

MEMS from the nanoscale up

Before microsystems can fulfill their promise, engineers have to understand that the macroscale rules don't necessarily apply.

by Arthur C.
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Over the past decade, silicon microelectromechanical systems technology has gradually increased its foothold in mechanical engineering. Favored for their low cost, reliability, and small size—qualities inherited from the integrated circuit manufacturing process—relatively simple MEMS devices began finding their way into consumer applications a decade and a half ago.

Something else was happening back then. At the time that the market was benefiting from microscale automotive airbag sensors and inkjet modules, considerably more complex microsystems were being considered for use in space applications, where miniaturization is a prime goal in the design of military and non-military payloads alike. Such payloads are limited in terms of mass and volume, so when a new function needs to be added to the system, it must be accomplished through miniaturization.



Researchers believe microsystems can become mighty mites.



Administration.)

Sandia then had a state-of-the-art microelectronics fabrication facility that would provide the physical environment, and much of the engineering talent, to take on this new initiative. The 74,000-square-foot Microelectronics Development Laboratory included 12,500 square feet of Class I clean room space. With the growing interest in silicon MEMS technology, part of these new facilities was turned over to the new enterprise, and a new cadre of scientists and engineers began to start work on advanced microsystems that could "sense, think,

It was not surprising, then, that beginning in the late 1980s, Sandia National Laboratories began to look at MEMS for solutions in its continuing mission to improve and modernize ordnance systems required for the U.S. nuclear stockpile. (Sandia is operated by Sandia Corp., a Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security

act, and communicate."

While focused on the needs of the U.S. nuclear weapon complex, it could be assumed that these innovations would also spur new developments in the commercial arena: automotive and consumer products, telecommunications, radio-frequency applications, and medical care.

Out of Proportion

Sandia's new MEMS team began work on a number of relatively complex designs in the early 1990s, and in 1994 demonstrated a micro steam engine that used resistive heating to provide steam from a drop of water. The engine seemed at first to require simply scaling from meters to microns.

Remarkably, it worked without seals because the attractive interfacial force between surfaces was sufficient to prevent the loss of steam. The increased surface-to-volume ratio with decreasing size led to the self-sealing nature of the design. This was an important early indicator that, as structures are scaled to smaller and smaller size, elements of mechanical, optical, and chemical understanding needed to be revisited.

In fact, the micro steam engine gave early notice that, if you really want to excel in MEMS, you need to understand the dominant transport processes and material interactions at the micro- and, more likely, at the nanoscale. Certain processes, such as chemical mechanical polishing to planarize polysilicon layers, were inherited from standard microelectronics fabrication procedure. But new "fixes" had to be found as the fledgling MEMS industry moved farther from its parent technology, and the design assumptions derived from observation of large-scale phenomena became less dependable.



At about this time, Sandia also was tackling a couple of major problems in the design of

Silicon-based MEMS devices must be constructed in clean rooms, such as this one at Sandia's Microelectronics Development Laboratory.

micromechanical actuators. While MEMS sensors were already a marked success, the micro-actuators of the time suffered from low torque and an inherent difficulty in coupling tools to engines. Sandia's solution was revolutionary: a new, four-layer polysilicon micromachining process that made it possible to make the more complex devices that were needed to solve the actuator riddle.

The process incorporated three movable levels of polysilicon in addition to a stationary layer for a total of four layers of polysilicon. These were separated by sacrificial oxide layers, and an additional friction-reducing layer of silicon nitride was placed between the bearing surfaces. When completed, the resulting micro-engine consisted of two sets of comb-drive actuators that drove a pair of linkages that in turn drove a pair of rotary gears. The smaller gear (0.03 mm in diameter) was successfully operated at speeds in excess of 300,000 rpm, and the larger (1.6 mm diameter) gear as fast as 4,800 rpm. Unfortunately, scanning electron microscopy images taken after only 477,000 cycles clearly showed the buildup of silicon debris, abraded from moving parts of the device.

