Molecular dynamics of phonon relaxation of an SWNT

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SWNT is expected to have large thermal conductivity, therefore suggested for thermal devices. This has motivated extensive researches on thermal conductivity of SWNT using both experimental and numerical methods [1,2].

Generally, heat conduction of an SWNT strongly depends on the transport of acoustic phonons: LA, TA and TW. The aim of this research is to estimate the contribution of each acoustic phonon mode to heat conduction. The contribution of each acoustic phonon mode to heat conduction was quantified by exciting the mode and then monitoring the phonon relaxation process. The energy of a phonon mode is extracted by calculating the phonon energy spectra. Figures 1-2 demonstrate the case when a LA phonon mode is excited. Here, the spectra are calculated by taking two-dimensional Fourier transfer of atom velocity in the axial direction of SWNT. The dependence of the relaxation on the phonon branch, wave number, temperature of SWNT, kinetic energy of excited phonon and tube length will be discussed.

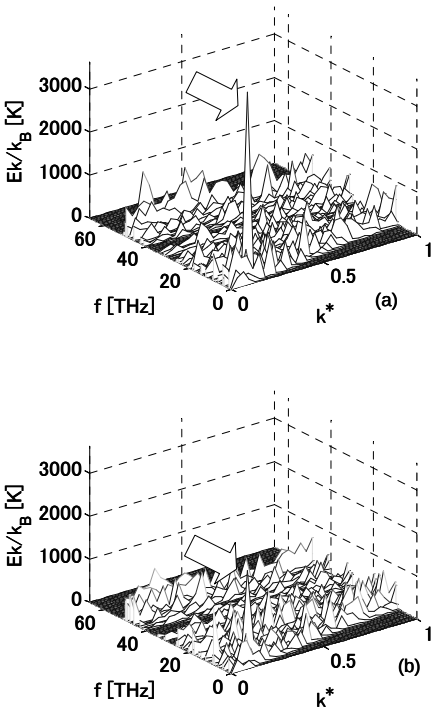

Fig.1 Excited phonon energy spectrum E_k (f, k^*) of an SWNT at (a) t=0.0 and (b) t=0.21 ns.

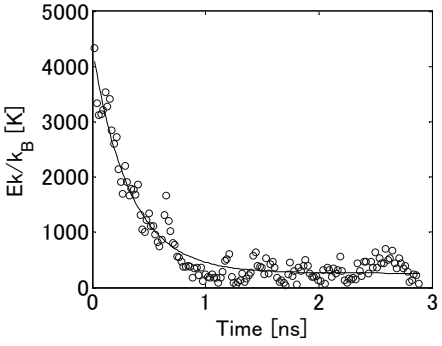

Fig. 2 Relaxation of excited LA phonon. The fitting line is denoted in solid.

[1]. C. Yu et.al., Nano Lett. 5,. (2005) 1842.

[2]. Maruyama, Physica B, 323 (2002)193.

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