Thermal boundary resistance at an SWNT hetero junction

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Single-walled carbon nanotubes (SWNTs) are expected to possess high thermal conductivity. While experimental attempts to characterize thermal conduction of SWNT encounter technical difficulties, the classical molecular dynamics simulations hold advantage as the heat conduction is phonon-dominated. The heat conduction can be altered by local thermal resistance due to defects, hetero-junctions and isotope impurities. By using non-equilibrium molecular dynamics, we have previously demonstrated that the hetero-junction of different isotopes or chirality can cause the thermal boundary (Kapitza) resistance (TBR) even with combination of tubes with similar mass or diameter. As an extensional study, we have recently simulated isotope superlattices i.e., periodically connected ^{12}C-SWNT and ^{13}C-SWNT, and investigated the dependence of thermal conductivity on the period thickness. Present report aims to study TBR at SWNT hetero-junctions in terms of phonon scattering dynamics. As the SWNT has the quasi-one dimensional structure with absence of phonon scattering at wall boundary and with the junction roughness confined in an atomic monolayer, the dynamics of TBR should be simpler than those for 3 dimensional cases. Here, we focus on relatively short-wavelength phonons which are expected to play an important role in the local events at the junctions.

In order to investigate the propagation of the short-wavelength phonons, we perform non-stationary molecular dynamics simulations with pure ^{12}C-SWNTs, where the heat pulse is generated as coherent fluctuations by connecting the local cell to a thermostat. Resulting spatio-temporal evolution of energy field (Fig. 1) exhibits non-Fourier heat conduction. The dominant energy is transported in the form of heat waves. There are two major energy streaks which propagate with different group velocity. By performing wavelet transformation, both energy streaks can be assigned to different radial phonon bands. Intensity of each phonon band decays exponentially hence the heat waves can be characterized with the relaxation time and the group velocity. These values showed minute variation with respect to temperature of the heat pulse. With these effective properties, together with the known heat capacity, the contribution of the short-wavelength phonon to the heat conduction can be described.

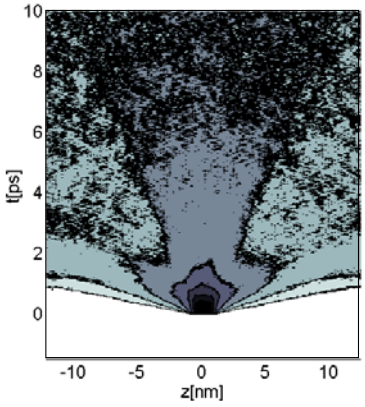

Fig. 1 Spatio-temporal contours of isotherms. The heat pulse is applied at (z,t)=(0,0)

On calculating the thermal boundary resistance in terms of phonons, the key property would be the phonon transmission coefficient. The transmission coefficient can be probed by passing the above mentioned heat pulse through a junction. Here, our intension of applying a heat wave instead of certain selected phonon mode is to take unharmonic effects into account. The result will be compared with the value of TBR obtained by stationary non-equilibrium molecular dynamics simulations and will be discussed together with the conventional transmission models.

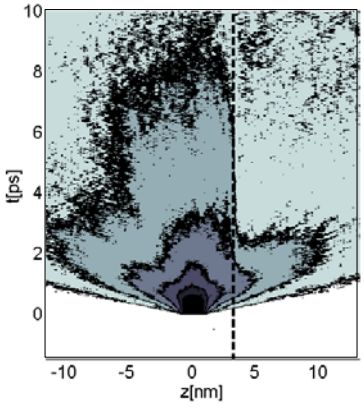

Fig. 2 Spatio-temporal contours of isotherms. Dotted line indicates the junction between ^{12}C-SWNT (left) and ^{13}C-SWNT (right).