PHONON SCATTERING DYNAMICS OF SLIDING MOTION IN CARBON NANOTUBE OSCILLATORS

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ABSTRACT

Nanomechanical devices often involve sliding atomic surfaces with complex interface dynamics. The interface phenomena can be understood in terms of the interplay between low-frequency mechanical motions and high-frequency vibrational modes of sliding surfaces. The focus of this thesis is to develop a phonon dynamics based understanding of how structure and dynamics of sliding atomic surfaces affect energy dissipation and how phononically-driven motion may be generated and controlled in nanomechanical devices. Co-axially sliding carbon nanotube (CNT) oscillators are studied using phonon wave packet molecular dynamics simulations. Single-mode phonon wave packets are prepared using computed phonon dispersion relations and are allowed to propagate through the outer CNT to analyze the interaction mechanism with the inner CNT.

Anomalous longitudinal acoustic phonon scattering in low to moderate energy ranges is found to be responsible for initiating thermophoretic motion in CNT-oscillators. The repeated scattering of a train of single-mode longitudinal acoustic phonon wave packet near the ends of inner nanotube provides a net unbalanced force that, if large enough, initiates thermophoresis. The thermodiffusion coefficients obtained for a range of thermal gradients and core lengths suggest that longitudinal acoustic phonon scattering is the dominant mechanism for thermophoresis in longer cores while for shorter cores it is the highly diffusive mechanism that provides the effective force.

Further, the phonon mode contributions in frictional dissipation dynamics in co-axially sliding CNTs are investigated. The radial breathing mode and twisting acoustic modes displayed ideal transmission throughout the spectrum and could be the major reason for ultra-low friction in relative sliding of CNTs. Three other modes—longitudinal acoustic, transverse acoustic and first-order flexural optic mode—are responsible for major part of the dissipation in CNT-oscillators. Phonon transmission functions of these dissipative modes display a significant dip in the rather narrow frequency range of 5-15 meV. The distinct dissipation mechanism of each mode resulted in a strong geometry dependence of interfacial phonon scattering.

Finally, sliding velocity dependent frictional dissipation is investigated. Coherent phonon generation of radial breathing mode, which occurs at particular sliding velocities (800-875 m/s), is found to be the origin of enhanced phononic dissipation.

Keywords: Nanomechanical devices; Phonons in carbon nanotubes; Vibrational energy transfer; Atomic scale friction; Vibrations at solid surfaces and interfaces