

# Thermal Conductance between SWNT and Other Materials

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Thermal conductance between an SWNT and other materials were estimated from classical molecular dynamics simulations. Simulation systems are shown in Figures 1-3. In Figure 1, a bundle of SWNTs were simulated with the Brenner potential between bonding carbon atoms and Lennard-Jones potential between non-bonding carbon atoms. Initially, all SWNTs were kept at 300 K for 100 ps. Then, the temperature of the central SWNT was suddenly heated to various temperatures using velocity scaling method. After stopping all the temperature control, the temperature change of central and surrounding SWNTs were measured in the constant energy condition. The time history of the temperature difference was well approximated by an exponential function. This exponential decay was compared with the lump heat transfer equation as following:

$$T_{hot} - T_{cold} = T_0 \exp\left(-\frac{t}{\tau}\right) = T_0 \exp\left(\frac{-KS}{\rho c V} t\right),$$

where  $K$  [MW/m<sup>2</sup>K] was defined as the thermal conductance. Irrespective of the initial heating temperature, the thermal conductance was estimated to be about 10 MW/m<sup>2</sup>K.

Thermal conductance between an SWNT and water inside the nanotube can be calculated in the similar way with the simulation system shown in Figure 2. Furthermore, the thermal conductance between an SWNT and surrounding gas, liquid, and solid of Lennard-Jones fluid was calculated as in Figure 3. The systematic change of the Lennard-Jones potential parameter gave an insight on the physical mechanism of the thermal conductance.

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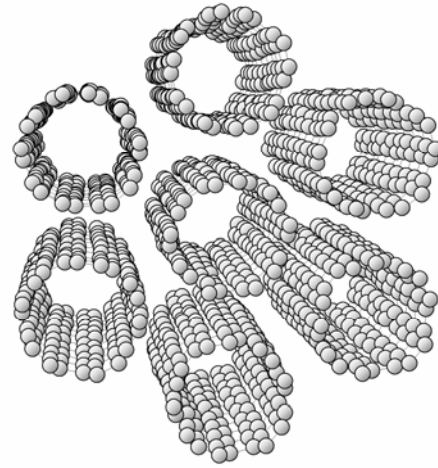


Figure 1 Simulation of a bundle of (5, 5) SWNTs (total 2800 atoms)

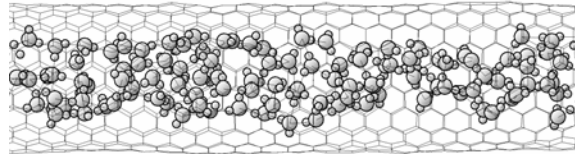


Figure 2 Simulation of water-SWNT system

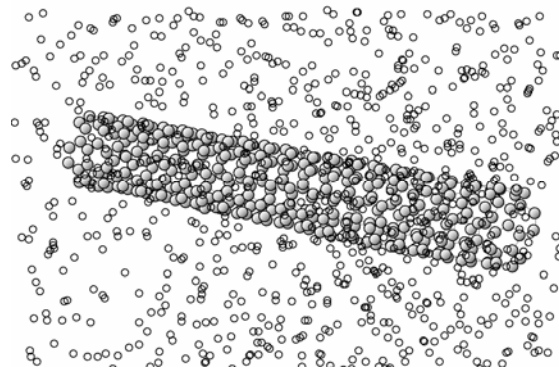


Figure 3 Simulation of an SWNT in Lennard-Jones fluid