Coupling of Length Scales and Atomistic Simulation of MEMS Resonators

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ABSTRACT

We present simulations of the dynamic and temperature dependent behavior of Micro-Electro-Mechanical Systems (MEMS) by utilizing recently developed parallel codes which enable a coupling of length scales. The novel techniques used in this simulation accurately model the behavior of the mechanical components of MEMS down to the atomic scale. We study the vibrational behavior of one class of MEMS devices: micron-scale resonators made of silicon and quartz. The algorithmic and computational avenue applied here represents a significant departure from the usual finite element approach based on continuum elastic theory. The approach is to use an atomic simulation in regions of significantly anharmonic forces and large surface area to volume ratios or where internal friction due to defects is anticipated. This corrects the expected, but previously unquantified, failure of continuum elastic theory in the smallest MEMS structures. Peripheral regions of MEMS which are well-described by continuum elastic theory are simulated using finite elements for efficiency. Thus, in central regions of the device, the motion of millions of individual atoms is simulated, while the relatively large peripheral regions are modeled with finite elements. The two techniques run concurrently and mesh seamlessly, passing information back and forth. This coupling of length scales gives a natural domain decomposition, so that the code runs on multiprocessor workstations and supercomputers. We present novel simulations of the vibrational behavior of micron-scale silicon and quartz oscillators. Our results are contrasted with the predictions of continuum elastic theory as a function of size, and the failure of the continuum techniques is clear in the limit of small sizes. We also extract the Q value for the resonators and study the corresponding dissipative processes.

Keywords: MEMS, silicon resonators, coupling of length scales, atomistic simulation, molecular dynamics

1. THE FAILURES OF STANDARD FINITE ELEMENTS FOR SMALL DEVICES

The design of MEMS relies on a thorough understanding of the mechanics of the device itself. As system sizes shrink, MEMS are forced to operate in a regime where the assumptions of continuum mechanics are violated, and the usual finite element (FE) models fail. The behavior of materials begins to be atomistic rather than continuous, giving rise to anomalous and often non-linear effects:

- The devices become less stiff and more compliant than FE predicts.
- The roles of surfaces and defects become more pronounced.
- Anharmonic effects become more important.
- New mechanisms for dissipation become evident.
- Statistical Mechanics becomes a key issue, even to the point that thermal fluctuations cannot be neglected.

The inadequacy of FE for these phenomena will be an obstacle to further miniaturization of MEMS.
1.1. Micro-Resonator

The failings of continuum elastic theory are evident in many ways for micro-resonators. Gigahertz resonators (cf. Fig. 1) are roughly of the size $0.2 \times 0.02 \times 0.01$ microns. Devices of this size and smaller are so miniscule that materials defects and surface effects can have a large impact on their performance. Atomistic surface processes which would be negligible in large devices are a major source of dissipation in sub-micron devices, leading to a degradation in the Q-value of the resonator. Additionally, bond breaking at defects can produce plastic deformations. These effects vary with temperature, and in the smallest devices, the atomicity shows up through stochastic noise. Systems smaller than about 0.01 microns are too small to be in the thermodynamic limit, and anomalous statistical mechanical effects are important. These effects are beyond continuum elastic theory.

![Figure 1. Silicon micro-resonator. Length: approx. 0.2 microns. Courtesy Prof. M. Roukes, Cal Tech.](image)

1.2. Micro-Gears

The anomalies are also evident in articulated devices. The effects of wear, lubrication and friction can be expected to have profound consequences on the performance of micron-sized machines, where areas of contact are a significant part of the system. An archetypical example is the gear train, something at the heart of many micro-machines of the future (See Fig. 2). The process of micro-gear teeth grinding against each other cannot be simulated accurately with FE. All of the failings listed above are evident. The teeth are predicted to be too rigid. Large amplitude high-frequency resonant modes may be missed. Bond breaking and formation at the point of contact can only be treated empirically.

2. COUPLING OF LENGTH SCALES

Sub-micron MEMS require atomistic modeling, but atomistic simulations are very computer intensive. The active region of a device whose dimensions approach a micron may be modeled with atomistics, but it is beyond the capabilities of even the largest supercomputers to model the entire region of interest of a micron-scale device. The coupling of the active region to the substrate is important, and this may involve volumes of many cubic microns and billions of atoms. Thus, many sub-micron MEMS are too small for finite elements and too large for atomistics.

