Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Phonon-fluid coupling and energy dissipation in single-walled carbon nanotubes SUBHADEEP DE, NARAYANA ALURU, University of Illinois, Urbana Champaign — We elucidate the role of phonons, fluid and phonon-fluid coupling in the dissipation of high frequency carbon nanotube (CNT) resonators using molecular dynamics (MD) simulation. To investigate the dissipation mechanisms, we consider different simulation setups consisting of a single-walled CNT and confined argon. First, we consider a flexible CNT in vacuum and show that the intrinsic dissipation due to phonons is governed by the Akhiezer theory. The parameters for the Akhiezer model - phonon relaxation times and the Grneisen parameter are computed using Quasi-harmonic methods. Next, we introduce a new formulation for viscous dissipation due to the fluid in terms of a force-response function using Linear response theory. The developed relation is validated for a rigid CNT (no phonons) with confined argon. Finally, we consider a flexible CNT with confined argon and incorporate the effect of phonon-fluid coupling on the Akhiezer model parameters and force-response function to explain the net dissipation. We observe reduction of the overall dissipation with increase in fluid density at low excitation frequencies. This counter-intuitive behavior is shown to be a direct consequence of phonon-fluid coupling.

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Date submitted: 11 Nov 2016 Electronic form version 1.4