This failure mechanism provided an invaluable lesson for the Sandia design team. The search for an in-depth understanding of wear mechanisms in dynamic silicon MEMS—so elusive and yet so important—would drive an ambitious wave of leading-edge research into microscale

science and engineering, distinct from that which prevailed at the mesoscale.

The design of multilevel two-dimensional silicon devices (so-called 2.5-D designs) continued apace. Before long, these complex computer-aided designs evolved from four to five levels (trademarked by Sandia as SUMMiT IV and SUMMiT V, respectively). But as these designs became more complex, performance issues associated with adhesion, friction, wear, strength, toughness, impact tolerance, fatigue, and creep phenomena became increasingly important.

Significant Forces

Stiction, the combined effects of sticking and friction between surfaces, proved particularly troublesome in MEMS devices from the outset. For structures with thicknesses of a few tenths to several micrometers and lateral dimensions of tens to hundreds of micrometers, significant forces are required to pull apart two surfaces in contact and to initiate motion. Additionally, controlling surface adhesion for materials with high surface energies like polysilicon requires special consideration.

There are two aspects to stiction. The first is the surface tension of the meniscus of liquids, which can pull the surfaces of micromechanical parts together as they are removed from liquid during wet processing (critical steps in SUMMiT IV and SUMMiT V MEMS production). The second problem is the tendency of surfaces to stick together once they touch. Sandia successfully used strategies such as drying in supercritical CO₂ and freeze sublimation to deal with the first problem.

The second problem was alleviated through the application of coatings with low energy surfaces at the final stages of fabrication. The application of self-assembled monolayers like octadecyltrichlorosilane, which adheres strongly to SiO₂ surfaces and presents a surface monolayer of tail groups that have low sticking and friction properties, lowered demonstrated adhesive forces by orders of magnitude.

Failure provided an invaluable lesson. Anti-adhesion design, supercritical drying, and hydrophobic surface

The search for an

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monolayers all help to treat the headaches that occur when van der Waals forces "glue" silicon to silicon. But stiction remains a troublesome problem despite these improvements, and continues to be an important contributor to device failure.

For this reason, newer Sandia MEMS designs minimize the contact of moving parts wherever possible, during normal operation and in the event of abnormal occurrences such as mechanical shock and electrostatic discharge. This can be a very difficult goal. For example, while reducing the amount of surface area rubbing during operation to a minimum is a worthy objective, no method for doing this has yet been devised.

Sandia designers were now taking on the challenges of incorporating changes in behavior into new machine principles at the microdomain, rather than struggling with problems arising from conventional designs. For several years now, a large-scale effort has been devoted to increasing the understanding of surface phenomena (i.e., van der Waals, electrostatic, capillary forces) operating in submicrometer silicon structures. Here, computational simulation has been important to understanding MEMS performance. Adhesion and electrostatic models have been added to Sandia-developed finite element simulation codes such as Adagio and Presto to model structural deformations.

Shedding Light on Heat

Thermal management is similarly important because surface micromachined (SMM) electrothermal actuators rely on thermal processes to deliver work. Modeling phonon-phonon, phonon-grain boundary interactions, and "non-continuum" heat transfer in gases have all proven to be important in predicting the overall, systemic behavior of MEMS devices.

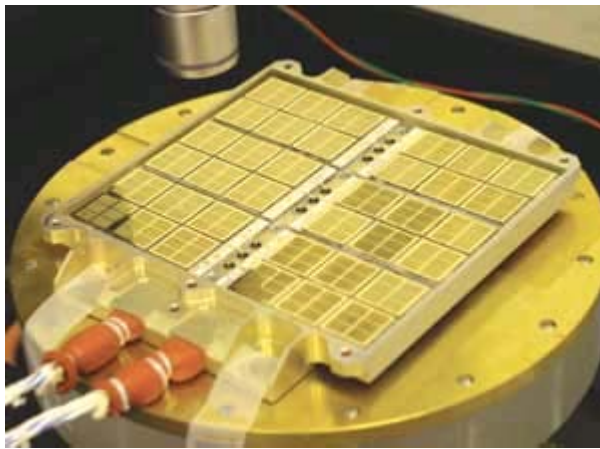
For example, non-continuum heat transfer in gases occurs when the typical distance between gas molecular collisions becomes comparable to the system length scale.

