The form of Abstract

Molecular dynamics simulations of diffusive-ballistic heat conduction in carbon nanotubes

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On considering device applications of single-walled carbon nanotubes (SWNTs), one of the primary tasks is to characterize their thermal properties not only for thermal devices but also for electrical devices since they determine the affordable amount of electrical current in the system. In this study, we have calculated SWNT heat conduction by using classical molecular dynamics (MD) simulations. The MD simulations serve to probe detailed heat conduction characteristics and to gain fundamental understanding of heat conduction in quasi-one-dimensional systems.

The phonon mean free path of an SWNT is expected to be extraordinary long due to the strong carbon bonds and quasi-one-dimensional confinement of phonons. As a consequence, the ballistic phonon transport regime stretches beyond the realistic length in many applications even at room temperature. Hence, phonon transport exhibits complex diffusive-ballistic feature, which gives rise to unique steady and unsteady heat conduction characteristics, such as non-Fourier heat conduction in a pulse heated SWNT [1] and minimum thermal conductivity in the SWNT isotope superlattice structures formed by periodically connecting ^{12}C-SWNT and ^{13}C-SWNT [2].

In this study, particular attention is paid on the length effect of the thermal conductivity (or thermal conductance) due to its practical importance [3, 4]. By using non-equilibrium MD simulations, we have calculated the thermal conductivity at room temperature and characterized a gradual transition from nearly pure ballistic phonon transport to diffusive-ballistic phonon transport [4]. It is shown that the thermal conductivity does not converge in the range of nanotube lengths examined in the current work (L<1.6 μm). In addition, in the long nanotube regime (L>100 nm), the power-law length dependence was observed. The trend will be discussed in connection with the scattering dynamics of long wave phonons and the effect of low-dimensional confinement.

In addition to the above studies on isolated SWNTs, we have recently investigated heat conduction of an SWNT in contact with surrounding materials, which is of a great importance in practical situations [5]. The primary results from equilibrium MD simulations suggest a strong influence of the surrounding materials on the transport of long wave phonons. The mode-dependent phonon boundary scattering will be discussed by investigating the heat flux correlations.

[1]. J. Shiomi and S. Maruyama, *Phys. Rev. B*, **73**, 205420 (2006). [2]. J. Shiomi and S. Maruyama, *Phys. Rev. B*. **74**, 155401 (2006). [3]. S. Maruyama, *Micro. Thermphys. Eng.* **7,** 41 (2003). [4]. J. Shiomi and S. Maruyama, *Jpn. J. Appl. Phys*. (in press). [5] S. Maruyama, *etal*., *J. Therm. Sci. Tech.* **1**, 138 (2006).

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