Theoretical nanomechanics: From cells to solids

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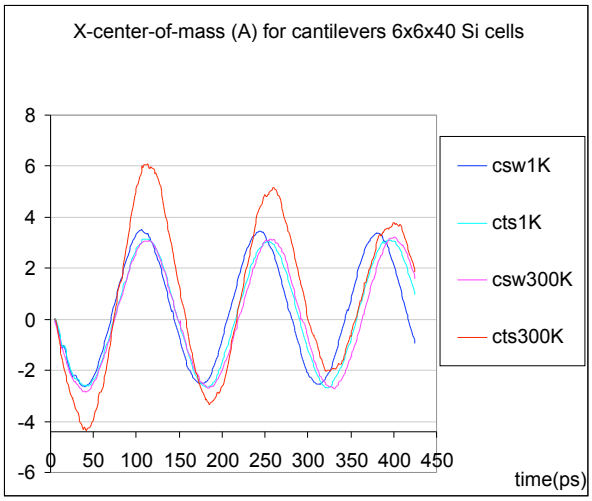
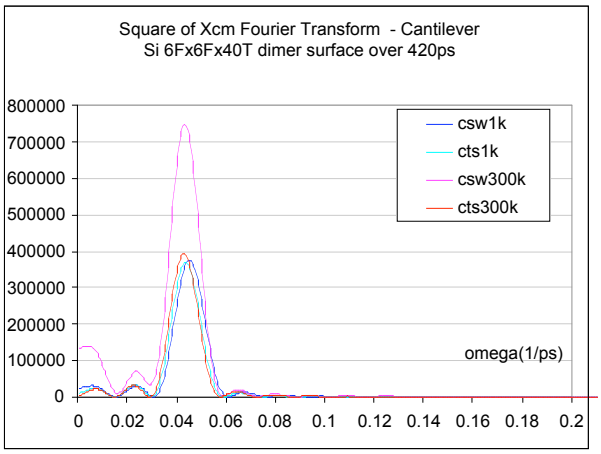
We are investigating the mechanical behavior of nanoscale crystalline solids, biological materials, and combined solid-state/biological systems. These systems have the common feature that their mechanical properties depend essentially on that of critical components with nanoscale dimensions, together with that of larger-scale constituents, and in many cases on the interplay of mechanical properties on both scales. Our approach has been to attempt to develop broadly applicable theoretical and computational methods by examining three specific classes of nanomechanics problems. The first class of problems concerns friction and energy dissipation in nanoelectromechanical systems (NEMS), especially nanomechanical resonators. The quantum limit of NEMS has also been investigated. The second is the development of new mechanical models for biological materials and machines, including DNA, biomembranes, bacterial flagella, and ion channels. The third class of problems involves the design and simulation of bio-functionalized NEMS devices and related bio-nanomachines, with applications to chemical and biological sensing. This includes a new kind of scanning probe device proposed by us, a scanning thermal-conductance microscope.

Our main focus on NEMS has been on the Q factor problem and on the origin of dissipation in nanomechanical resonators. We are conducting extensive finite-temperature molecular dynamics simulations of Si resonators and have confirmed that our codes reproduce the bulk properties of Si accurately. These simulations will allow us to calculate “bulk” contributions to dissipation, including material nonlinearity and defect motion.

The figure on the left shows the time evolution of the center of mass for a cantilever at 1K and 300K using Stillinger-Weber potential and Tersoff potential respectively. The figure on the right shows the Fourier transform of the center of mass for a cantilever. The Q factor can be extracted from this figure.





We have also developed a general formalism for calculating the acoustic radiation emitted by a NEMS resonator into a support substrate, and are testing this using finite-element method simulations.

