Editors: Ken Hass, khass1@ford.com
Thomas L. Tysinger, tlt@fluent.com

COMPUTATIONAL MATERIALS SCIENCE AND INDUSTRIAL R&D: ACCELERATING PROGRESS

By Sharon C. Glotzer and James A. Warren

COMPUTATIONAL MATERIALS RESEARCH HAS MADE MAJOR ADVANCES OVER THE PAST DECADE IN ACCELERATING THE DESIGN, PROCESSING, AND PROPERTY OPTIMIZATION OF TECHNOLOGICALLY IMPORTANT MATERIALS. MATERIALS SIMULATION IS still in its infancy, however, as the nature of materials problems are so complex. Fortunately, as computational power has grown, so too has our ability to attack increasingly challenging materials problems and pose increasingly difficult questions. To fully capitalize on these advances and accelerate the integration of computational materials science into day-to-day R&D, we must work to strengthen the infrastructure for computational materials research and identify, develop, and focus the resources and talents of the computational materials science research community.

The road to come

For the foreseeable future, molecular and materials simulation will play an increasingly important role in guiding materials R&D. Advances in computational quantum chemistry, forcefield development, molecular and mesoscale simulation, and the bridging of atomistic, mesoscopic, and macroscopic scales will both improve the processing and facilitate the rational design of new and better materials. Because of this, industrial R&D labs are hiring more computational scientists today than ever before, and these numbers promise to increase as our ability to make relevant and accurate predictions and provide useful insight continues to grow. Despite great successes, however, substantial barriers to progress remain that must be addressed for materials computation to become a regular part of day-to-day R&D in all industry sectors.

Education. The widespread application of materials simulation is predicated on the existence of an appropriately educated scientific workforce. Thus, a particularly important bottleneck to progress is in the area of education. Recruiting computationally inclined students to the discipline of materials research is an ongoing challenge both in US companies and abroad. Students need to be informed about the growing demand for computational materials researchers, particularly in this age of unprecedented dot.com and Wall Street career opportunities for computational scientists. In light of this demand, the academic research community must make greater efforts to integrate materials modeling and simulation into the undergraduate and graduate core curriculum. Eventually all research scientists will need to know something about modeling and simulation, if only to interact and col-

Useful links

To learn more about the programs discussed in this article as well as roadmapping activities relevant to computational materials science, please visit these Web sites:

www.oit.doe.gov/chemicals/page9.shtml
http://itri.loyola.edu/molmodel/welcome.htm
www.cse.dl.ac.uk
www.ctcms.nist.gov
http://cmpweb.ameslab.gov/ccms
http://psi-k.dl.ac.uk
www.susqu.edu/facstaff/B/brakke/evolver/evolver.html

laborate with their computational colleagues. In industry, where research is done in teams, this will be especially true as computational scientists become an integral part of these teams. For this reason, we must increase access to education and training in materials modeling and simulation. Finally, because materials research is by its nature multidisciplinary, the curricula that we develop in materials modeling and simulation must be multidisciplinary as well.

Tools. Even the best-trained artisans cannot perform their craft without the proper tools. In the area of materials modeling and simulation tools, there are several Web sites that distribute codes benevolent developers have donated. You should generally use these codes with a certain sense of caveat emptor, however, because they usually come with no guarantee with regard to accuracy or validity. The same can be said of many of today's commercial codes—despite enhanced GUIs that make these tools easier to use for experts and nonexperts alike. Today, most materials research codes are still developed in-house for a particular research problem or application, and they are typically easily used only by the person who wrote the code. Thus, revolutionary progress in materials computation will require our community to address issues of "code development infrastructure," such as

- standards for data structures, I/O, and GUIs;
- code standards for portability and interoperability;
- object-oriented programming and materials simulation toolboxes;
- systematic validation of codes, methods, and force fields;
- benchmarks for validation and quantification of uncertainties;
- problem-solving environments and expert systems for materials modeling and simulation;
- scalable codes to facilitate the use of multiprocessor machines;
- software tools to interact with, mine, and extract knowledge from large data sets ("mat-informatics"); and
- materials modeling and simulation Web portals for increased access to tools.

Finally, as a community, we must strive to bridge the gap between academic and commercial codes and encourage competition in the commercial materials modeling and simulation software industry.