In this case, our normal continuum assumptions like Fourier's law of heat conduction and the continuous-temperature boundary condition—that the gas temperature equals the solid temperature at their interface—begin to break down. Normally, this isn't a concern, since gas molecules travel less than a tenth of a micrometer between collisions—but for microsystems dimensions of one micrometer or less are encountered and we can no longer ignore these phenomena.

Similarly, non-continuum heat transfer in solids begins to appear when phonon-collision length scales become comparable to system dimensions. Left without the convenience of our continuum assumptions, prediction of non-continuum heat conduction requires the simulation of individual quantized lattice vibrations or phonons as they move and interact—typically using statistical (Monte Carlo) techniques.



Heat management is an important concern for satellites such as the Space Technology 5 (above), launched last year. An array of MEMS-based shutters installed onboard the satellite open and close via moving microscale actuators.



Based on the results of these complicated (and time-intensive) methods, subgrid analytical models can be built to capture these non-continuum effects and to couple with standard continuum finite element models for large-scale system analysis.

Progress has been made both in improving the SMM design and in qualifying its performance as a result of accurately capturing these non-continuum phenomena in thermal analysis codes. By incorporating more reliable models in design, the number of design-testing cycles has been reduced, and pretest predictions are becoming more reliable.

Explaining Failures

In 2004, Sandia demonstrated a coupled-physics analysis code to simulate electrical, thermal, and mechanical response of SMM microactuators. These "bent-beam" devices operate when current is pushed through an anchored V-shaped beam, expanding the beam with Joule heating (due to the electrical resistance of the structures) and causing the apex to move forward. Joule heating is also a function of voltage, current density, specific resistivity, and geometry. Such devices will operate at up to 60 million cycles without failure at moderate operating temperature—that is, less than 600 K. At temperatures greater than 900 K (1,600°F) and with an increasing number of cycles, stresses within the structural members will change and cause failure. One explanation for the failure suggests the grain sizes in the material increase and surface topology becomes roughened.

The number of Comparison of code predictions

unknowns that remain is substantial, and grows larger as designs become more complex. But the problems are by no means insurmountable; they are just taking longer to solve than we anticipated.

resistivity and conduction, using Raman spectrometry diagnostics to obtain measurements at the submicron scale. And while continuum models predicted that the temperature is continuous at the beam-air interface, Direct Simulation Monte Carlo "non-continuum" simulations showed that the opposite was the case. That is, a temperature jump occurred at the beam-air interface.

This "non-continuum" effect again showed the stark differences between micro- and meso-scale physical effects in structural dynamics, and the folly of assuming that models for processes that are useful in designing relatively large devices can be applied to dynamic MEMS geometries.

We also found that "gas damping" between MEMS structures and the substrate, within the sealed package, can cause serious nonlinearities. While this doesn't lead to failure in the classic sense, it may make it harder to close a switch. On the plus side, gas damping can provide a cushion that enables a MEMS device to survive surprisingly high shock loads.

Growing Pains

The quest to ensure the reliability of complex MEMS devices has yielded impressive results at Sandia and elsewhere, as illustrated by manufacturing and packaging improvements and increased understanding of the physical phenomena that affect reliability at the submicron level. The relative infancy of MEMS manufacturing disciplines, and to some extent the

from a "non-continuum" thermal model with a "continuum" thermal model yielded striking results. In analyzing the heat transfer in the resistivity-heated microscale beam actuator, the traditional "continuum" model predicted a beam temperature (after cycling) of 750 K, while the "non-continuum" technique model predicted a temperature of 900 K. Researchers experimentally confirmed the higher temperature, a consequence of grain scale property changes including

restrictions posed by corporate proprietary protection of its intellectual property and the painfully slow emergence of industry standards, has resulted in slower MEMS technology development and infusion into the commercial sector than was expected in the 1990s.

