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Coarse-Grained Molecular Dynamics and Multiscale Modeling of NEMS Resonators

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ABSTRACT

We review concurrent multiscale simulations of dynamic and temperature-dependent processes found in nanomechanical systems coupled to larger scale surroundings. We focus on the behavior of sub-micron Micro-Electro-Mechanical Systems (MEMS), especially micro-resonators. These systems are often called NEMS, for Nano-Electro-Mechanical Systems. The coupling of length scales methodology we have developed for MEMS employs an atomistic description of small but key regions of the system, consisting of millions of atoms, coupled concurrently to a finite element model of the periphery. The model, Coarse-Grained Molecular Dynamics (CGMD), builds a generalized finite element formalism from the underlying atomistic physics in order to ensure a smooth coupling between regions governed by different length scales. The result is a model that accurately describes the behavior of the mechanical components of MEMS down to the atomic scale.

Keywords: concurrent multiscale modeling, MEMS, flexural resonator

1 NEMS AS MULTISCALE SYSTEMS

As mechanical systems are miniaturized to the nanoscale, new physics can arise due to the atomic nature of matter. Systems that would appear to be continuous media at larger sizes are able to sense the discrete atoms. The continuum mechanics suitable for large systems must be corrected and the completely supplanted by atomistic mechanics as the typical length scale transitions from macroscopic to nanoscopic sizes. New modeling techniques must be devised to simulate systems in the transitional regime. In this article we discuss the use of concurrent multiscale simulations to explore how the behavior of microsystems changes as they are miniaturized into the nanoscale.

We are particularly interested in concurrent multiscale modeling of dynamic and temperature-dependent processes found in nanomechanical systems coupled to larger scale surroundings. [1], [2] We focus on the behavior of sub-micron Micro-Electro-Mechanical Systems (MEMS), especially micro-resonators. The coupling of

length scales methodology we have developed for MEMS employs an atomistic description of small but key regions of the system, consisting of millions of atoms, coupled concurrently to a finite element model of the periphery. The model, Coarse-Grained Molecular Dynamics (CGMD) [3], builds a generalized finite element formalism from the underlying atomistic physics in order to ensure a smooth coupling between regions governed by different length scales. The result is a model that accurately describes the behavior of the mechanical components of MEMS down to the atomic scale.

The miniaturization of mechanical devices is the primary theme in the development of MEMS. The qualitatively new possibilities afforded by these systems arise because of the precision of microscopic components, the economy of scale in semiconductor fabrication, and the emergence of new phenomena in the scaling to small sizes. The vast majority of MEMS mechanical devices operate at engineering scales of microns and larger, but a new class of MEMS devices are being developed at the nanoscale. [4]–[6] Fundamental challenges to MEMS design arise for these ultrasmall devices, because the conventional rules for device engineering based on continuum mechanics are violated by the atomic nature of materials: the atomic-level discreteness of matter affects the behavior of ultrasmall MEMS.

This work is a theoretical and computational study of atomistic phenomena in the context of silicon MEMS micro-resonators. The challenge of modeling these devices is compounded by the fact that the atomic-scale effects cannot be separated cleanly from larger-scale phenomena, and the system exhibits strongly-coupled multiscale behavior, governed by the interplay between physics at the Angstrom, nanometer and micron scales. A direct, atomistic simulation of the billions of atoms involved is prohibitive, and it would be inefficient. Instead, we have developed a new concurrent multiscale methodology, which uses finite elements to model processes in the substrate and atomistics to model processes in the smallest features of the device. The two are run concurrently to attain a self-consistent model of the entire system. [1], [7]

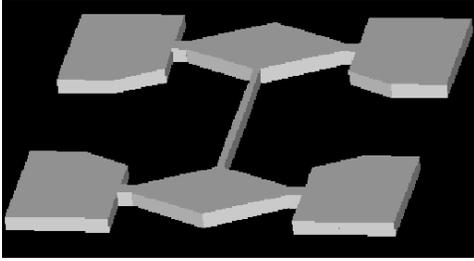


Figure 1: Three dimensional model of the bridge-type flexural microresonator. The device oscillates out of the plane of the substrate. The geometry is modeled on a device fabricated by Prof. Roukes and coworkers [4].

2 FORMULATION OF CGMD

In this Section and the next we review some of the general issues involved in concurrent multiscale simulation, including recent advances in CGMD allowing the suppression of spurious reflections of out-going waves. The geometry of the sub-micron resonator, as simulated, is shown in Fig. 1. This three dimensional geometry is based on a device fabricated by the Roukes group at Caltech. [4] Once the geometry is defined, a mesh is introduced in order to specify which regions are to be coarse grained, as shown in Fig. 2. In particular, the resonating bar and the immediate periphery are modeled using atomistics—the nodes of the mesh and the equilibrium sites of the atoms coincide and are in one-to-one correspondence. Then the mesh size increases moving out further into the peripheral regions. Here each node of the mesh corresponds to many atoms. It is this reduction in the number of degrees of freedom that increases the efficiency of multiscale simulations.

