MOLECULAR DYNAMICS SIMULATION OF QUASI-BALLISTIC HEAT CONDUCTION IN CARBON NANOTUBES

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In device applications of carbon nanotubes, characterization of the heat transfer is essential. While experimental attempts to characterize heat conduction of carbon nanotubes encounter technical difficulties, the classical molecular dynamics (MD) simulations hold an advantage as the heat conduction is phonon-dominated. Single-walled carbon nanotubes (SWNTs) are expected to possess high thermal conductivity. Furthermore, the effective thermal conductivity exhibits size effects in the realistic length scale. This suggests a significant contribution of ballistic phonon transport in the actual scale of the applications. The ballistic aspect of phonon transport can also be observed by forming an isotope superlattice by periodically connecting ^{12}C-SWNT and ^{13}C-SWNT. The critical period thickness that minimizes the effective thermal conductivity reflects the length scale of phonon tunnelling.

In order to investigate the phonon propagation, we have performed non-stationary MD simulations, where a heat pulse is generated as coherent fluctuations by connecting the local cell to a thermostat for duration of the order of a picosecond. Consequently, the spatio-temporal evolution of energy field exhibits non-Fourier heat conduction, where the dominant energy is transported in the form of waves. By performing wavelet transformations, the energy flux can be assigned to different phonon bands. Diffusive or ballistic feature of the phonons is wavelength dependent. On paying particular attention to relatively short-wavelength phonon bands, with an aim to extend the analysis to probe the intrinsic thermal resistance, the intensity of each phonon band decays exponentially and can be characterized with the relaxation time and the group velocity. The relaxation characteristics of short wavelength phonons are strongly influence by the anharmonic effects. This aspect was examined by altering the bulk temperature.

The analysis methodology described above can be used to study phonon dynamics of thermal boundary resistance at a heterojunction of different isotope SWNTs, where phonons with the wavelength of the order of the atomic scale roughness are expected to play an important role. On calculating the thermal boundary resistance, the key property is the transmission probability. The transmission probability can be probed by passing the above mentioned heat pulse through the junction. The results were compared with the conventional transmission models.

The phonon probing technique is also useful when analysing non-localized sources of thermal resistance. Here, we demonstrate the computation of phonon relaxation and its alternation due to the interaction between SWNTs and surrounding materials. Investigation of the attenuation of SWNT heat conduction due to surrounding materials is of a prior importance in practical applications. For example, as SWNTs form a bundle in many cases, the influence of the inter-tube interaction on the heat conduction is of an interest. In addition, we consider an SWNT confining an ice-tube with finite length and, as a general case of interactions with surrounding materials, an SWNT surrounded by matrix of Lennard-Jones molecules.