Coupling of Length Scales and Atomistic Simulation of a MEMS Device

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ABSTRACT

We simulate the dynamic and temperature dependent behavior of two different 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, by combining the power of an atomistic simulation with the efficiency of finite elements. This work studies the dynamics of a silicon micro-gear train and the vibrational behavior of a micron-scale quartz oscillator. The work provides a new paradigm for device design and prediction, and for the relevance of atomistic simulation.

Keywords: Molecular Dynamics, Atomistic Simulation, Silicon Resonator, Coupling of Length Scales, MEMS

The Problems with Standard Finite Elements for Small Devices

The design of MEMS relies on a sound understanding of the mechanics of the device itself. As system sizes shrink, MEMS are forced to operate in a regime where many of 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.

- 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 a major obstacle to further miniaturization of MEMS.

Micro-Gears

The problems are particularly 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. 1). 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.

Figure 1: Example of a MEMS nickel gear train. Dimensions: approx. 200 microns. Courtesy Prof. H. Guckel, University of Wisconsin. [1]

Micro-Resonator

The failings of continuum elastic theory are also evident for micro-resonators (See Fig. 2). These devices are typically much smaller than the micro-gears. They are so miniscule that materials defects and surface effects can have a large impact on the performance of the device. Bond breaking at defects can lead to 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.
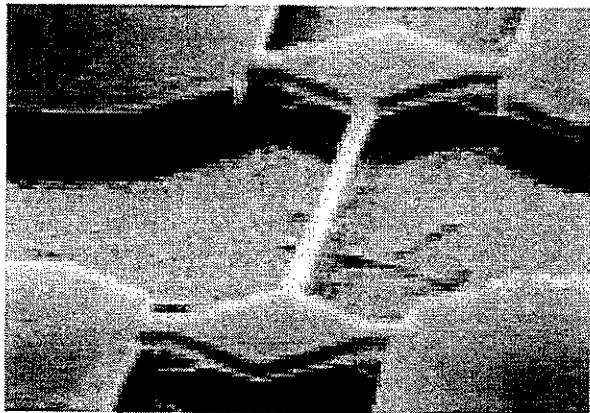

Figure 2: Silicon Micro-Resonator. Length: approx. 0.2 microns. Courtesy Prof. M. Roukes, CalTech. [2]

Coupling of Length Scales

Surfaces and other regions of micro-gears and micro-resonators in which these effects are critical can be modeled accurately with an atomistic simulation. Finite elements then 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. We have developed an algorithm which combines electronic, atomistic and finite element 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.

Our codes employ electronic and atomistic simulation in the regions of bond-breaking, 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. The increased compliance at small sizes arises naturally in the simulation. No special phenomenology is required for effects due to surface relaxation, bond breaking and asperities.

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.

In this paper we describe the simulation of interacting gear teeth, both with and without lubricant. The lubricant will take the form of surface self-assembled monolayers. We also present the results of a simulation of the vibrational behavior of a micron-scale quartz oscillator. Our findings 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.

Technical Approach

Micro-Gears

Fig. 1 shows an example of micro-gear technology. [1] 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.

Our technical approach 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.

Fig. 3 illustrates the domain decomposition for the micro-gear train. We imagine an inner region including the shaft which is treated by finite elements. FE uses the energy density that comes from constitutive relations for the material of interest to produce a force on each nodal point which drives the displacement field at that point using an algorithm which looks just like molecular dynamics. We are also developing improved codes based on Coarse Grained Molecular Dynamics, in which the FE equations of motion are determined directly from the MD potential [3]. The timestep used by the FE region has to be in lock step with the MD region (and also therefore with the TB region). The handshaking

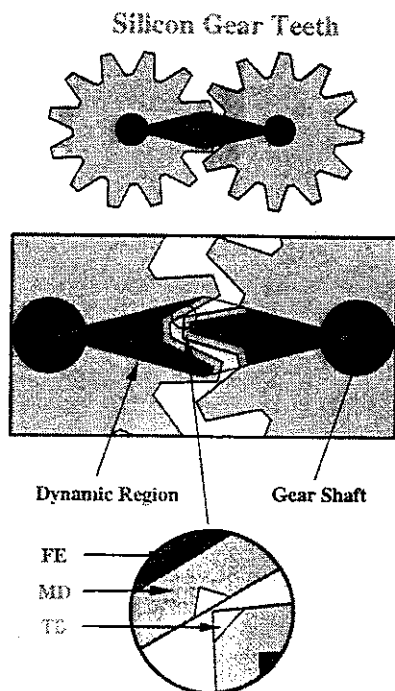Silicon Gear Teeth

Dynamic Region   Gear Shaft

FE
MD
TB

Figure 3: Illustration of dynamic simulation zone and domain decomposition for coupling of length scales: from continuum (FE), to atomistics (MD) to electronic structure (TB).

between the FE and MD region is accomplished using a self-consistent overlap region.

