SEMI Modeling and Simulation Roadmap

In this article we introduce the “Modeling and Simulation” chapter of the International SEMI MEMS/MST/Micromachining (M3) Technology Roadmap. The purpose of this article is to provide a framework to initiate discussion with the Microsystems Technologies (MST) community, and thereby solicit input from practitioners in all facets of this technology. Over the coming months, we anticipate integrating input from a variety of sources to develop this critical chapter of the roadmap.

Executive Summary

With the exponential growth in the power of computing hardware and software, modeling and simulation is becoming a key enabler for the rapid design of reliable Microsystems. One vision of the future microsystem design process would include the following primary software capabilities:

1. The development of 3D part design, through standard CAD packages, with automatic design rule checks that guarantee the manufacturability and performance of the microsystem.
2. Automatic mesh generation, for 3D parts as manufactured, that permits computational simulation of the process steps, and the performance and reliability analysis for the final microsystem.
3. Computer generated 2D layouts for process steps that utilize detailed process models to generate the layout and process parameter recipe required to achieve the desired 3D part.
4. Science-based computational tools that can simulate the process physics, and the coupled thermal, fluid, structural, solid mechanics, electromagnetic and material response governing the performance and reliability of the microsystem.
5. Visualization software that permits the rapid visualization of 3D parts including cross-sectional maps, performance and reliability analysis results, and process simulation results.

In addition to these desired software capabilities, a desired computing infrastructure would include massively parallel computers that enable rapid high-fidelity analysis, coupled with networked compute servers that permit computing at a distance.

We now discuss the individual computational components that are required to achieve this vision. There are three primary areas of focus: design capabilities, science-based capabilities and computing infrastructure. Within each of these areas, there are several key capability requirements.

Design Capabilities

Geometry Capture/System Layout/Standard Cell Libraries
Micromechanics provide real challenges to the design/geometry capture infrastructure. Unlike microelectronics, micro-mechanical systems are not laid out on “Manhattan” geometry. Furthermore, the lithographic nature of the processes forces the designer toward creating 2D mask layouts. Machine design will be greatly enhanced by the creation of tools that allow the designer to work in either 2D or 3D and use incorporated process information to convert between them. The design tool should also provide a seamless path to 3D analysis tools and contain a robust library of standard parts and components.

Visualization
A challenge to designers in multilevel processes is to visualize the results of processing on each level and understand the interdependencies. Designs would greatly benefit from a visualization tool that built a visual model of the final product using process information and all masks definitions. The tool would have greater utility if it provided both 3D representation and arbitrary cross sectional capability.
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Basic functionality/Parametric Design/Tradeoffs

There are two types of users of analysis tools: designers and dedicated analysts. Designers are interested in exploring the solution space quickly and will frequently give up precision while doing so. Their goal is to understand basic cause-and-effect and to quantify design parameters. The designer desires to perform parametric studies and places a premium on model flexibility. Near the end of the detailed design phase, the design is frequently passed to a dedicated analyst. Analysts create models with more detail than designers. Their efforts are used for design qualification and troubleshooting. The analyst's tools must be capable of solving larger problems and with more complex subgrid physics. The suite of tools used by designers and dedicated analysts should be completely compatible so that the models created by the designers can be readily shared with dedicated analysts and vice versa.

Artificial Intelligence Design Rule Checking

Microelectronics designers use design rule checkers (DRC) to insure that their designs do not violate fabrication rules of the foundry. Micromachine designers would benefit from similar tools. A DRC would provide feedback about aspect ratios, etch release systems, side wall angles, etc. The utility of the tool would be enhanced if it included process variability information with a mechanical tolerance algorithm.

Science-Based Capabilities

Material Properties

Material microstructure takes on added significance at the microscale where grain size can become comparable to part dimensions. In these situations, material properties can become highly nonuniform and anisotropic. Accurate determination of these material properties is critical to science-based simulations of component performance and reliability.

