Mechanism of thermal boundary conductance between SWNTs and surrounding materials

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Thermal boundary conductance (TBC) between SWNTs and surrounding materials is one of the crucial characteristics for various electrical and thermal devices applications. Although there have been many reported studies that experimentally and numerically investigated the TBC for specific systems [1,2], the mechanism of the interfacial energy transfer is far from being understood.

In this study, we investigate the TBC between an SWNT and the various surrounding materials in wide density and temperature ranges (Fig. 1). Our primary aim here is to identify the general scaling law that explains the TBC for various surrounding materials. Such a general law would be of practical importance to predict and design the interfacial thermal transport and also would serve to identify its mechanism.

We employed classical molecular dynamics (MD) simulations to investigate the TBC between a 25 nm long SWNT and a surrounding Lennard-Jones (LJ) medium, as shown in Fig. 1. Using the non-stationary approach, the TBC can be obtained adopting the lumped-heat-capacity method [3]. Figure 2 shows typical density dependence of the TBC for various interfaces, where the axes are nondimensionalized based on the bulk properties of the LJ medium. Different scalings will be tested to identify the general law and to investigate the mechanism of the interfacial energy transfer. Furthermore, the analysis will be extended to examine more complicated aspects such as influence of phase change of the medium and bundling of SWNTs.

References

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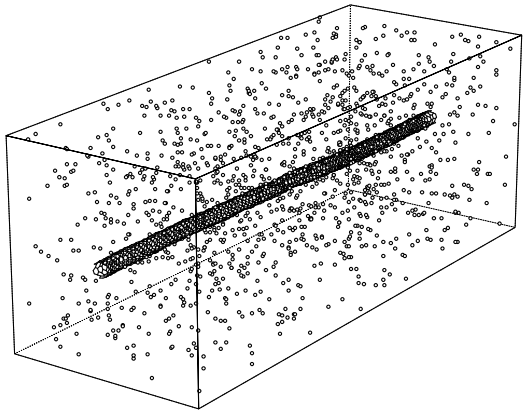

Fig. 1 Snapshot of the simulation.

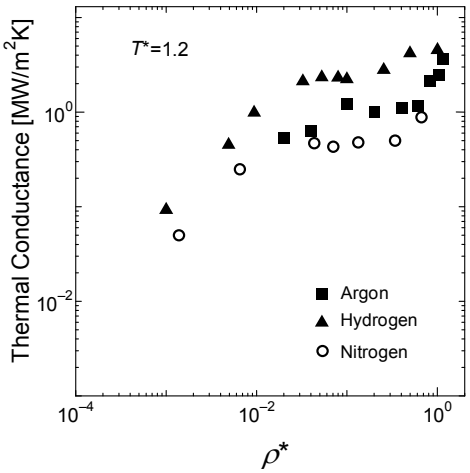

Fig. 2 Density dependence of TBC between SWNT and L-J molecules.