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Abstract

TITLE:
Thermal conductivity of single-walled carbon nanotubes with carbon 13 isotopes and with junctions.

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ABSTRACT BODY:
The theoretically high thermal conductivity (k) of single walled carbon nanotubes (SWNTs) plays a key role in the many of the prospective industrial applications. In the actual applications, SWNTs may have defects, impurities and junctions, which may limit the values of 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. The decrease of k is considered to result from the scattering of phonons at structure interfaces, when the operated temperature is below the Debye temperature.

In the current study, molecular dynamics simulations were performed to investigate the nano-scale axial heat conduction of (5,5)-SWNT by visualizing the spatio-temporal behavior of phonons. The carbon interactions in an SWNT were expressed by the Brenner potential. The defective nano-structures were represented by mixing C13 isotopes to a C12-SWNT either at random or in order. 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 in the latter part of the present study.

The random mixing of C13 isotopes to C12-SWNTs results in the decrease of k. The results show not only that k decreases against the fraction of mixed C13, but also that the value of k is dependent on the structure of C13 clusters, seemingly on their sizes. However, the random nature of the study leaves us with uncertainties of the size dependence.

In order to highlight the influence of axial scales of the defects, another set of simulations were performed by mixing C13 in order. In this case, SWNTs consist of C12 and C13 periodically connected with certain interval thickness. By shortening the interval length from about 10 nm, k was observed to decrease with the interval thickness. Consistently to the experiment reported by Huxtable for Si/SiGe super-lattices, the phonon scattering increased with the number of intervals per unit length. The simulation allowed us to decrease the interval thickness further which resulted in finding the critical interval thickness (2 nm) below which k begins to increase. The spectral analysis reveals that, below the critical interval thickness, the system behaves not as connections of cells with individual dispersion

relations, but rather as a diatomic crystal with continuous spectra in axial direction.

When nano timescale heat transport phenomena in SWNT system take place, since the timescale becomes comparable to the relaxation time of the heat flow, Fourier's assumption should not hold any more. The non-Fourier aspect of the heat transfer in SWNTs was examined by applying a local heat pulse with duration ranging from 40 fs to 4 ps. The results of the simulations exhibit the heat waves of selected phonons traveling from the heated end of the SWNT to the other. The characteristic properties of the heat flow will be discussed.

(No Table Selected)