It is convenient to distinguish between two regions of the simulation. The region in which the nodes are in one-to-one correspondence with the atoms is called the molecular dynamics (MD) region; the region with many atoms per node is called the coarse-grained (CG) region. The equation of motion for the atoms in the MD region is just the usual MD equation of motion based on a classical, empirical potential. Stillinger-Weber [8] and Tersoff [9] potentials have been used for the silicon resonators. [1] In the CG region, the equation of motion is of the finite element form:

$$M_{ij}\ddot{\vec{u}}_j = -K_{ij}\vec{u}_j + \dots \quad (1)$$

where M_{ij} is the mass matrix, K_{ij} is the stiffness matrix and \vec{u}_j is the displacement at node j . The mass and stiffness matrices are derived from the underlying atomistic model. The details are given in Ref. 3.

Coarse-grained molecular dynamics has proven very effective in permitting large volumes of the system to be simulated with a reduced number of degrees of freedom. This has allowed larger systems sizes than would oth-

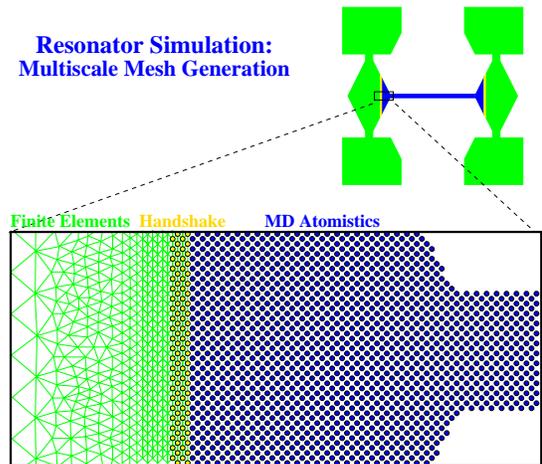


Figure 2: The decomposition of the microresonator system into molecular dynamics (MD) and finite element (FE) or coarse-grained molecular dynamics (CGMD) regions. A narrow handshaking region is used to couple the FE and MD regions; in the case of CGMD, the crossover to atomistics for atomic-sized cells is completely smooth and no handshaking region is required. [1]

erwise be possible with the given computer resources. Also, CGMD has proven to be advantageous over a straight finite element/molecular dynamics hybrid approach. Conventional finite elements does not automatically give the MD equation of motion as the cell size is reduced to the atomic scale; CGMD does. The result is a higher quality interface between the MD and CG regions. Unwanted elastic wave scatter is reduced, although not completely eliminated (see the discussion below). The elastic wave spectrum is better represented in the CG region. Effects such as thermal expansion are treated properly. CGMD is more expensive computationally than conventional finite element modeling, but in many instances this additional cost is warranted in order to achieve a higher quality simulation.

3 ATOMISTIC EFFECTS IN NEMS

We have conducted simulations of the vibrational behavior of micron-scale oscillators. We have found anomalous surface effects that are due to atomistic processes. [10] They show up in temperature-dependent shifts of the resonant frequency, degradation of the quality factor (increased dissipation) and extreme compliance. These 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 nanoscale MEMS.

The conventional description of the mechanical components of MEMS is based on continuum mechanics im-

plemented in a finite element model. [11] The oscillations of a resonator, for example, are dictated by the geometry of the system, the properties of the materials and the applied forces. In linear elastic theory, the material properties are just the elastic constants and the mass density of the material. These properties are taken to be independent of size, an assumption that is valid as long as the variations of the elastic fields occur over lengths that are large compared to the characteristic lengths of any microstructure. For example, the material properties would differ for a resonator a meter long and one a micron long, if the material had a characteristic grain size of 10 microns. In one case, the material would behave as a polycrystal; in the other it would be a single crystal.

We are primarily interested in NEMS bulk micromachined from single crystal silicon. At first glance, this appears to be a homogeneous system, and the material properties should be scale independent. This is not the case, however, because the lattice constant (the inter-atomic spacing) sets a scale. The width of the smallest NEMS resonators is on the order of 100 atoms wide, so the properties of the resonator can be affected by the discrete, atomic lattice.

Another issue is the fact that the surface area-to-volume ratio increases as systems are miniaturized, and surface effects become more important. This fact has long been appreciated in the MEMS community.[12] It takes on new significance for NEMS. One of our results is that the Young’s modulus, the elastic constant that enters the resonant frequency of a flexural resonator, becomes scale dependent due to atomistic surface effects. These results are explained in detail elsewhere [2], [13], and are not repeated here. The basic result is that for a resonator that is 100 atoms wide, the computed deviation from the continuum Young’s modulus is about 1%. It increases as the system size is decreased, but this is the limit of the current fabrication techniques. A direct verification of this 1% change is not possible due to other uncertainties in the fabrication process, but it is possible to measure shifts in the resonant frequency of a single device that are much less than 1%, so an indirect measurement may be possible.