The MD region is partitioned into subregions, each of which is assigned to a separate processor. The FE regions (one per gear) at present comprise one processor each, since they are not excessively computationally intensive. The MD region uses an empirical potential suitable for the material of interest; in this case, since the material is silicon, it is that due to Stillinger and Weber [4].

Lastly, in regions at the gear-gear contact point in the non-lubricated case, a tight-binding description is used. When we study the lubricating properties of SAMs, the TB region is not required, since bond breaking is not an issue. Each TB region spreads across multiple processors. Tight binding is a fast electronic structure method—with careful parameterization, it can be very accurate. We use the parameterization due to Bernstein and Kaxiras [5]. The effectiveness of this coupling of length scales has been demonstrated previously in simulations of a crack opening in silicon. [6]

As Fig. 3 indicates, we can concentrate upon the contact between gear teeth. It is not necessary to simulate the two gear wheels in their entirety; instead, using a methodology akin to periodic boundary conditions, we can focus on that part of the system of direct interest. Using a moving reference frame, material leaving the top of the figure is fed back up from the bottom. This

will be implemented in future versions of the gear simulation in order to study larger systems. In the direction (z) into the page, we use standard periodic boundary conditions to represent a cog of infinite z-extent.

Micro-Resonator

A similar approach is used in the case of the quartz crystal oscillator. 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. 4, 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. The electronic, atomistic and continuous regions are joined seamlessly to form the complete simulation.

Coupling of Length Scales
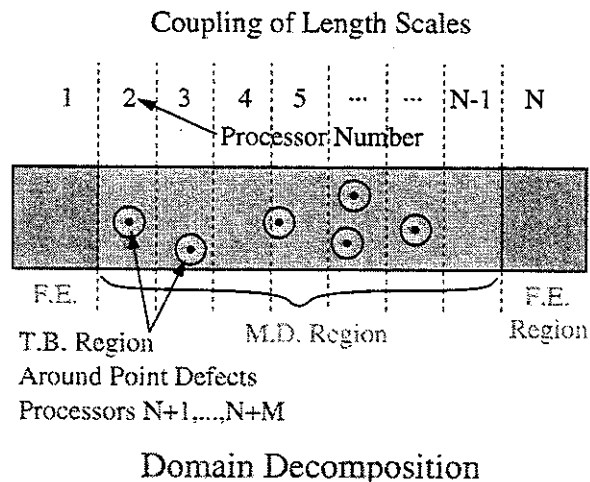
Domain Decomposition

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.

Coupling length scales 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 submicron 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. Our simulations have been limited to relatively small defect densities, so the multimillion 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.
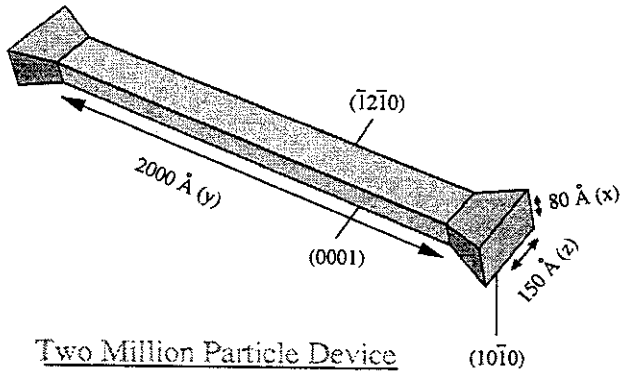
Figure 5: Size and aspect ratio of the quartz oscillator, as simulated.

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. 5. The results are shown in Figs. 6 and 7. The figures show 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 [10]. 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 response of the oscillator with 1% vacancies is also anomalous. The vacancies have caused a substantial plastic deformation in both runs, and again at 300K the response is highly anharmonic.

