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Anisotropic heat transfer of carbon nanotubes: Non-Fourier heat conduction and thermal boundary resistance with surrounding materials

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Characterization of thermal properties of carbon nanotubes is one of the primary issues towards their device applications. The current work aims to provide various anisotropic thermal properties of single walled carbon nanotubes (SWNTs) by means of non-equilibrium molecular dynamics. Firstly, Non-Fourier heat conduction is investigated by applying local heat pulse with duration of sub-picoseconds to SWNTs. Prominent heat waves originated from the radial breathing mode are identified with certain relaxation time. Secondly, thermal boundary resistance between an SWNT and surrounding Lennard-Jones (LJ) materials is considered. The entire SWNT was subjected to a heat pulse to observe the interfacial heat transfer. The resulting trend of thermal resistance suggests that the key physics for heat transfer depends on the phase of the LJ material. For the gas phase, heat transfer is diffusive where random molecular collisions are in charge. On the other hand, in the solid phase, the d ominant part of heat transfer can be attributed to certain modal interactions which can be modeled by the convolution of lattice vibrations of the nanotube and the LJ matrix. Finally, anisotropy of SWNT heat transfer is characterized by comparing the thermal boundary resistance (conductance) with axial conductivity under influence of surrounding matrix and bundles.