Molecular dynamics of low-dimensional heat and mass transport in carbon nanotube systems

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Single-walled carbon nanotubes (SWNTs) have caught much attention as materials realizing various low-dimensional transport properties with their quasi-one-dimensional structures. The confined dynamics gives rise to unique heat and mass transport that are beneficial for applications. The current study highlights the confined dynamics by means of classical molecular dynamics (MD) simulations.

The importance of probing SWNT heat conduction has attracted many recent researches in ideal environment, which have revealed remarkable heat conduction properties at low and high temperatures. While these properties encourage thermal and electric device applications of SWNTs, their sensitivities to the defect, impurity, and environment become key issues in practice [1]. In this study, following a demonstration of the diffusive-ballistic heat conduction of an ideal SWNT (Fig. 1) [2, 3], the sensitivity of the heat conduction to the environment will be discussed by modeling an SWNT surrounded by simple fluid.

Internal space of an SWNT can be thought as an ideal quasi-one-dimensional channel, a key system in bioscience, where thermofluid dynamics is severely restricted. Here, we firstly investigate the phase transition of a water cluster confined in an SWNT to an ice-nanotube. The transition temperature T_m and its diameter dependence obtained by the simulations (circles) agree well with those of experiments (squares) [4] (Fig. 2). T_m of ice-nanotubes was observed to take a maximum value of around room temperature with the number of the ice-ring members n=5 [5]. Secondly, we investigate transport of a water cluster through an SWNT under longitudinal temperature gradient. It is demonstrated that the water cluster is transported with an average acceleration proportional to the temperature gradient. On the other hand, the transport simulations with a junction of two different SWNTs suggest that an angstrom diameter difference may result in a significant drag for small diameter SWNTs (Fig. 3).

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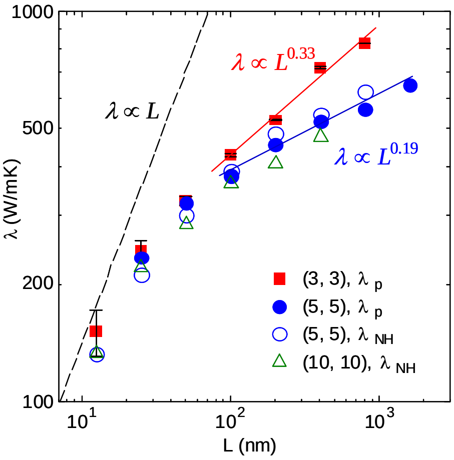

Fig. 1 Length and diameter effects of SWNT thermal conductivity.

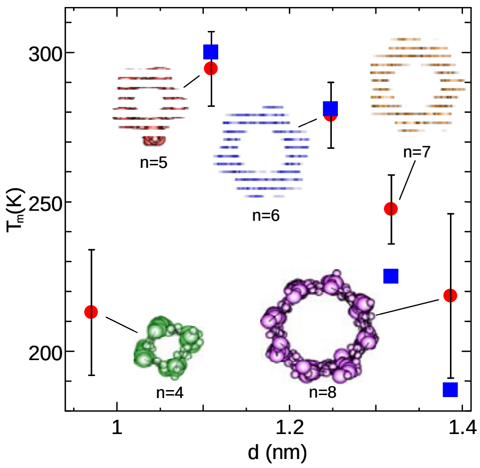

Fig. 2 Transition temperature of ice nanotubes formed inside SWNTs with various diameters.

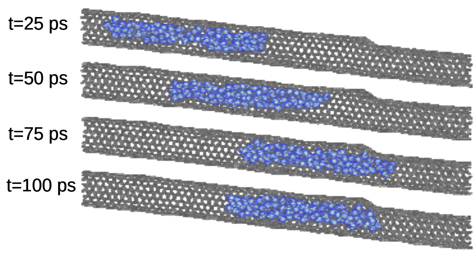

Fig. 3 Thermally driven water transport in an SWNT with a junction.