Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Influence of temperature and adsorbates on a carbon nanotube resonator by molecular dynamics simulations HEEYUEN KOH, JAMES CANNON, SHIGEO MARUYAMA, JUNICHIRO SHIOMI, the University of Tokyo — The bending modes of carbon nanotube have been studied for ultralow mass and force sensing and its tunable resonance frequency. On the other hand, the nonlinear damping of flexural mode has been shown to be vulnerable to temperature and adsorbates. For this reason, we have studied the interaction between mechanical and thermal characteristics in a carbon nanotube cantilever resonator observing the phase space trajectories, strain-stress distributions, and lattice vibrational spectra for various temperatures and adsorbate conditions. 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 result. 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, 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.

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Date submitted: 15 Dec 2011 Electronic form version 1.4