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Abstract Proof**CONTROL ID:** 128269**CONTACT (NAME ONLY):** Shigeo Maruyama**Abstract Details****PRESENTATION TYPE:** Invited Speaker**SYMPOSIUM:** DD: Heat and Mass Transport at Nanoscale-From Fundamentals to Devices**KEYWORDS:** Single-Walled Carbon Nanotubes, Molecular Dynamics Simulation, Thermal Boundary Resistance.**Abstract****TITLE:**

Molecular Dynamics Simulation of Thermal Boundary Resistance between a Carbon Nanotube and Surrounding Materials.

AUTHORS (ALL): [Maruyama, Shigeo](#)¹.**INSTITUTIONS (ALL):** 1. Dept. of Mech. Eng., The University of Tokyo, Tokyo, Japan.**ABSTRACT BODY:**

Several kind of thermal boundary resistance 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. 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.

For the thermal boundary resistance between SWNTs in a bundle, 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. The decay of the temperature difference of central and surrounding tubes is well approximated with a single 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.

Then, the thermal boundary resistance between an SWNT and water was considered. 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 quadrupole 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 20.118x10x10 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. Finally, the thermal boundary resistance between a nanotube and Lennard-Jones fluids in different thermodynamics conditions was examined. The general mechanism of thermal boundary resistance is thought.

(No Table Selected)

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