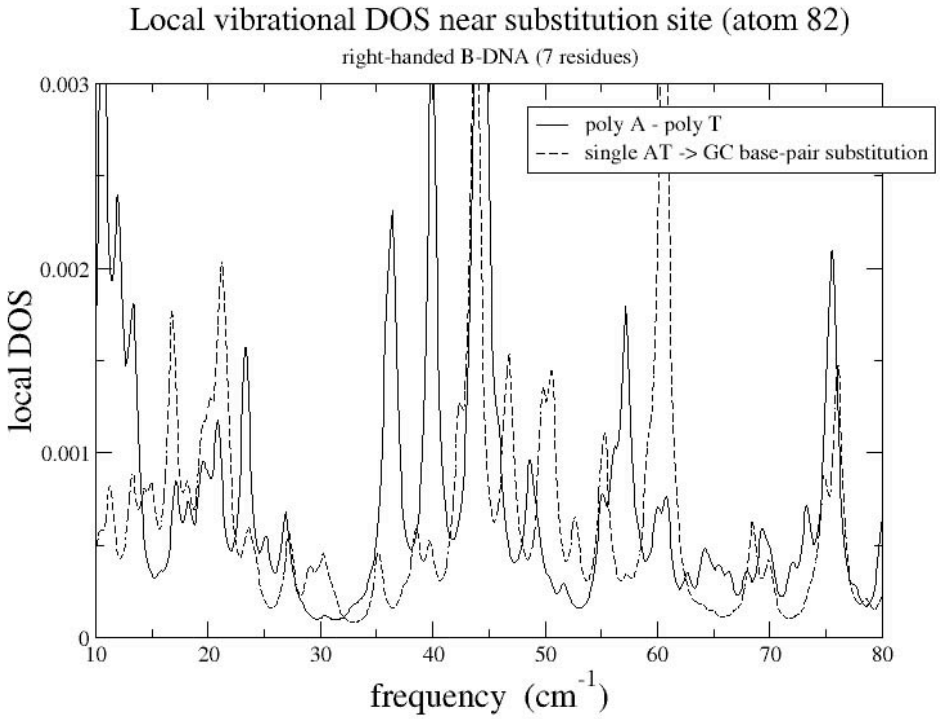
The quantum limit of NEMS resonators has also been investigated. We have shown how to experimentally manipulate the quantum states of a nanomechanical resonator by coupling it to a Josephson junction [1] or to a Cooper-pair box [2]. The use of a NEMS resonator as a long-lived quantum state memory device has also been investigated [3]. Studies of friction in NEMS resonators have thus far focused on energy relaxation only (the T_1 time in NMR language); we are currently using concepts from quantum information science to design an experimental protocol for measuring the corresponding T_2 time.

A new, general purpose multi-scale algorithm was developed and tested on single crystals of Ni [4]. The method is a course-grained alternative to molecular dynamics, but is still based on an underlying accurate molecular-dynamics force field. We hope to apply this method to NEMS devices soon.

Bacteria such as *E. coli* use rotating helical flagella to swim. These filaments are about 20 nm in diameter and 10 nm in length, are being proposed as nanomachines for pumping, mixing, and actuation in microfluidic devices. To calculate the response of the filaments to external stress in these devices, one would like to use continuum beam theory for the filament. However, under external stress, mechanical phase transitions between left- and right-handed states arise from slight, Angstrom-scale changes in the conformation of the flagellin subunits that constitute the filament. These transitions may also be caused by changes in pH, ionic strength, or by amino acid substitution. We have successfully carried out a multi-scale approach combining atomic-scale structural information with continuum mechanics to model these flagella [5].

We have also carried out theoretical investigations of other nanomechanics problems occurring in molecular biology, including elastic nonlinearity in highly curved DNA [6], Bacteriophage DNA packing and ejection [7], and membrane-protein interaction [8].

Finally, we have been designing a new device called a scanning thermal-conductance microscope, which is a thermal analog of a scanning tunneling microscope and which can measure the local vibrational density of states of a material with atomic scale resolution. The microscope makes use of the nature of thermal energy transport at low temperatures [9,10].



This figure shows the local (vibrational eigenfunction weighted) phonon density of states of two model DNA strands differing only by a single base-pair substitution. These quantities are calculated using molecular dynamics with the AMBER force field. The two DNA segments are clearly distinguishable by their local vibrational spectrum (which is not the case for their ordinary global or thermodynamic vibrational spectrum). A scanning thermal-conductance microscope should therefore be able to sequence a single strand of DNA.

As part of our outreach efforts we will be running summer school on nanomechanics at Caltech in July 2007.

References

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