We have developed a novel hybrid methodology which solves this problem. Surfaces and other regions of micro-gears and micro-resonators in which atomistic effects are critical can be modeled accurately with an atomistic simulation. Finite elements offers an adequate and efficient model of other regions such as the body and the axle of the micro-gears and the peripheral regions of the micro-resonator. Then the two, finite elements and atomistics, are melded together to run concurrently through consistent boundary conditions at the handshaking interface. Our multiscale algorithm combines atomistic, finite element and even electronic simulations into a seamless, self-consistent monolithic simulation. This coupling of length scales strikes a balance between computational accuracy and efficiency. This is part of our DOD HPC Grand Challenge project to model the dynamical behavior of MEMS. The project gives us vast computational resources at the Maui Supercomputer Center, where we are developing codes to simulate the behavior of the next generation of MEMS.
2.1. Hybrid of electronic structure, atomistics and continuum

Our codes employ electronic and atomistic simulation in the regions of bond-breaking and bond-deformation (large strain), so they are free from the assumptions of continuity that lead to the failure of FE. Instead, the codes are based on well-tested interatomic potentials and electronic parameterizations. The simulation tracks the motion of each individual atom as it vibrates or perhaps diffuses in thermal equilibrium. This means that the simulation automatically includes a wide range of phenomena. The increased compliance at small sizes arises naturally, and when the stresses are large enough to induce plastic deformation, this is simulated, too. No special phenomenology is required for effects due to surface relaxation, bond breaking and asperities.

The technique involves a state-of-the-art atomistic simulation (molecular dynamics, MD) augmented self-consistently with concurrent FE and electronic simulations (tight-binding, TB). This coupling of length scales is a novel finite temperature technique in materials simulation. It has never been attempted before, especially on parallel machines, and it allows the extension of an essentially atomistic simulation to much larger systems. Effects such as bond-breaking, defects, internal strain, surface relaxation, statistical mechanical noise, and dissipation due to internal friction are included. The trick is that the gear train is decomposed into different regions, FE, MD and TB, according to the scale of the physics within that region.

Our current codes will not run on existing desktop workstations, although they may in five years. Several factors will make this possible. First, the intrinsic speed and capacity of workstations will increase exponentially with time (Moore’s Law). Second, multiprocessor workstations will become more common, so parallel codes will offer the same advantage to workstations that they currently offer only to supercomputers. And third, our codes will become more efficient as we continue to make algorithmic advances.

The ultimate goal of this work is to understand the important atomistic effects both qualitatively and quantitatively. To quantify the effects, we have calculated new constitutive relations appropriate for sub-micron resonators. They include terms that describe atomistic surface effects, and other contributions to the energy of the structure. These constitutive relations provide the starting point for continuum and finite element models. Of course, the resulting models do not contain all of the information from the atomistic simulation, so they are only valid for a restricted range of device sizes and geometries, but the resulting finite element computations could be carried out on a workstation. This may be very useful for device design.
Figure 3. Schematic diagram of Coupling of Length Scales for a micro-resonator. An atomistic simulation (MD) is used in the regions of the device with moderate strain oscillations, while finite elements (FE) is used in the peripheral regions where changes in the strain are small. The two are joined through a consistent boundary condition in the handshaking region, and both are run concurrently in lock-step.

2.2. Coarse-grained molecular dynamics

The coupling between atomistics and finite elements described above works very well for many applications. For example, in simulations of crack propagation in silicon, the strain fields and elastic waves emanating from the crack tip pass fairly smoothly from the atomistic region into the finite element region. In particular, there is little coherent backscatter of elastic shock waves from the MD/FE interface, a problem that has plagued pure atomistic simulations of cracks. It is clear, however, that finite elements does not connect perfectly smoothly with atomistics in the limit that the element size becomes atomic scale. Finite element analysis assumes that the energy density is spread smoothly throughout each element, but at the atomic scale, the potential energy is localized to the covalent bonds of silicon and the kinetic energy is localized largely to the nuclei. This small atomic scale mismatch can cause problems in some types of simulation.

We have developed a substitute for finite elements which does connect seamlessly to molecular dynamics in the atomic limit. It also reproduces the results of finite elements (with slight improvements) in the limit of large element size. This new methodology is called Coarse-Grained Molecular Dynamics (CGMD).

CGMD has been constructed to provide a consistent treatment of the short wavelength modes which are present in the underlying atomistics but are missing from the coarse finite element mesh. These modes can participate in the dynamics and the thermodynamics of the device. In many situations, the short wavelength part of the spectrum is relatively unpopulated, and the missing modes are irrelevant to the behavior of the device. But this is not true for sufficiently small devices, or when there is a strong source of high frequency elastic waves (such as a propagating crack or when two micro-gears grind against each other). In addition to offering well-behaved thermodynamics, CGMD also models the elastic wave spectrum more accurately than conventional finite elements. Furthermore, CGMD includes non-linear effects that are compatible with the atomistics; i.e. it effectively provides non-linear constitutive equations that are derived from the atomistics without any free parameters.

