Thermal conductance between an SWNT and Lennard-Jones fluid

○Yasuhiro Igarashi, Junichiro Shiomi and Shigeo Maruyama

Department of Mechanical Engineering, The University of Tokyo
7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

Thermal conductance between an SWNT and Lennard-Jones fluid is studied by classical molecular dynamics simulations. As the initial condition, a 5 nm length SWNT surround with Lennard-Jones molecules was placed in the simulation cell as shown in Fig. 1. The carbon-carbon interaction in the SWNT was expressed with Brenner potential [1] in the simplified form [2]. Lennard-Jones molecules were located randomly around the SWNT with the density set as 1.0~2000.0 [kg/m^3], from supercritical vapor to solid. At the first stage of simulation, system temperature was controlled to 300 K for 100ps. After that, the temperature of only SWNT was heated up to 600 K and all temperature control was stopped. Then, the temperature difference between the SWNT and Lennard-Jones fluid decayed exponentially. This decay of temperature difference was well expressed with the following equation.

$$T_{SWNT} - T_{LJ} = \left(T_{0\,SWNT} - T_{0\,LJ}\right)\exp\left\{-\left(\frac{1}{\rho_{SWNT}c_{SWNT}V_{SWNT}} + \frac{1}{\rho_{LJ}c_{LJ}V_{LJ}}\right)KSt\right\} \qquad (1)$$

Using this equation, the thermal conductance K was estimated to 0.01~10 [MW/m^{2}K] depending on the density of Lennard-Jones fluid. Fig. 2 shows the density dependence of thermal conductance. The thermal conductance was proportional to σ$^{0.8}$. This dependency was the same as for the case with doubled ε value of Lennard-Jones energy. Reason for this dependence may be explained by the thermal energy transferred by common vibration mode of an SWNT and Lennard-Jones fluid. Fig. 3 shows the vibration mode of SWNT in radial direction and Lennard-Jones molecules adhering the SWNT.

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

Corresponding Author: Shigeo Maruyama
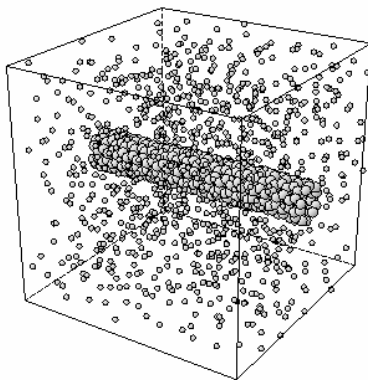E-mail: maruyama@photon.t.u-tokyo.ac.jp   Tel/Fax: +81-3-5800-6983

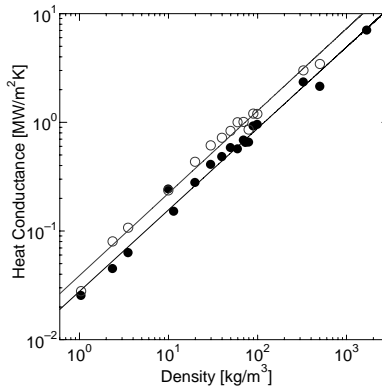Fig. 1 A snapshot of the simulation

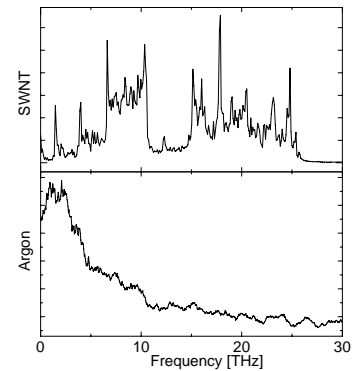Fig. 2 Density dependence of thermal conductance between SWNT and Lennard-Jones Fluid.

Fig. 3 Radial vibrational mode of SWNT and Lennard-Jones fluid near the SWNT.