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HEAT TRANSFER PROBLEMS RELATED WITH CARBON NANOTUBES BY MOLECULAR DYNAMICS-BASED SIMULATIONS

Yasuhiro Igarashi, Yasushi Shibuta and Shigeo Maruyama

The University of Tokyo, Tokyo 113-8656, Japan
E-mail: maruyama@photon.t.u-tokyo.ac.jp

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ABSTRACT

Several heat transfer problems related to single-walled carbon nanotubes (SWNTs) are considered using molecular dynamics (MD) simulations. The Brenner potential (Brenner, 1990) with the simplified form (Yamaguchi and Maruyama, 1998) is employed as the potential function between carbon and carbon within a nanotube. MD simulations of thermal conductivity along a nanotube, isotope effect in longitudinal thermal conductivity, and thermal boundary resistance in a junction of nanotubes are reviewed. Then, the heat transfer from an SWNT to various surrounding materials is simulated by MD simulations. Heat transfers between nanotubes in a bundle of nanotubes and between a nanotube and water are considered. The heat transfer rate can be well expressed by the thermal conductance (or thermal boundary resistance) at the boundaries. The value of thermal conductance of various systems such as nanotube-junction, SWNT bundle and water-nanotubes are compared.

1. INTRODUCTION

With a strong motivation to characterize the thermal properties for ever-expanding application of single-walled carbon nanotubes (SWNTs), in this paper, the thermal properties and heat transfer issues are considered by means of molecular dynamics (MD) simulations.

Our preliminary results showed that thermal conductivity was strongly dependent on the nanotube length for realistic length scale for device applications (Maruyama, 2002; Maruyama, 2003). In addition to the thermal conductivity along a SWNT, heat transfer from a nanotube to the surrounding material is quite important for the practical applications using carbon nanotubes as electrical devices or composite materials. In this paper, in addition to a review of simulations of thermal conductivity, isotope effect, and thermal conductance of a junction, the heat transfer from an SWNT to various surrounding materials is simulated by MD simulations. Heat transfer between nanotubes in a bundle of nanotubes and between water and a nanotube are considered.

2. THERMAL CONDUCTIVITY OF SWNTs

In our previous reports (Maruyama and Choi, 2001; Maruyama, 2002; Maruyama, 2003), thermal conductivity was calculated from the measured temperature gradient and the heat flux obtained by the energy budgets of phantom molecules. Combined with the temperature gradient, the thermal conductivity λ can be calculated through the Fourier's equation. Although the thermal conductivity for a finite length nanotube was calculated to be lower than the previously reported result; 6600 W/mK at 300 K (Berber et al., 2000), the thermal conductivity is much higher than highly thermal-conductive metals. The dependence of the thermal conductivity on the nanotube length is summarized in Fig. 1. The thermal conductivity was diverging with the power-law of the nanotube length at least up to the 0.4 μm long nanotube for (5, 5). As the result resembles the one-dimensional model calculations of thermal conductivity (Lepri, 2000, Livi and Lepri, 2003) where the divergence of λ with the power of 0.35 or 0.4 is discussed, the one-dimensional feature of heat conduction seems to be possible with the real material: the small diameter carbon nanotube.

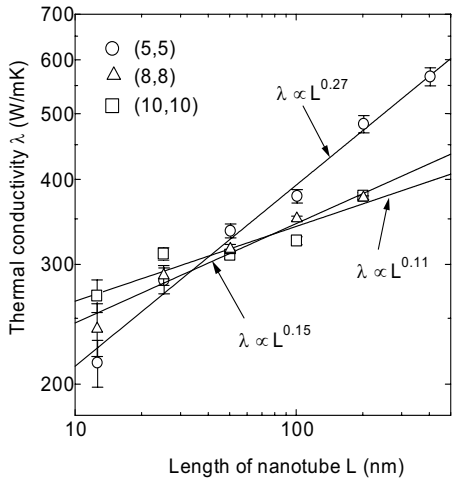

Fig. 1 Dependence of thermal conductivity on length of nanotubes for 300 K.

