Thermal conductivity of single-walled carbon nanotubes with isotopes

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Single walled carbon nanotubes (SWNTs) may have defects, impurities and junctions, which may limit the expected high thermal conductivity (k). These nano-scale defective structures, having scales of the order of the phonon mean free path, are expected to have strong influence on thermal properties of the bulk material. In this study, we investigate the influence on k in terms of the scattering of phonons at the structure interfaces.

Molecular dynamics simulations were performed to investigate the heat conduction of (5,5)-SWNT by visualizing the spatio-temporal behavior of the phonons. The Brenner potential with the simplified form was employed as the potential function between carbon and carbon within a nanotube. The defective nano-structures were represented by mixing ^{13}C isotopes to a ^{12}C-SWNT. Following our previous studies where the random mixing of ^{13}C isotopes to ^{12}C SWNT was shown to results in the decrease of k, in the current study, the influence of axial scales of the defects were investigated by mixing ^{13}C in order. Here, SWNTs consist of cells of ^{12}C and ^{13}C periodically connected with certain interval thickness.

By shortening the interval length from about 10 nm, k was observed to decrease with the interval thickness (Fig. 1). The phonon scattering increases with the number of intervals per unit length. By decreasing the interval thickness further, we find the critical interval thickness (~ 2 nm) bellow which k increases against the thickness. The spectral analyses (Fig. 2) reveal that, below the critical interval thickness, the system behaves not as connections of cells with individual dispersion relations, but of rather as a diatomic crystal with continuous spectra in the axial direction. When the system is at equilibrium, k can be well computed through the Fourier's law. Non-Fourier aspects of the heat transfer in the non-equilibrium SWNTs are also examined.

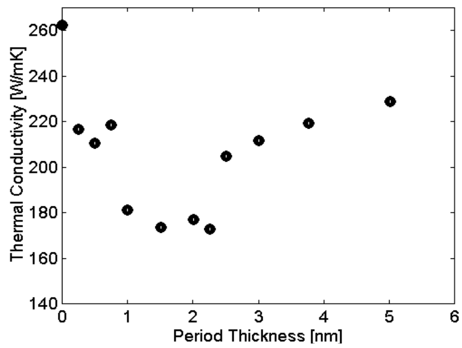

Fig. 1. The thermal conductivity for various interval thickness of the ^{12}C-^{13}C isotope carbon nanotubes.

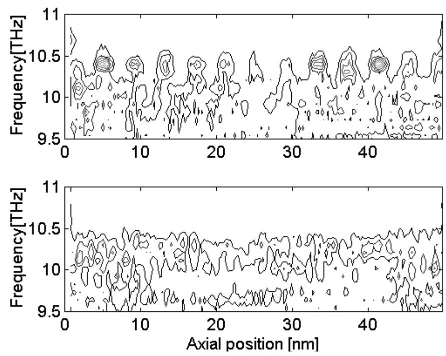

Fig. 2. Contour plots of radial velocity power spectral bands corresponding to the radial breathing modes, with interval thickness of 2 (top) and 0.8 nm (bottom).

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