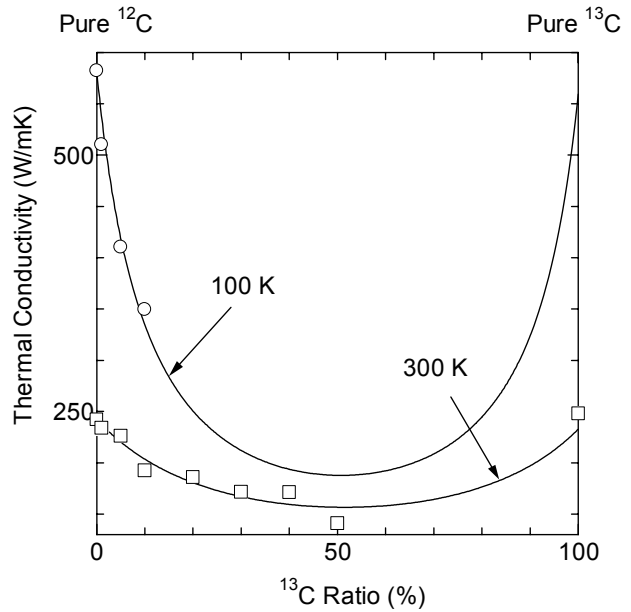


Fig. 3 Effect of  $^{13}\text{C}$  isotope on thermal conductivity of SWNT

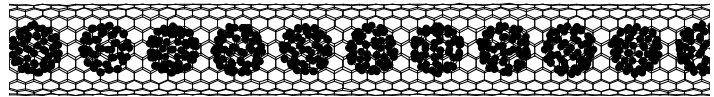


Fig. 4. Peapod structure,  $\text{C}_{60}$  in (10, 10).