Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Understanding Heat Dissipation in Carbon Nanotube Resonators: New Insights from Molecular Dynamics Simulation RAJAMANI RAGHUNATHAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, P. ALEX GREANEY, School of Mechanical, Industrial and Manufacturing Engineering Oregon State University, Corvallis, OR 97331, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139 — Dissipation in carbon nanotube (CNT) resonators under conditions of steady state continuous driving has been simulated within classical molecular dynamics (MD) making use of a newly developed "Phonostat" algorithm. A previous study on heat flow in CNT resonators using MD simulation showed an anomalous heat dissipation and gateway kind of behavior was proposed. Here, we focus on characterizing the "gateway" modes and identify the pathways of heat dissipation by clamping such modes using our phonostat algorithm. In this present study we see three or four different sets of heat flow behavior when different sets of gateway modes are clamped as against a single heat flow behavior presented in the previous study. Our new results are explained in terms of filling of different subsets of phonon modes and the magnitude of friction between them. Our simulation results show that controlling these gateway modes is the key to improve the quality factor (Q) of CNT resonators for sensing applications, which has been a major challenge till now.

Rajamani Raghunathan
Department of Materials Science and Engineering,
Massachusetts Institute of Technology, Cambridge, MA 02139

Date submitted: 28 Dec 2011 Electronic form version 1.4