

Influence of temperature on a carbon nanotube resonator by molecular dynamics simulations

Heeyuen KOH, James CANNON, Shigeo MARUYAMA, and Junichiro SHIOMI

Department of Mechanical Engineering

The University of Tokyo

7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656

JAPAN

Abstract

Phonon related multi-scale problems are very challenging but worthy of study to predict the thermal characteristics of nanomaterial composites on the continuum scale. For this reason, we have studied the interaction between mechanical and thermal characteristics in a carbon nanotube resonator by observing the phase space trajectories, strain-stress distributions, and lattice vibrational spectra. The calculation was based on molecular dynamics simulations using the REBO potential, where a carbon nanotube was excited by sinusoidal mechanical forcing at a tube end with constant-temperature boundary condition. The result confirms that the localized strain distribution is in agreement with previous high-resolution transmission electron microscopy results [1]. Particularly notable is the excitation near the 1st mode of resonance frequency which shows transient vibration with the beating frequency. Based on the simulations, the dynamic Young's modulus and the damping coefficient will be extracted in the frequency domain for different nanotube length and chirality, and will be compared with the continuum theories. In addition, by carrying out the calculations for various temperatures, the interaction between the first resonance mode and the background phonons will be discussed based on the obtained dissipated thermal energy and the phonon energy spectra.

[1] J. H. Warner et al., Resolving strain in carbon nanotubes at the atomic level, *Nature materials*, 2011.