

Influence of interfaces on diffusive-ballistic heat conduction of carbon nanotubes

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Characterization of thermal properties of single-walled carbon nanotubes (SWNTs) is one of the key issues 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. This gives rise to significant ballistic phonon transport for realistic nanotube length in many applications even at room temperature. 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 ballistic heat transport, the intrinsic phonon distribution function and thus effective heat conduction is expected to depend strongly on the mode-dependent phonon transmission and scattering dynamics at the interfaces. In the current study, this aspect is explored by using equilibrium and non-equilibrium molecular dynamics methods. Heat conduction of SWNTs in contact with other materials is calculated for various geometries; an SWNT bridging a heat source and a sink with realistic interfaces, an SWNT surrounded by and confining other materials.