Coarse-Grained Molecular Dynamics for Design of Nanomechanical Systems

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ABSTRACT

We give an overview of some of the unique challenges for computer modeling and simulation that arise from the development and design of nanoscale mechanical systems. Of particular interest are the dynamic and temperature-dependent processes found in nanomechanical systems. We focus on the behavior of sub-micron mechanical components of Micro-Electro-Mechanical Systems (MEMS), especially micro-resonators. The coupling of length scales methodology we have developed for MEMS employs an atomistic description of millions of atoms in relatively small but key regions of the system, coupled concurrently to a generalized finite element model of the periphery. The model, Coarse-Grained Molecular Dynamics (CGMD), describes the dynamics on a mesh of elements, but the equations of motion are built up from the underlying atomistic physics to ensure a smooth coupling between regions governed by different length scales.

Keywords: concurrent multiscale modeling, MEMS, NEMS, flexural resonator

1 NEMS DEVICES AND EMBEDDED NANOMECHANICS

There is growing interest in the development of nanoscale mechanical components for applications in Micro-Electro-Mechanical Systems (MEMS) and Nano-Electro-Mechanical Systems (NEMS). The vast majority of MEMS mechanical devices operate at engineering scales of microns and larger, but a new class of MEMS devices is being developed at the nanoscale. Their extremely small size produces extreme sensitivity to forces and displacements as well as ultra-low power consumption. Applications under development range from devices such as gigahertz resonators for communications applications [1]–[3] and ultra-sensitive scanning probe microscopes [4], [5], to devices to explore the esoteric worlds of quantum transport [6] and perhaps quantum information processing [7]. The former applications are in some sense a natural progression driven by the advantages of miniaturization; the latter are tapping into the dramatically new behavior accessible at the nanoscale.

Whether pushing the limits of miniaturization or searching for revolutionary functionality, the development and the design of nanoscale mechanical systems pose an array of challenges for computer simulation and modeling. One set of challenges arises from the need to miniaturize the mechanical components of MEMS to such an extent that the materials behavior becomes anomalous. The behavior of materials at the nanoscale need not be the same as that in macroscopic systems, either because the system size is less than characteristic length scales in the macroscopic material such as grain sizes, or because the form of the mechanics is sensitive to material properties that are irrelevant at the macroscale such as surface stresses. Anomalies have been identified in various aspects of materials behavior including elasticity, plasticity, fracture, fatigue and tribology. The occurrence of anomalous behavior together with what is often limited direct characterization of the properties at the scale of interest complicates materials selection and other aspects of device optimization.

Computer modeling offers the promise of guidance based on first-principles theory in the absence of complete experimental data. We are particularly interested in the application of concurrent multiscale modeling of dynamic and temperature-dependent processes found in nanomechanical systems coupled to larger scale surroundings. [8], [9] The ensuing discussion focuses on the behavior of sub-micron MEMS, especially micro-resonators. The coupling of length scales methodology we have developed for MEMS takes advantage of the heterogeneity of the MEMS components. It employs an atomistic description of small but key regions of the system, consisting of millions of atoms, and a finite element model of the periphery. The two are run concurrently to attain a self-consistent model of the entire system. [8], [10] The model, Coarse-Grained Molecular Dynamics (CGMD) [11], 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.

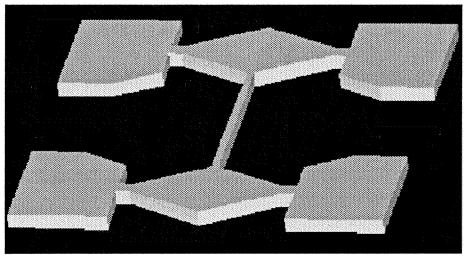

Figure 1: A three-dimensional model of the bridge-type flexural microresonator. The central semiconductor bar is attached only at its end points and hence free to oscillate. The oscillations are out of the plane of the substrate. The geometry is modeled on a device fabricated by Prof. Roukes and coworkers [1].

2 CONCURRENT MULTISCALE MODELING

In this Section we describe how concurrent multiscale modeling has been applied to model the behavior of some nanoscale mechanical components under development. It should be noted that several different approaches to the concurrent multiscale modeling of solid materials have been developed, each optimized for a particular kind of application.[10], [11], [13] The methodology we describe here has been optimized for use to simulation the dynamics of nanomechanical systems, including those at finite temperature. The goal is to model an important region of the system, consisting of thousands of cubic nanometers of material, with atomistic precision; surrounding regions of the system are to be modeled at a more coarse-grained level to capture the relevant part of the dynamics but at a much reduced level of computational expense.