What has emerged in the past decade is the recognition that more data on materials and on the underlying physics is needed to move MEMS technology forward. This will require that we make noninvasive, high-quality measurements at the scale of the devices—in itself an extremely difficult task because of the small size and the large influence of the surrounding structures.



The Microlab and Microfab facility was completed last year. Replacing a lab built in the 1980s, the building has space for more than 250 workers.

For example, if they are to optimize their designs, MEMS engineers need a greater understanding of the role of coatings and surface roughness on adhesion: Why is it that a rough surface with a few contacts may provide less friction than two smooth surfaces with high adhesion? Modeling and simulation can help with the answer, but only if the essential physics is captured in the model.

The bottom line in the MEMS engineering story is designing for reliability, to assure fatigue-free behavior over hundreds of millions of cycles, during which the physical properties of the device remain virtually indistinguishable from those of a newly minted device. To do this, we know that contacting surfaces should be minimized; that planar surfaces should be positioned to minimize contribution of van der Waals forces; that stress in polysilicon elements should be kept to 10 percent or less of the measured fracture strength for the material and process in use. And more. And we know that this is just the start of the quest.

The number of unknowns that remain as we unscramble the nano- and microscale mysteries of the MEMS phenomenon is indeed substantial, and grows larger as designs become more complex. But the problems are by no means insurmountable; they are just taking longer to solve than we had anticipated. A number of reliability-connected improvements have been noted above.

Microscale Enabled Solutions

In addition, modeling and simulation can provide valuable insights on how to enhance the MEMS device performance, discover flawed designs before fabrication, and enable design optimization. As an example, process improvements augmented after modeling and simulation were responsible for increasing yields from a mere 20 percent to more than 90 percent for the micromirror arrays, used for optical switching, made by the Sandia spin-off company MEMX. Each of these arrays contains more than 100,000 mechanical elements. Today they will function for more than half a trillion cycles at 70°C without failure.

While MEMS has not yet lived up to the optimism of the 1990s, enhanced understanding of scale-dependent physics is helping us to make progress toward the buoyant expectations voiced during those times. We are moving from the early, relatively unenlightened days of "making macro solutions smaller" to doing things a new way, through "microscale enabled solutions."

We have learned a lot. Engineering at the microscale introduces an appreciation of the complex physics at the feature scales of the devices. It demands the appreciation of a ground-up approach to design and problem-solving, and full acknowledgment of the importance of nano-phenomena that run from van der Waals forces to the collision of phonons with grain boundaries. Ideas like "micro-enabled solutions" and the related need for "scale aware" tools arise as modeling becomes accepted as an integral part of the product realization cycle.

As these new perspectives evolve into reality, a new breed of engineer is also coming into existence. In fact, the distinction among the computer scientist, the materials scientist, and the engineer is becoming blurred. Mechanical engineering cannot help but benefit from this

exciting new horizon. MEMS is here to stay, and it will transform the future.

CAD for MEMS

The lack of computer-aided design infrastructure held back early work in silicon microelectromechanical systems technology.

While MEMS drew heavily on existing integrated circuit technology, the related CAD packages were not very compatible with integrated microsystems, which employ much more complex shapes.

For example, they were not well suited for describing a frame shape, which is in effect a rectangle with a smaller rectangular hole in it, and were quite inadequate when designing something as complicated as a gear with involute gear teeth and 1,000 etch release holes. A similar problem existed in the case of simulation packages, which were excellent in simulating electrical behavior, but ineffective when mechanical, optical, or other structures were introduced onto the chip.

While companies such as Microcosm Technologies and Tanner Research made early progress in addressing these issues, much of the design work was guided primarily by rules of thumb.

Since those days, the challenges of scale have been addressed by applying an increased understanding of the nanoscale physics that becomes an increasingly important factor in device reliability as feature sizes become smaller. To a very large degree, this increased knowledge is being enabled by computational simulation.

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