Programs

Like the Japanese government and the European community, the US government has recognized the need to increase support for computational science. In particular, programs such as the National Science Foundation's Information Technology Research program, the new National Nanotechnology Initiative, and the Department of Energy's new program in Scientific Discovery Through Advanced Computing will help accelerate progress in the development of materials modeling and simulation infrastructure.

There have been several recent reports and roadmapping activities in computational chemistry and molecular and materials modeling and simulation. One of the outstanding needs identified is the coordination of activities in computational materials science. This should come from a neutral party that can pull together key people across disciplines, identify critical bottlenecks and challenges, focus goals and objectives, and organize efforts toward progress on precompetitive research topics. Several government-sponsored programs have taken a first step in this direction. One example is the newly established DOE Computational Materials Science Network (cmpweb.ameslab.gov/ccms). Another is the Center for Theoretical and Computational Materials Science (CTCMS) at the National Institute of Standards and Technology (NIST) in Gaithersburg, Maryland. Founded in 1994, the CTCMS's mission is to accelerate progress in computational materials science and its impact on US industry. To achieve its mission, the CTCMS holds and sponsors workshops on computational materials science methods and applications, identifies key problems in materials research where modeling and simulation could enable real progress and multidisciplinary efforts offer the best attack, and assembles teams ("working groups") of researchers from universities, industry, and government and national labs to attack the problem collaboratively. By providing small amounts of "glue money," the CTCMS helps enable collaboration between the team members.

The goals of each CTCMS working group are different. They might include several of the following: developing a computational tool or technique, designing a piece of software, facilitating the simulation of a particular process or set of material properties, gaining insight or understanding on a particular problem, or developing a set of rational design principles. The format for collaboration varies from group to group and evolves to fit both the group's dynamics and the needs of the project. To illustrate how the CTCMS facilitates progress in computational materials science, we review three examples of CTCMS working groups.

Micromagnetic modeling of materials. The micromagnetic modeling of materials (μmag) working group developed out of a need for validated software tools capable of accurately predicting the domain structures of magnetic materials for devices such as disk drives. At an Intermag meeting in 1995, NIST sponsored an evening symposium aimed at determining the state of the art in current modeling tools the community uses, many of which were home grown and some of which were developed by commercial software vendors. The consensus of the roughly 60 attendees was that in the absence of validated micromagnetic-modeling tools, future progress would be delayed because the current tools' users had no simple and reliable way of confirming the validity of the predictions of the tools they were using in the context of real-world applications. To gauge the current software's accuracy and validity, the attendees agreed on a standard problem that each would solve using his or her favorite micromagnetic modeling software package.

They submitted their solutions to the NIST principal investigators, who posted the results anonymously on the CTCMS Web site (www.ctcms.nist.gov/mumag). That none of the solutions agreed confirmed the community's suspicions (see Figure 1). As a result, a CTCMS working group was formed with three goals: establish a forum for developers and users of micromagnetic modeling tools; identify standard problems to serve as benchmarks and provide a vehicle for validating software; and develop public-domain, validated, standard reference micromagnetic-modeling software that could be used alone or to validate commercial or in-house software.

