Molecular Dynamics Simulation of Heat Transfer Issues of Nanotubes.

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Heat transfer between single-walled carbon nanotubes (SWNT) in a bundle was studied with the molecular dynamics method. The Brenner potential [1] with the simplified form [2] was employed as the potential function between carbon and carbon within a nanotube. The van der Waals force between carbon atoms in different SWNTs was expressed by Lennard Jones potential. Fig. 1 shows the initial condition with 7 SWNTs of 5 nm length. Initially, the whole system was kept at 300 K for 100 ps. Then, the temperature of only the central SWNT was suddenly increased to 1000 K using the velocity scaling method. Soon, all temperature control was stopped and temperature change of central and surrounding SWNT were observed.

Fig. 2 shows temperature change of central (hot) and surrounding (cold) tubes, whereas the temperature difference is shown in Fig. 3. The temperature difference is well approximated by an exponential function. Comparing this approximated function with the lump heat transfer method as in the following equation.

$$T_{hot} - T_{cold} = T_0 \exp\left(-\frac{t}{\tau}\right) = T_0 \exp\left(\frac{-St}{R\rho cV}\right)$$

The thermal boundary resistance R between SWNTs was estimated to be about 6.46×10^{-8} [m^2K/W]. The length to which axial thermal resistance and radial one become equal was defined as characteristic length of TBR, which was 0.105 μm. In other words, when the length of SWNT is 0.105 μm, the radial heat transfer is comparable to longitudinal heat conduction.

[1] D.W. Brenner, *Phys. Rev. B*, **42** (1990) 9458.
[2] Y. Yamaguchi, *Chem. Phys. Lett.*, **286** (1998), 336.

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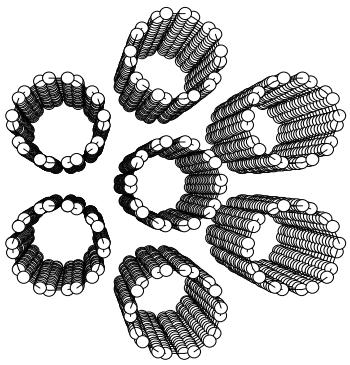

Fig. 1 Initial condition.
(5, 5) SWNTs (total 2800 atoms)

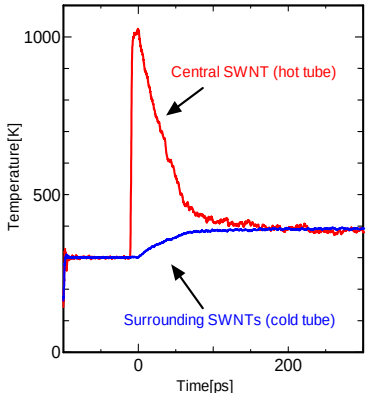

Fig. 2 Temperature change of central and surrounding tubes.

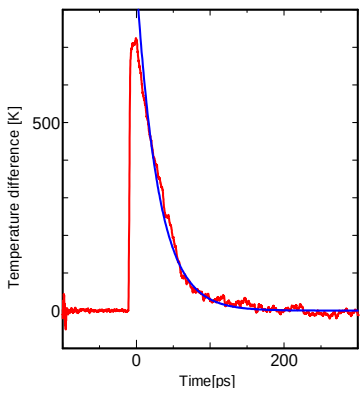

Fig. 3 The temperature difference and exponential fit.