# Influence of surrounding materials on heat conduction of carbon nanotubes: Molecular dynamics simulations

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Characterization of thermal properties of single-walled carbon nanotubes (SWNTs) is a key issue for their prospective electrical and thermal device applications. An SWNT is expected to be a good heat conductor with the extraordinary long phonon mean free paths [1-3]. As a result, phonon transport exhibits complex diffusive-ballistic feature for realistic nanotube-length in many applications even at room temperature. This gives rise to unique steady and unsteady heat conduction characteristics [4-8]. Especially, the length effect of the thermal conductivity or conductance [4,5,8] has caught particular attentions due to its practical importance and there are ongoing discussions on the scattering dynamics of long wave phonons and the effect of low-dimensional confinement.

Although the characteristics of intrinsic heat conduction of SWNTs have been explored extensively for ideal thermal boundary conditions, in practical situations, interfacial heat transfer between SWNTs and heat sinks/sources is expected to determine the overall heat transfer performance. Such interfaces not only give rise to thermal boundary resistances but also influence the intrinsic heat conduction. 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. In the current study, this aspect is explored by using equilibrium and non-equilibrium molecular dynamics methods. The boundary scattering and its influence on the long wave heat flux correlations is discussed.

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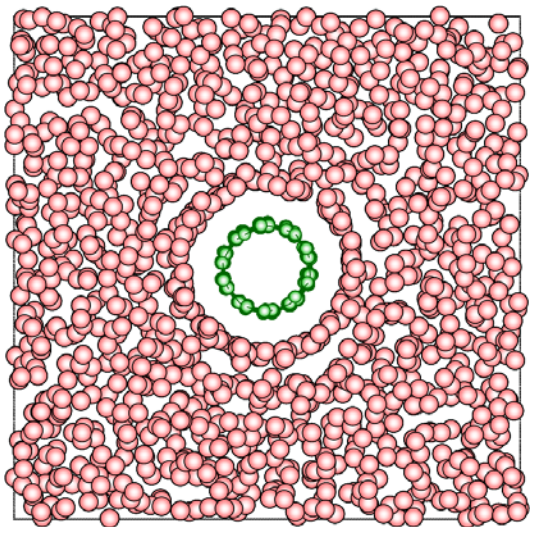

Figure 1. (5, 5) SWNT surrounded by matrix