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Multiscale Modeling of Dissipation and Failure in MEMS Resonators

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Abstract:

This work studies multiscale phenomena in silicon micro-resonators which comprise the mechanical components of next-generation Micro-Electro-Mechanical Systems (MEMS). Unlike their larger relatives, the behavior of these sub-micron MEMS is not described well by conventional continuum models and finite elements, but it is determined appreciably by the interplay between physics at the Angstrom, nanometer and micron scales. As device sizes are reduced below the micron scale, atomistic processes cause systematic deviations from the behavior predicted by conventional continuum elastic theory. [1] These processes cause anomalous surface effects in the resonator frequency and quality factor--even for single crystal devices with clean surfaces due to thermal fluctuations. They also lead to unconventional failure mechanisms.

The simulation of these atomistic effects is a challenging problem due to the large number of atoms involved and due to the fact that they are finite temperature phenomena. Our simulations include up to two million atoms in the device itself, and hundreds of millions more are in the proximal regions of the substrate. A direct, atomistic simulation of the motion of this many atoms is prohibitive, and it would be inefficient. The micron-scale processes in the substrate are well-described by finite elements, and an atomistic simulation is not required. On the other hand, atomistic processes in the device are inherently coupled to the micron-scale strain fields which extend out into the substrate. In order to capture physical effects at both length scales simultaneously, we have developed a multiple-scale simulation methodology. [2,3,4]

The computational technique applied here represents a significant departure from the usual finite element approach to MEMS modeling based on continuum elastic theory. When ordinary finite elements are refined to the atomic scale, the forces acting at the nodes do not resemble the true forces between atoms. Finite element models assume that the potential and kinetic energies are spread smoothly throughout each element. In reality, the potential energy is localized in covalent bonds and the kinetic energy is localized at the nuclei. Our multiscale approach uses finite elements in the peripheral regions where continuum elastic theory is valid, but it replaces finite elements with an atomistic model in regions of significantly anharmonic forces and large surface-area-to-volume ratios and where internal friction due to defects is anticipated. The different regions are joined seamlessly and run concurrently within a single simulation.

In this talk we present simulations of the vibrational behavior of micron-scale oscillators. We find anomalous surface effects that are due to atomistic processes, both in terms of temperature-dependent shifts of the resonant frequency and degradation of the quality factor (increased dissipation). Systematic experimental studies have seen anomalous dissipation at a somewhat larger scale where it has been attributed to surface degradation. [5,6,7] We also study the failure mechanisms in micro-resonators, which differ from those at large scale due to the instability of dislocations. These results are compared with

the structural transitions seen in nanowire experiments. [8] We also study the failure mechanisms in these devices, which are unconventional due to the interaction of the dislocations with the surfaces in close proximity. Dislocations are crystal defects which are the microscopic agents of plasticity, and they govern all modes of failure apart from pure cleavage. The fact that sub-micron devices have a large surface area to volume ratio implies that dislocation nucleation must take place near a surface, where they are energetically unfavorable and suppressed. The failure of sub-micron devices is therefore dramatically different that that of conventional MEMS devices.

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Key words: atomistic modeling, multiscale, MEMS, dissipation, MEMS device failure

Biography:

Dr. Rudd received his his Ph.D. from Princeton in Theoretical Physics in 1992. Later at the Naval Research Lab in Washington DC, Dr. Rudd together with Jeremy Broughton pioneered the use of new atomistic techniques to model MEMS devices, research that he continued as a Lecturer at the University of Oxford. In 2000 he took a position at the Lawrence Livermore National Laboratory in California where he is building a group in multiscale modeling of MEMS, nanoscale structures and materials failure.