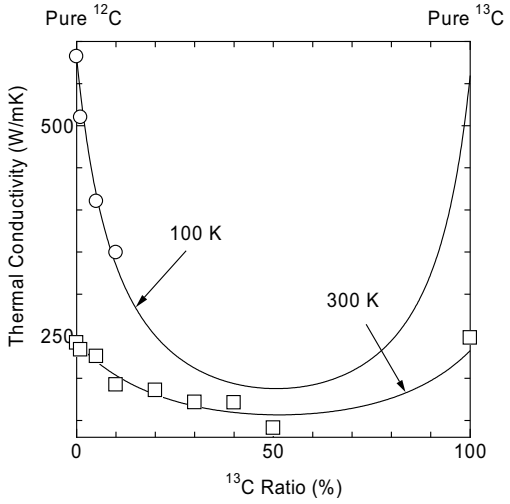

Fig. 2 Effect of ^{13}C isotope on thermal conductivity of SWNT

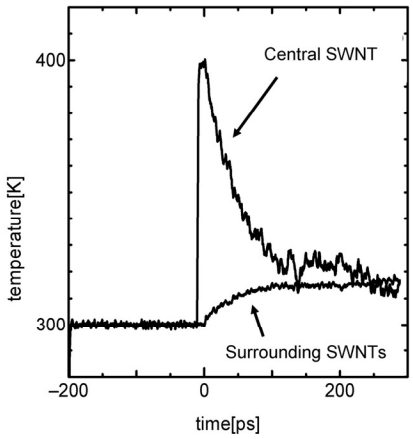

Fig. 3 Time history of the temperature difference.

3. EFFECT OF ISOTOPE FOR HEAT CONDUCTION.

Thermal conductivity of nanotube with randomly distributed ^{13}C with various ratios was calculated in our previous paper (Maruyama et al, 2003). A preliminary result is shown in Fig. 2. Here, (5, 5) nanotube with about 50 nm was tested. The dependence of thermal conductivity on isotope ratio was well explained with the following equation as the fit lines in Fig. 2.

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

where β is the ratio of ^{13}C, $\lambda_{pureC^{12}}$ is the thermal conductivity for pure ^{12}C, and C_1 is the fitting parameter. It is also noted that the thermal conductivity at 100 K is not realistic in Fig. 2 because the classical simulation cannot reproduce the correct change of heat capacity at low temperature. The mechanism of the decrease of thermal conductivity with isotopes should be further discussed.

4. THERMAL CONDUCTANCE OF AN SWNT BUNDLE

Now, we consider a 5 nm SWNT bundle, which consists of 7 armchair type (5, 5) SWNTs with the diameter of 0.693 nm. In addition to the Brenner potential between carbon atoms within an SWNT, van der Waals force between carbon atoms in different SWNTs was expressed as 12-6 Lennard-Jones potential.

After keeping the whole system at 300 K for 100 ps, the temperature of only the central SWNT was suddenly increased to 400 K using the velocity scaling method for a time period of 10 ps.

In order to examine the heat transfer, temperature difference of central and surrounding tubes is drawn in Fig. 3. The monotonic decay of temperature difference in Fig. 3 was well approximated by an exponential function. This encourages us to consider an SWNT as a solid material and express the heat transfer from the central tube to surrounding tubes by thermal conductance. Adopting the lumped capacity method since the characteristic length of an SWNT is extremely small, the thermal conductance was estimated.

5. THERMAL CONDUCTANCE AT SWNT-WATER BOUNDARY

Water molecules were expressed by SPC/E potential (Berendsen et al., 1987) The potential function between water molecules and carbon atoms are represented by Lennard-Jones function and the quadropole interaction term (Walther et al., 2001).

One (10, 10) SWNT with length 20.118 nm and 192 water molecules inside it were prepared in the 20.118×10×10 nm fully-periodic simulation cell. At the initial stage of simulation, water molecules and the SWNT were equilibrated at temperature of 300 K. Then, only the temperature of the SWNT was suddenly heated up to 400K. And all temperature control was stopped.

The temperature difference between SWNT and water exhibited the exponential decay in a similar manner to the previous case of SWNT bundle simulation. The thermal conductance is estimated using the lump method similarly to the previous case.

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Y. Igarashi received the B.E in 2003. He is currently a Matster's student in the University of Tokyo. His research topic includes molecular dynamics studies of heat transfer phenomena of carbon-nanotube systems.

Y. Shibuta received the B.E. (1998), M.E. (2001) and D.E. (2004) from the University of Tokyo. JSPS Research Fellow. His research topic includes the molecular dynamics studies of formation process of carbon nanotubes.

S. Maruyama received the B.E. (1983), M.E. (1985) and D.E. (1988) from the University of Tokyo. Associate Professor of Deparment of Mechanical Engineering, The University of Tokyo. His current interests include science and technology of carbon nanotubes, and molecular dynamics studies of nano-scale heat transfer.