The second aspect of NEMS behavior that we have investigated is the dissipation. Dissipation leads to a degradation of the quality factor of the resonator, Q , that determines the width of the peak at resonance. A high Q and a correspondingly narrow peak are desirable for applications like frequency standards and filters because it ensures that the frequencies are well defined. [6] Scaling arguments predict that sub-micron bridge-type oscillators could be made to resonate in the GHz regime, something that would be very useful for communications applications. [6], [4] Most GHz resonators have a very low Q , but the use of single crystal resonators would

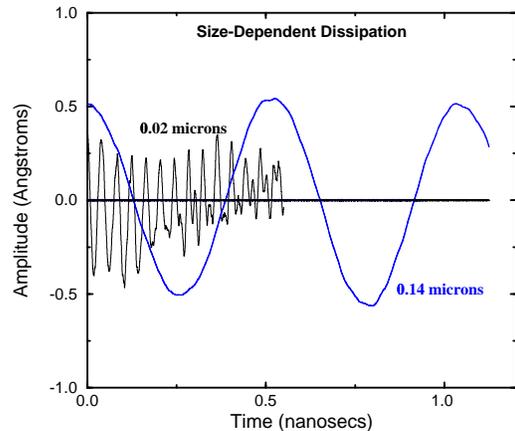


Figure 3: Comparison of the oscillations of resonators of two different sizes but with the same aspect ratio. Both are at room temperature. Note the increased dissipation in the smaller resonator. This is due to a mode-mixing effect coming from lattice anharmonicity. [2]

eliminate many dissipative processes and hold the hope of relatively high Q values. In fact, our simulations [2] and experiments [14] have found that Q decreases as devices are miniaturized: the dissipation, $1/Q$, scales roughly like the surface area-to-volume ratio.

We have investigated dissipation using atomistic and multiscale simulations. The results from two such simulations are shown in Fig. 3. [2] The curves represent the oscillations of systems of two different sizes with the same aspect ratio. The two systems contained 20 thousand and 2 million atoms in the MD region. The larger system exhibits longer period oscillations, corresponding to a frequency of about 2 GHz. The smaller system has a resonant frequency of about 24 GHz. The oscillations of the larger system are sinusoidal throughout the 1 ns simulation time, whereas the oscillations of the smaller system begin sinusoidally, but rapidly degenerate into a noisy motion. This degeneration is the result of dissipation. Energy is transferred from the fundamental mode, the initial state, into the other normal modes of the oscillator. In the Fourier transform of the oscillations (not shown) an appreciable amount of the first excited mode (and some of the second) is evident by the end of the simulation. These modes are coupled through anharmonic interactions that are enhanced by the surface. The result is dissipation that increases as the surface area-to-volume increases.

4 EXTENSIONS OF CGMD

The original formulation of CGMD was as a Hamiltonian system. Thermal effects were present, but not the random, dissipative forces due to the heat bath of

modes that were integrated out. Energy was conserved. Recently, a non-conservative version of CGMD was developed [15] in order to remove unphysical elastic wave reflection. In a conservative framework, elastic waves are reflected from regions of the mesh where the mesh spacing exceeds the wave length. Basically, energy is conserved, so the energy in the wave must go somewhere. If the mesh spacing is too large, the wave cannot be supported on the mesh: it is reflected. Projection operator techniques were used to derive a generalized Langevin equation that solves this problem.

Another issue is the fact that CGMD assumes small fluctuations about a perfect lattice in the coarse-grained region. One of the remaining challenges in concurrent multiscale modeling is to allow lattice defects to propagate from the atomistic region into the coarse-grained region. These could be point defects (vacancies, interstitials, substitutional defects, etc.), line defects (dislocations, disclinations, etc.) or planar defects (grain boundaries, surfaces, etc.). The need for a solution is particularly acute in the case of dislocations because they are highly mobile. In dynamic fracture simulations, for example, dislocations have been observed to propagate across a simulation box containing one million atoms in just 20 ps. [16] After this very short amount of time, the simulation departs from the behavior of a crack growing in a macroscopic system. One way to avoid this finite-size effect would be to embed the system in a coarse-grained region and to allow the dislocations to propagate across the interface into the coarse-grained region. Some progress has been made recently with the development of techniques to locate dislocations in finite temperature molecular dynamics simulations [17], but this is still an open problem.

There are of course many other applications for concurrent multiscale modeling. We are just at the start of what promises to be a very interesting development.

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