Abstract id: 470

Sorting Category: X. Thermal and mechanical properties

Low dimensional heat and mass transport in carbon nanotubes

Junichiro Shiomi, Shigeo Maruyama

1: Department of Mechanical Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, 113-8656, Japan

Keywords: Single-walled carbon nanotube, Thermal transport, Mass transport, Interface

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 molecular dynamics gives rise to unique heat and mass transports that are beneficial for applications. Here we introduce some of our recent works on the confined dynamics by means of molecular dynamics (MD) simulations.

Characterization of thermal properties of SWNTs is a key issue for their prospective electrical and thermal device applications. 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. The heat conduction exhibits complex diffusive-ballistic feature for realistic nanotube-length in many applications even at room temperature. As a consequence, unique steady and unsteady heat conduction characteristics manifest [1,2], which is particularly evident in the length effect of the thermal conductivity or conductance [3,4]. The possibility and trend of heat conduction divergence with respect to the tube length have been discussed in relation with the scattering dynamics of long wave phonons and the effect of low-dimensional confinement.

While these properties encourage the device applications of SWNTs, their sensitivity to the surrounding environment becomes a key issue in practice [5]. The question is how much of the ballistic heat conduction is preserved in a practical environment. In a system with significant contribution from ballistic heat transport, the intrinsic phonon distribution function and thus effective heat conduction is expected to depend strongly on the mode-dependent scattering dynamics at the interfaces [6]. The sensitivity of the diffusive-ballistic nature of the SWNT heat conduction to the environment has been investigated by modeling molecular dynamics of an SWNT surrounded by simple fluid. The MD simulations suggest that the heat conduction suffers significantly from the presence of the surrounding material. The surrounding fluid was found to selectively attenuate the transport of long range phonons, the main heat carriers of an SWNT.

As water intrusion into hydrophobic SWNTs has been demonstrated to be possible, possibilities of using SWNTs as molecular transporter and filters have been explored with a merit of realizing fast transport even in a nanoscale pore attributing to the exceptionally large slip-length at the hydrophobic and atomically smooth interface. In this course, we have investigated the 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 [7].

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Submited Date: 2009-4-20