Phenomenology

As the size of a mechanical system decreases, its surface-to-volume ratio increases. In Microsystems, surface phenomena such as adhesion, friction, and interfacial dynamics can become more dominant than bulk phenomena such as inertia and body forces. When modeling the behavior and response of a microsystem, surface effects need to be captured accurately in order to obtain reliable predictions. The present understanding and modeling capability of surface phenomena in Microsystems is only adequate. For example, studying stiction requires calculation of the adhesion energy for any given contact surfaces under various conditions. Currently very limited data and validated models exist.

To prevent stiction during the final stage of the release process or to minimize wear during the operation conditions, the surfaces of Microsystems are usually treated by applying either a self-assembly-monolayer (SAM) coating, a coated diamond film, or any coating that can harden the surface. Thus the characteristics of the coated surface and its interfacial dynamics under various environments and the evolution of its microstructure with time (aging effect) are very important. Research activities on this model development and validation are required.

Modeling and simulation can advance the fabrication and manufacturing processes of Microsystems including the process of surface coatings. It can identify the dominant parameters in chemical vapor deposition (CVD) reactor dynamics, micro-feature development, and coating mechanism. With better understanding and control, process variations can be minimized, which in turn will result in more reliable materials for Microsystems.

Analysis & Solver techniques

In general, the computational analysis tools required to simulate microscale phenomena will be different than those required to simulate macroscale phenomena. Even if continuum mechanics are still applicable, the assumptions of material homogeneity and isotropy will fail when length scales approach those of the
mean free path in fluids and approach the grain scale for solids. However, the continuum assumptions of fluid and thermal transport will also fail at sufficiently small scale. Therefore, in analyzing microscale systems, careful analysis of the appropriate transport equations and material properties is required to ensure that the governing physics is captured.

For those cases in which modeling the microstructure becomes necessary or the continuum assumptions become invalid, particle simulation techniques such as molecular dynamics or the DSMC approach may become appropriate. However, these approaches can become computationally intensive necessitating the need for coupling of these particle techniques to continuum approaches, where appropriate. Work is required to establish analysis approaches for bridging between the continuum and non-continuum limits.

**Coupled phenomenology**

The simulation of manufacturing processes and component performance typically involves the solution of coupled physics. For example the simulation of LIGA electroplating involves the coupled simulation of fluid flow, electrochemistry, electrodynamics and thermal transport. The simulation of electrostatically driven microsystems can involve the simulation of coupled solid mechanics, structural dynamics, fluid mechanics, electrostatics and thermal transport. These coupled physical phenomena require robust solution strategies that can capture the disparate time and length scales characteristic of multi-physics.

**Verification and Validation**

Advanced computational tools require ongoing verification of the software and validation of the material models, phenomenology and integrated tools. Verification is the process of confirming that the software accurately represents the scientific model used to describe the phenomena. Validation is the process of confirming that the scientific model accurately captures the relevant physics.

**Computing Infrastructure**

**Evolution of Platform Capability**

The continuing evolution of computing platform capability permits a continuous evolution in our desktop capabilities and high-performance computing capabilities. In particular, the high performance computing capabilities of today become the desktop capabilities of tomorrow. In 1983, high performance computing was defined by the Cray 1S computer. This computer has less compute power than today’s low end Intel Pentium class processors. Today’s high-performance parallel computers have six orders of magnitude more compute power than the supercomputers of the early 1980s. It is anticipated that today’s Teraflop high performance massively-parallel computers will become the desktop machines of the future. As this evolution of computing capacity continues, the fidelity of our computational models will continue to evolve providing the desktop designer with ever-more sophisticated design tools.

**Interactive distributed infrastructure**

With the continued evolution of high-speed networking, object oriented programming and high performance computing, we anticipate that interactive distributed design infrastructures will become more prevalent. Within this infrastructure, component design, manufacturing process design, and optimization of design and process will occur concurrently across multiple platforms driven by a designer at his desktop. These complex distributed simulation tools will share a common interface permitting interoperability of modules and allowing rapid implementation of new and enhanced design and manufacturing modules. This capability will dramatically reduce the design cycle time for new microscale components.

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