3. TECHNICAL APPROACH
3.1. Micro-Resonator

The goal of a multiscale simulation is to balance accuracy with efficiency in an inhomogeneous system. An atomistic simulation is employed in regions of significantly anharmonic forces and large surface area to volume ratios or where internal friction due to defects is anticipated. As shown in Fig. 3, the atomistic simulation models the central region of the resonator. This corrects the expected, but previously unquantified, failure of continuum elastic theory in the smallest MEMS structures. Regions of the micro-resonator which are well-described by continuum elastic theory are simulated using finite elements. These peripheral regions include the coupling to the outside world, a substrate at a given temperature. Electronic structure calculations are used in regions of very large strain and bond breaking, such as at defects. The electronic, atomistic and continuous regions are joined seamlessly to form the complete simulation.

![Coupling of Length Scales](image)

**Figure 4.** Illustration of the domain decomposition of the long, thin resonator showing coupling of length scales. The smallest regions are electronic structure simulations of the vicinity of defects, implemented with tight-binding (T.B.). The intermediate regions are molecular dynamics (M.D.) simulations and the end caps depict part of the large finite element (F.E.) simulation. The simulation is decomposed according to the scale of the physics in each region, and then the simulation is distributed among the processors on a supercomputer in order to optimize the overall efficiency.

Coupling length scales for the micro-resonator is accomplished as follows. Any defects, the only regions of breaking bonds, are of necessity described by electronic structure methodology. These are coupled to the statistical mechanics of sub-micron system sizes (to provide necessary fluctuations) via conventional molecular dynamics. This region, in turn, is coupled to micron and larger scales via finite elements. In each case the coupling between the regions amounts to a set of consistent boundary conditions that enforce continuity.

This formulation of the coupling of length scales gives a natural domain decomposition to divide the computational load among parallel processors, as shown in Fig. 4. The MD region is partitioned lengthwise into subregions, each of which is assigned to a separate processor. The FE regions (one at each end of the resonator) at present comprise one processor each, since they are not excessively computationally intensive. Each electronic structure domain consisting of about 20 atoms is assigned to a separate processor. The MD region uses an empirical potential suitable for the material of interest; in this case, since the materials are silicon and quartz, the potentials are those due to Stillinger and Weber and Vashishta, respectively.

Our simulations have been limited to relatively small defect densities, so the multi-million atom atomistic region of the resonator requires the majority of the processors. Even though the electronic structure calculation is intrinsically a much more expensive computation, the total TB expense is less because there are relatively few TB atoms. Our codes are written in FORTRAN and MPI and run on IBM SP2s, allowing atomistic regions of millions of atoms coupled, of course, to large finite element regions, if necessary.
3.2. Micro-Gears

Fig. 2 shows an example of micro-gear technology. Such devices can presently be made on the 100 micron scale and rotate at speeds of 150,000 RPM. Materials may be either polysilicon or nickel, depending upon the method of manufacture; we concentrate on silicon. We can expect next-generation devices to reach the 1 micron level. The speed with which they could be made to rotate is a subject for our research.

**Figure 5.** Illustration of dynamic simulation zone and domain decomposition for coupling of length scales: from continuum (FE), to atomistics (MD) to electronic structure (TB).

The effectiveness of this coupling of length scales has been demonstrated previously in simulations of a crack opening in silicon.

4. RESULTS

We have simulated micro-resonators with various sizes, defect concentrations and temperatures, for comparison. The dimensions of the largest oscillator are shown in Fig. 6. All of the devices have the same aspect ratio, 25:2:1. The motion of the resonator is simulated as follows. The initial configuration of the atoms is taken to be a single crystal of stoichiometric quartz in the desired device geometry (with some fraction of the atoms removed at random, if vacancies are to be modeled). The system is brought to thermal equilibrium in 100,000 time steps. Then the
resonator is deflected into its fundamental flexural mode of oscillation, and released. Once released, the thermostat is turned off, and no further energy is put into the system.

Various properties of the resonator have been studied. Fig. 6 shows the Young’s modulus as a function of size. The resonant frequency of the oscillator is proportional to the square root of the Young’s modulus. The dashed lines in the figure indicate the bulk value, whereas the solid lines indicate the best fit to a constitutive equation which includes a surface term. Atomistic effects are clearly evident for devices less than 0.2 microns in length. Note that this is true even for the single crystal device at T=10K. This device is essentially a perfect crystal, disrupted only by the surfaces. But it is the surface relaxation which produces deviations from the bulk behavior.

