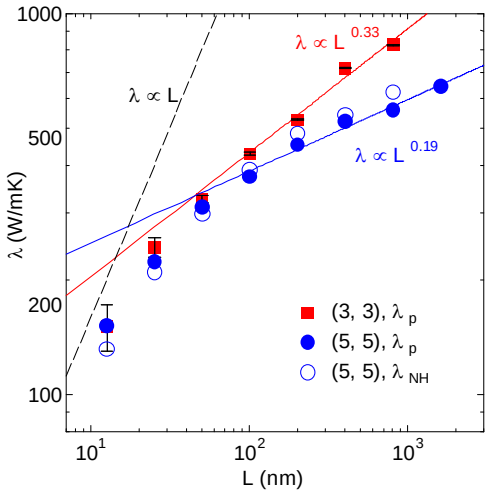
単層カーボンナノチューブの拡散・弾道熱伝導の分子動力学

Molecular Dynamics of Diffusive-Ballistic Heat Conduction in Single-Walled Carbon Nanotubes

東大院工　○塩見 淳一郎，丸山 茂夫
The University of Tokyo, Junichiro Shiomi, Shigeo Maruyama
E-mail: shiomi@photon.t.u-tokyo.ac.jp

Identification of heat conduction characteristics of single-walled carbon nanotubes (SWNTs) is one of the primary issues towards their thermal and electric device applications. In this study, diffusive-ballistic heat conduction of finite-length single-walled carbon nanotubes has been studied by means of non-equilibrium molecular dynamics simulations.[1] The length-dependence of thermal conductivity is quantified for a range of nanotube-lengths up to a micrometer 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 with the tube-length of a micrometer. Furthermore, the diameter dependence of thermal conductivity suggests considerable suppression of phonon scattering effect as the diameter decreases. The mechanism of the length and diameter dependcences will be discussed in terms of scattering dynamics of long wave phonons.

[1] J. Shiomi and S. Maruyama, Jpn. J. Appl. Phys. (in press)



Length and diameter effects on SWNT thermal conductivity.