For the discussion of the methodology, we focus on the application to a sub-micron flexural resonator. The geometry of the bridge-type resonator, as simulated, is shown in Fig. 1. This three dimensional geometry is based on a device fabricated by the Roukes group at Caltech. [1] 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 farther 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

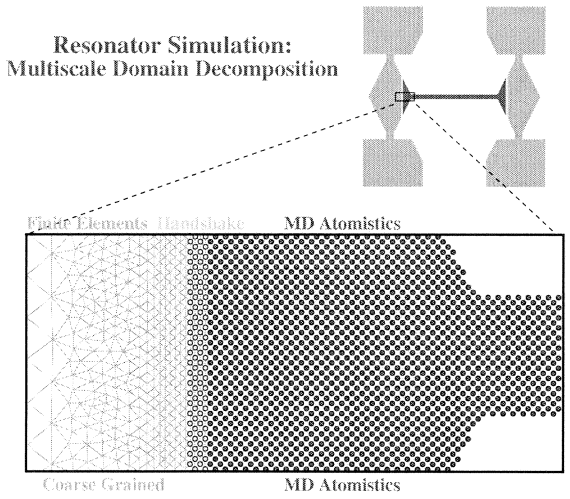

Figure 2: An example of a multiscale domain decomposition. The microresonator system is partitioned into molecular dynamics (MD) and finite element (FE) or coarse-grained molecular dynamics (CGMD) regions. A narrow handshaking region is used to couple the FE and MD regions; in the case of CGMD, the cross-over to atomistics for atomic-sized cells is completely smooth and no handshaking region is required. [8]

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 many-body potential that gives the forces between atoms. Stillinger-Weber [14] and Tersoff [15] potentials have been used for the silicon resonators. [8] In the CG region, the equation of motion is of the finite element form (cf. [16]):

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

where M_{ij} is the mass matrix, K_{ij} is the tensorial stiffness matrix and $\vec{u}_j$ and $\ddot{\vec{u}}_j$ are the displacement and acceleration at node j, respectively. The ellipses indicate additional terms arising from external and anharmonic forces. [8], [17]

In conventional finite element modeling, the mass and stiffness matrices are determined from the density and elastic constants of the material, together with a specification via shape functions of how the displacement is interpolated between nodes of the mesh. In CGMD, the mass and stiffness matrices of Eq. (1) are derived directly from the underlying atomistic model without recourse to continuum properties like the elastic constants. This is done through the constraint that the positions of the atoms should agree with the interpolated nodal displacements in a best-fit sense, but internal relaxation and thermal fluctuations about this mean field are allowed. Statistical mechanics tools then

permit the analytic calculation of the CGMD energy in terms of the nodal variables, and hence their equations of motion. 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 allows the modeling of larger systems sizes than would otherwise be possible with the given computer resources. Also, CGMD has certain advantages over a straight finite element/molecular dynamics hybrid approach. Conventional finite element models do 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.

The original formulation of CGMD is a Hamiltonian system. Thermal effects are present, but not the random, dissipative forces due to the heat bath of modes that have been integrated out. Energy is conserved. Recently, a non-conservative version of CGMD has been developed [17] 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 have been used to derive a generalized Langevin equation that solves this problem.

3 ATOMISTIC EFFECTS IN NEMS

The conventional description of the mechanical components of MEMS is based on continuum mechanics implemented in a finite element model. [16] 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 the linear elastic theory of macroscopic beams such as resonators, 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.

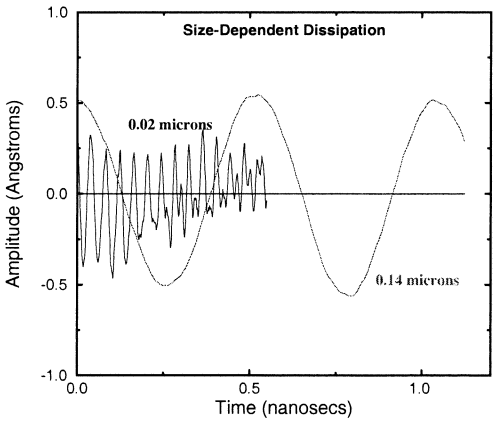

Figure 3: Comparison of the oscillations of resonators of two different sizes but with the same aspect ratio. Both are at room temperature. Note the increased dissipation in the smaller resonator. This is due to a mode-mixing effect coming from lattice anharmonicity. [9,19]

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 entirely the case, however, because the lattice constant (the interatomic 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.[18] 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 the contribution of surface stress in addition to the bulk elastic constants. These results are explained in detail elsewhere [9], [19] (see also [20]), 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. [3] 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. [3], [1] Most GHz resonators have a very low Q, but the use of single crystal resonators would eliminate many dissipative processes and hold the hope of relatively high Q values. In fact, our simulations [9] and experiments [21] 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. [9] 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, as energy is transferred from the fundamental mode into the other normal modes of the oscillator.

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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