Diffusive-Ballistic Heat Conduction in a Single-Walled Carbon Nanotube System

Shigeo Maruyama

Department of Mechanical Engineering, The University of Tokyo
7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan
E-mail address: maruyama@photon.t.u-tokyo.ac.jp

The extremely high and peculiar thermal conductivity of single-walled carbon nanotubes (SWNTs) is explored mainly by non-equilibrium molecular dynamics simulation approach. The diffusive-ballistic nature of heat conduction in finite-length single-walled carbon nanotubes is discussed. The length dependence of thermal conductivity [1] is quantified for a range of nanotube lengths up to 1.6 μm at room temperature. A gradual transition from nearly pure ballistic to diffusive-ballistic heat conduction was identified from the thermal conductivity profile. In the diffusive-ballistic regime, the profile exhibits power-law length dependence and does not converge even for a tube length of 1.6 μm [2]. The diffusive-ballistic phonon transport regime covers a wide range of nanotube-lengths in actual applications due to the extraordinary long phonon mean free path at room temperature. Here, the total thermal resistance between high-temperature thermal bath and low-temperature bath are separated into the diffusive thermal resistance of nanotube and two thermal boundary resistances between thermal baths and nanotube. The inevitable latter resistance may be explained by the Landauer energy flux determined by the difference in phonon density of states in thermal bath and nanotube. This gives rise to various unique stationary and non-stationary heat conduction characteristics [3,4]. Furthermore, several issues of heat transfer in practical situations are studied by molecular dynamics simulations [5].

References

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