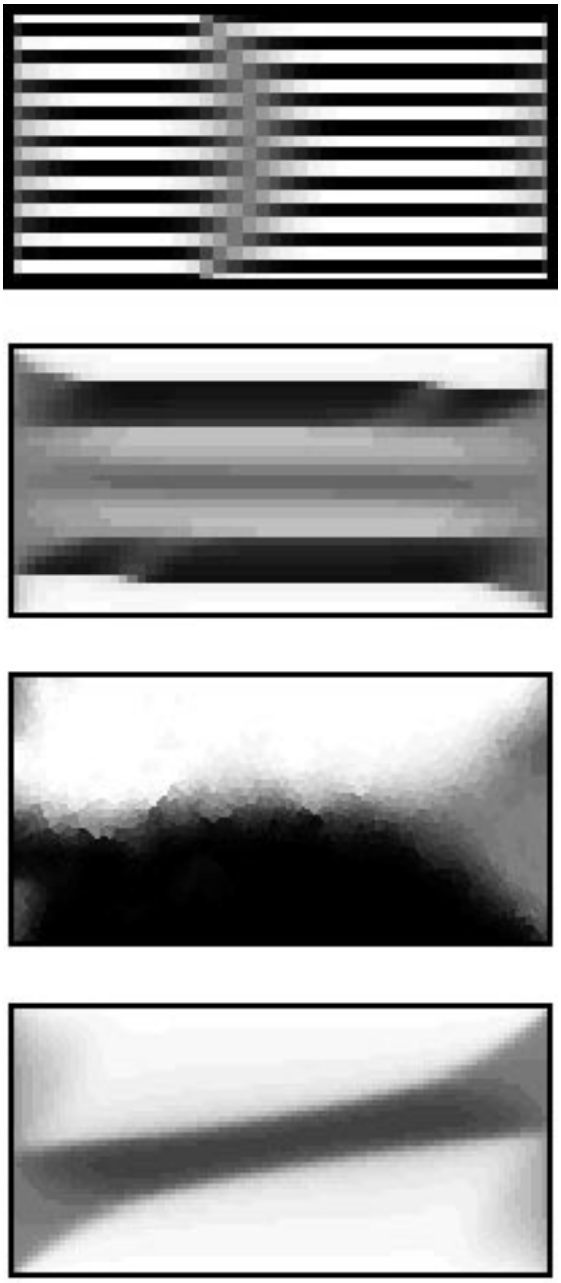

Figure 1. Comparison of four anonymously submitted solutions to μmag standard problem one. The images show the calculated *y*-component of the remnent state after field saturation along the short (*x*-) axis of a permalloy rectangle, as predicted by the submitters using their in-house or commercial codes. Submissions on other standard problems show better agreement.

For more information on this working group's activities, μmag standard problems, and the NIST-developed object-oriented micromagnetic-modeling framework OOMMF, visit www.ctcms.nist.gov/mumag.

The Solder Interconnect Design Team. NIST's Solder Interconnect Design Team (SIDT) was formed to address several pressing issues in the design and fabrication of circuit boards. The multibillion-dollar microelectronics industry depends on solder interconnects as the primary method for attaching chips to a circuit board. Over the past six years, the team of academic, industrial, and government researchers has established an agenda for solving modeling problems concerning equilibrium solder joint shapes and the resulting thermal and mechanical properties of the formed joint.

The SIDT's goal is to provide the industrial community with a suite of useful software tools for solder interconnect design and to provide standard reference problems. With this in mind, the SIDT actively supports the development of modeling tools based on the public-domain program Surface Evolver, which has proven to be extremely ef-

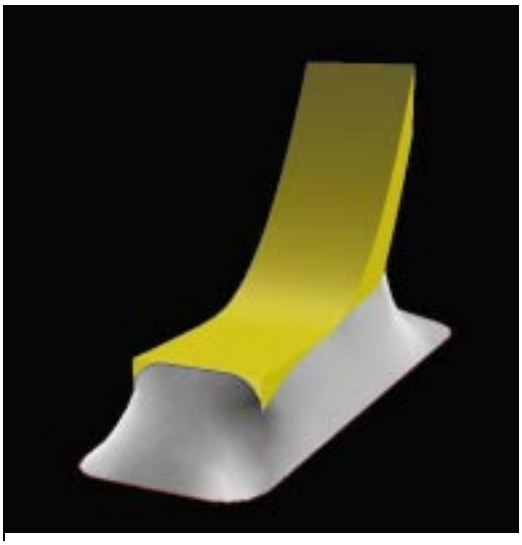

Figure 2. A Surface Evolver calculation of the geometry of a solder drop in a gull-wing lead configuration. The lead is shown in yellow, and the solder is shown in gray. (Figure courtesy of Daniel Josell, Daniel J. Lewis, and James A. Warren.)

