MOLECULAR DYNAMICS SIMULATION OF THERMAL BOUNDARY CONDUCTANCE BETWEEN SWNT AND SURROUNDING FLUIDS

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Single-walled carbon nanotubes (SWNTs) are expected to be used in various electrical and thermal device applications. In particular, the thermal boundary conductance (TBC) K between an SWNT and surrounding fluid –the inverse of thermal boundary resistance (TBR)– is one of the most important characteristics for thermal managements of SWNTs in various fields[1-5]. The cooling rate of SWNTs in electronic and optical devices and the improvement of thermal conductivity of nanotube-based composite are virtually determined by TBC.

In this study, we investigated the TBC between an SWNT and different surrounding fluids over wide density and temperature ranges using molecular dynamics (MD) simulations (Fig. 1) and adopting the lumped heat capacity method. Our primary purpose here is to identify a general scaling law which enables the prediction of TBC for various surrounding fluids at various thermodynamic conditions. We found that the "adsorption layer" (ordered fluid layer) on the outer surface of the SWNT shown in Fig. 2 is critical for the discussion of TBC. Taking into account the nominal density ρ_L of this adsorption layer, the nonlinear dependence of TBC on dimensionless density ($\rho^*=\rho\sigma^3/m$) can be simply linearized. The nominal density of the adsorption layer (ρ_L) is obtained from the calculated radial distribution function as in Fig. 2.

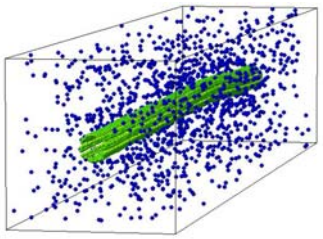

Fig. 1 Snapshot of a typical MD simulation of SWNT in argon fluid.

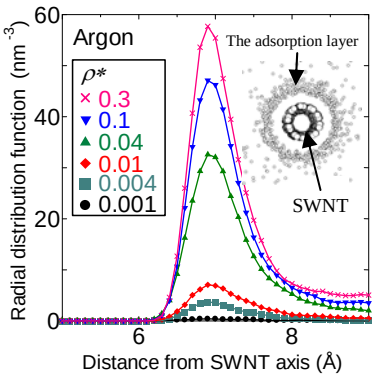

Fig. 2 Radial distribution functions of "adsorption layer" for various densities of fluid..

We also studied the TBC dependence on each parameter of the surrounding fluid, i.e., energy parameter ε, length parameter σ of LJ potential, and mass m. Here, we employed various hypothetical LJ fluid by modifying these parameters. Through these parametric studies, we obtained phenomenological description of TBC between an SWNT and a surrounding fluid as $K = 0.1\ \rho_L\,\varepsilon/m$. We verified the accuracy of this equation by comparing with values of the TBC obtained from MD simulations as in Figure 3. We will discuss the physics behind this simple model.

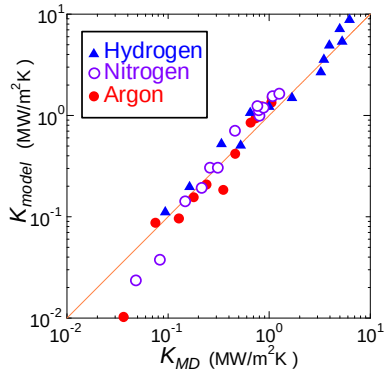

Fig. 3 Comparison the TBC obtained from MD simulation and by the model equation.

References:

[1] S. Maruyama, T. Kimura, *Therm. Sci. Eng.* **7** (1999) 63.
[2] S. T. Huxtable, *et al.*, *Nature Mater.* **2** (2003) 731.
[3] S. Maruyama *et al.*, *J. Therm. Sci. Tech.* **1** (2006) 138.
[4] M. Hu, *et al.*, *Appl. Phys. Lett.* **90** (2007) 231905.
[5] C. F. Carlborg, J. Shiomi, S. Maruyama, *Phys. Rev. B* **78** (2008) 205406.