This behavior could not be predicted from continuum elastic theory. The anharmonic response has been shown to be the result of surface effects, while the plastic behavior is due to relaxation of the lattice about the vacancies [10]. 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*
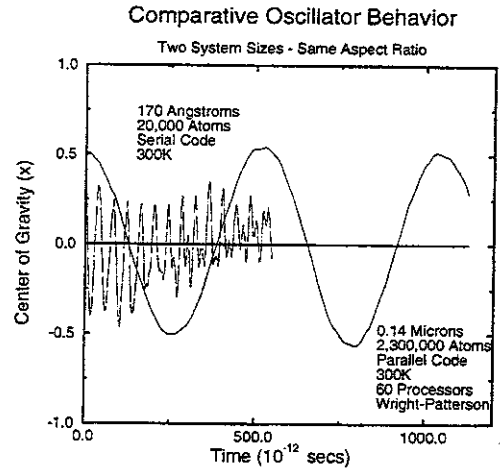

Figure 6: A comparison of a 170Å quartz crystal oscillator (QCO) and a .14 micron QCO. The smaller system shows anharmonic and surface effects.

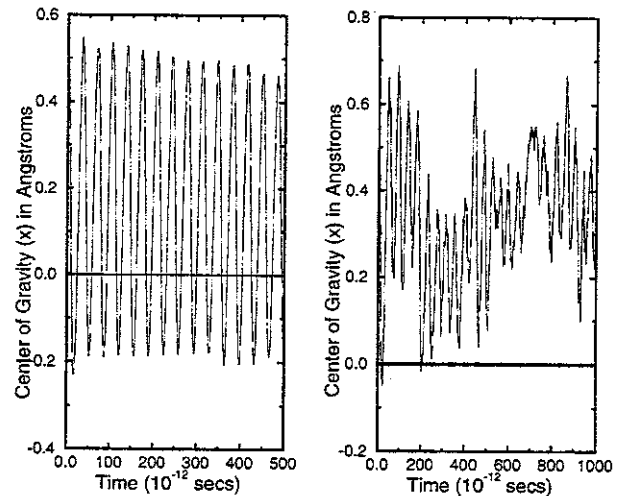*of length scales*, is able to make definitive predictions of device performance.

Figure 7: Behavior of 1% vacancy oscillator at two temperatures: (a) T = 10K and (b) T = 300K.

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 matter 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 exist for similar polymeric systems [7]. Technologically, such processing of the surfaces is very doable [8], and in fact has already been applied to micro-gears [9]. 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? Figs. 8 and 9 illustrate the concepts behind SAMs and also the envisaged simulation of SAM-covered gear teeth.
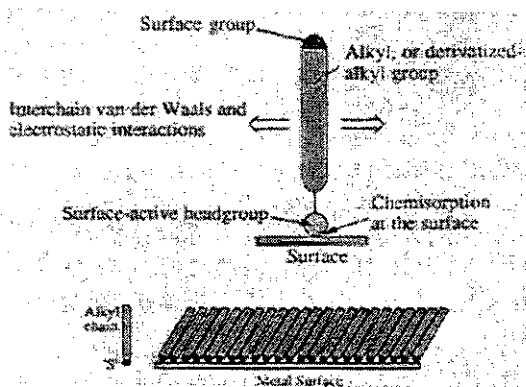

Figure 8: Conceptualization and basic ingredients of self-assembled monolayers.

Self-Assembled Monolayer on MEMS Gear Teeth

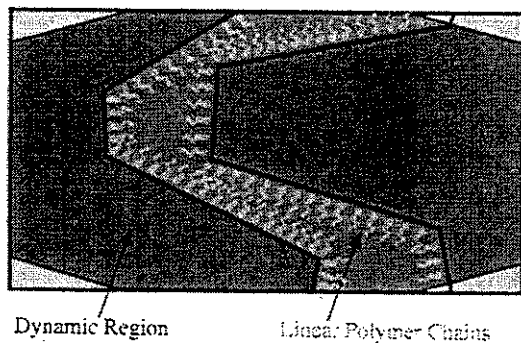Dynamic Region   Linear Polymer Chains

Figure 9: Illustration of simulation to reduce wear and friction in MEMS gear trains.

Conclusion

The algorithmic and computational avenue applied here represents a significant departure from the usual finite element approach based on continuum elastic theory. On submicron length scales, 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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