MOLECULAR DYNAMICS SIMULATIONS OF HEAT TRANSFER OF CARBON NANOTUBES

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Several heat transfer problems related to single-walled carbon nanotubes (SWNTs) are considered using molecular dynamics (MD) simulations. The Brenner potential [1] with the simplified form [2] 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 employing the thermal boundary resistance (TBR). The value of thermal boundary resistance is compared for nanotube-junction, bundle, and water-nanotubes cases.

HEAT CONDUCTIVITY OF SWNTs

In our previous reports [3-6], 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 [7]), the thermal conductivity is much higher than highly thermal-conductive metals. The dependence of the thermal conductivity on the nanotube length [5] is summarized in Fig. 1. The thermal conductivity was diverging with the power-law of the nanotube length [4, 5] 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 [8, 9] 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.

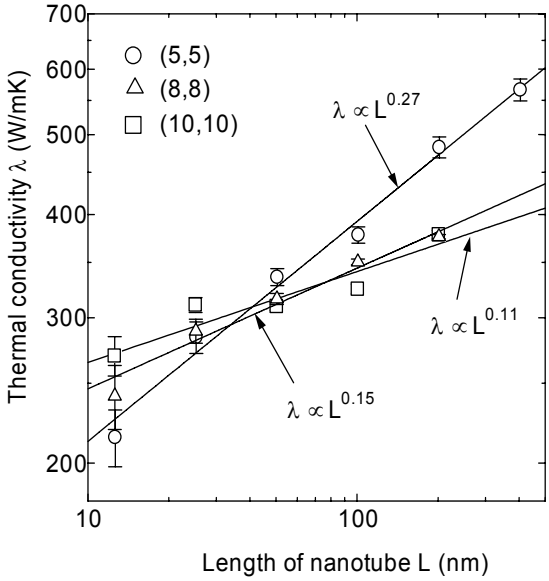

Fig. 1 Dependence of thermal conductivity on length of nanotubes for 300 K [5].

EFFECT OF ISOTOPE FOR HEAT CONDUCTION

Thermal conductivity of nanotube with randomly distributed ^{13}C with various ratios was calculated in our previous paper [6]. 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 [5]. The mechanism of the decrease of thermal conductivity with isotopes should be further discussed.

THERMAL BOUNDARY RESISTANCE OF A SWNT BUNDLE

Now, we consider a 5nm SWNT buddle, 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 300K for 100ps, the temperature of only the central SWNT was suddenly increased to 1000K using the velocity scaling method for a time period of 10ps.

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 heat transfer coefficient or thermal boundary resistance (inverse dimension of heat transfer coefficient). Adopting the lump method since the characteristic length of an SWNT is extremely small, the thermal boundary resistance was estimated.

One of the characteristics of heat transfer of SWNT is the strong anisotropy. By using the thermal resistance, axial and radial heat conductions are compared. The length of an SWNT, with which the thermal resistances in axial and radial directions are equal, can be the characteristic length of the thermal boundary resistance (L_{TBR}). Suppose using an SWNT as a promoter of heat conduction as a composite material, thermal boundary resistance determines the performance for a shorter nanotube than L_{TBR}.

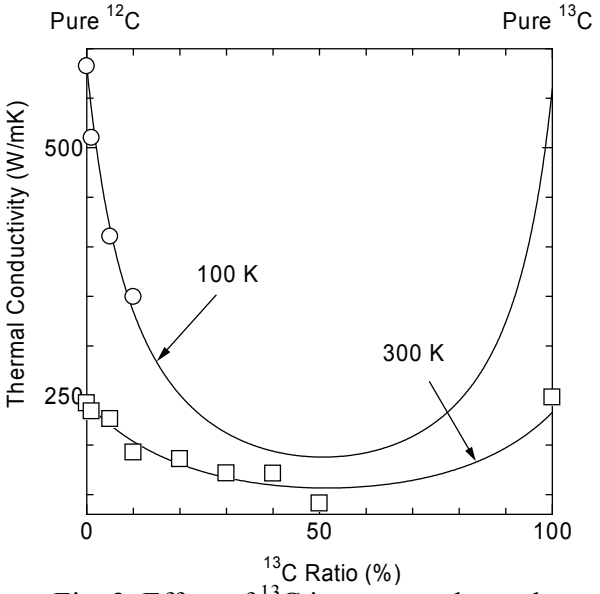

Fig. 2 Effect of ^{13}C isotope on thermal conductivity of SWNT [6].

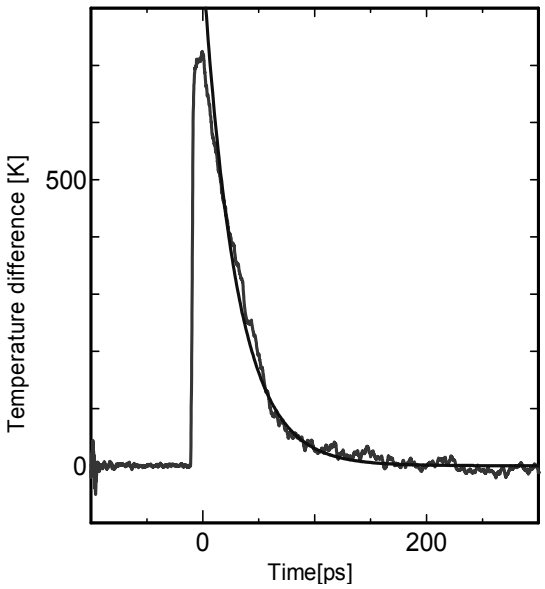

Fig. 3 Time history of the temperature difference.

THERMAL BOUNDARY RESISTANCE BETWEEN SWNT AND WATER

Water molecules were expressed by SPC/E potential [10]. The potential function between water molecules and carbon atoms are represented by Lennard-Jones function and the quadropole interaction term [11].

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 1000K. 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 boundary resistance is estimated using the lump method similarly to the previous case. The characteristic length of TBR between the SWNT and water molecules was also calculated.

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