Fig. 8 shows how the oscillator rings as a function of time when plucked in flexural mode. Note that relatively large deflections of the resonator are possible, as great as 0.2%, due to the increased compliance of the microscopic devices. The response of the oscillator at 300K shows marked effects of anharmonicity. There is a pronounced frequency doubling effect in the smaller oscillator, and even in the first few periods of the larger oscillator there are clear departures from a sinusoidal oscillation. The mode mixing is most apparent in the Fourier transform of the oscillations of the small device shown in Fig. 9. A significant amount of the first harmonic (as well as a bit of the second) has mixed into the spectrum. This is not the case for an identical simulation run at T=10K, where only the fundamental mode is present (not shown). Fig. 10 shows that the response of the oscillator with 1% vacancies is also anomalous. A substantial plastic deformation has resulted from the presence of vacancies at both temperatures, and again at 300K the response is highly anharmonic.

We can use simulations such as these to calculate the Q-value for the various resonators. The Q-value for the small devices at room temperature shown in Figs. 9 and 10 are Q=300 and Q=200, respectively, at their resonant frequency of 24 GHz. The simulation time for the large system captures too few oscillations for a direct computation of the Q-value, but a scaling analysis together with a fit to the dominant dissipative processes enables us to estimate this Q-value as well. The results will be presented elsewhere.

This behavior could not be predicted from continuum elastic theory. The anharmonic response has been shown to be the result of surface effects. The degradation of the Q-value of small resonators is also due to a surface effect. In large single crystal resonators, the primary sources of dissipation are bulk thermoelastic and phonon-phonon processes. Our results show that for small resonators at room temperature there is a new dominant source of dissipation at the surface. The reduction of Q for small resonators has been observed in experiments, where it has been attributed to flawed surfaces. Our results show that even for initially perfect single crystal devices, atomistic effects cause a significant degradation in Q at room temperature.

The plastic behavior is due to relaxation of the lattice about the vacancies. The only way these effects could be addressed using continuum elastic theory would be to construct empirical models that would extend the standard finite element analysis. However, this type of model simply does not afford the confidence necessary to push the frontiers of device design. Our methodology, coupling of length scales, is able to make definitive predictions of device performance.
Figure 7. A plot of the Young’s modulus as a function of the device size for a perfect crystal at two temperatures, T=10K and T=300K, and a crystal with 1% vacancies at T=300K. The dashed lines indicate the bulk value of the Young’s modulus. The solid curved lines are the best fit to a constitutive relation which includes terms for atomistic surface effects.

Figure 8. A comparison of a 170Å and a .14 micron quartz crystal oscillator. The smaller system shows anharmonic and surface effects.

5. WORK IN PROGRESS

We are in the process of setting up the micro-gear simulation. We have chosen to study silicon gear teeth because (a) a good TB parameterization exists and (b) because gear teeth are often made of polysilicon. The issues to be investigated are: (a) When two clean surfaces are brought together they “cold weld” - thus when two teeth are in contact, bonds will form across the opposing interfaces. As the gears rotate, these bonds will break. How much
Figure 9. A plot of the oscillations and corresponding frequency spectrum of the 0.017 micron device at room temperature (T=300K). The device is initially excited in the fundamental mode (0). Appreciable components in the first (1) and second (2) harmonics have resulted from mode mixing due to anharmonic lattice effects.

Figure 10. Behavior of 1% vacancy oscillator at two temperatures: (a) T = 10K and (b) T = 300K. Note that the oscillations have shifted in the positive (x) direction in both cases, due to a plastic deformation.

mater is transferred? How rough is the newly exposed surface? (b) Suppose we affix linear polymer chains to the surfaces of the gears (self-assembled monolayers) of length (say) 12 carbon atoms, does this significantly reduce wear and friction? The monolayer molecules in question are the alkyltrichlorosilanes. Interatomic potentials are available for similar polymeric systems. Technologically, such processing of the surfaces is very doable, and in fact has already been applied to micro-gears. How much energy is dissipated into the body of the gears when such surfaces rub? At what speed can we run a gear train before entanglement and relaxation times in the SAM polymer become an issue?

6. CONCLUSION

The algorithmic and computational avenue applied here represents a significant departure from the usual finite element approach based on continuum elastic theory. We have shown that atomistic simulation, and in particular multiscale atomistic simulation, offers significant improvements for the modeling of MEMS on sub-micron length
scales. It is at these scales that some of the assumptions of continuum mechanics fail. The issue is at what system size and in what way they fail. These are issues that we are able to answer unambiguously using atomistic simulation and coupling of length scales.

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