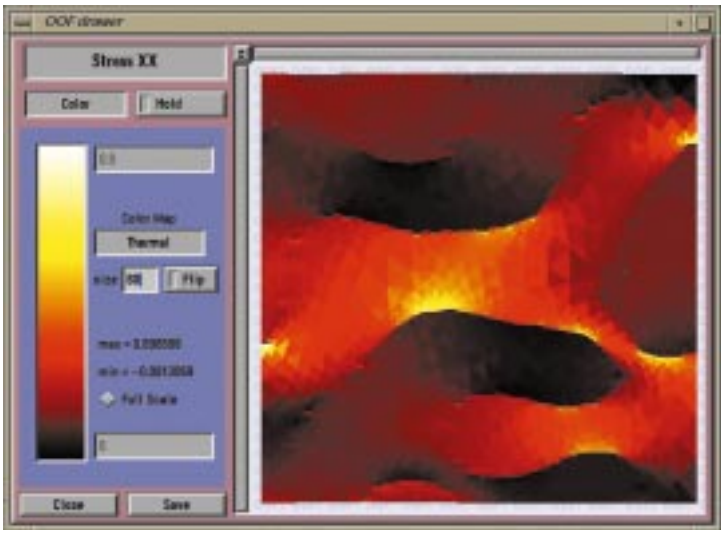

Figure 3. An example of an OOF mechanical property calculation on a simulated microstructure of an ultrathin polymer blend film resulting from phase separation. The microstructure has been subjected to a small longitudinal deformation. The bright spots indicate regions of high local stress and occur in the lower modulus phase. (Figure courtesy of Sharon C. Glotzer, Edwin R. Fuller, and Charles C. Han.)

fective for computing equilibrium solder meniscus shapes (see Figure 2).

The NIST CTCMS has established and fostered an industry–academia–government laboratory working group on solder joint design for the exchange of information and collaboration on topics of special importance. The SIDT acts as a forum for discussion of Evolver calculations and models, and, through the CTCMS, it provides access to software through the Internet. Software downloads from the SIDT Web site number in the thousands per year. The SIDT also seeks to hold workshops and symposia to promote collaboration and bring the community toward a consensus on the features required for a useful solder modeling system.

Object-oriented modeling tools for materials microstructures. In an effort to provide the materials community with a software tool capable of predicting properties of materials directly from their microstructures, W. Craig Carter (now at MIT), Edwin R. Fuller, A.R. Roosen, and Steven A. Langer of NIST invented OOF, which actually consists of two computer programs, `oof` and `ppm2oof`. `ppm2oof` reads a microstructure's image, either an experimental micrograph or a simulation's output, and lets the user assign material properties (such as elasticity moduli and thermal expansion coefficients) to the different phases or grains. The code generates a finite element mesh, which `oof` then reads. `oof` lets the user perform virtual experiments on the microstructure (such as applying forces or changing the temperature) and observe the micro- and macroscopic effects (such as local stresses and strains or global effective elastic properties; see Figures 3 and 4).

OOF's object-oriented framework allows new material properties to be added quickly and easily. OOF is already being used as a research tool in industry and academia, as a teaching tool in undergraduate and graduate materials science and physics courses, and as a measurement tool, ensuring that manufactured microstructures have the desired properties. Users can add modules to OOF and connect it to their own code, either using it as a postprocessor (to analyze simulation results) or a preprocessor (to generate stressed microstructures for analysis by an external program).

Currently, OOF deals with thermoelastic responses to stress, strain, and uniform temperature fields. Properties that OOF can calculate include macroscopic expansion, maximum and minimum stresses, rudimentary fracture and damage initiation, and transformation stresses.

OOF received an *Industry Week*

"Technology of the Year" award in 1999, being cited as one of the top 25 technologies of 1999 most likely to "make a difference in the global economy." The next version of OOF, now under development at NIST, will facilitate the incorporation of new fields and models by OOF users. (You can download `oof` and `ppm2oof` at www.ctcms.nist.gov/oof.)

In addition to the three working groups described here, there are several other CTCMS working groups, including groups focusing on problems in soft materials and complex fluids. Other tools developed under the auspices of the CTCMS include Wulffman (a 3D crystal shape constructor) and the Green's Function/Boundary Element Method Web site. Visit www.ctcms.nist.gov for more information on CTCMS activities.

Many outstanding opportunities in materials modeling and simulation exist. A major challenge for the future is the first-principles prediction of properties and behavior of soft materials, including polymers, foams, liquid crystals, emulsions, and colloids. Because of the hierarchy of complexity inherent to these classes of materials, the bridging of insight, information, and techniques over many length and time scales will be crucial for progress. Mesoscale modeling—which covers the broad range of length scales between atomistic and macroscopic—is a frontier that will see substantial growth over the next decade and which will have a major impact on the prediction of microstructures in materials. Outstanding opportunities exist in the area of biomaterials and bioinspired materials, where computation has not yet played a dominant role, but will certainly do so in the future. In the area of nanoscience and nanotechnology research, computation will play a critical role in elucidating molecular and materials processes occurring on nanoscopic scales and in guiding the design and manipulation of nanostructured materials.

The opportunity for computation to make an impact on the critical outstanding problems of materials science is before us. We must combine our resources, collaborate effectively, and continue to build the computational and intellectual infrastructure necessary to accomplish our goals.

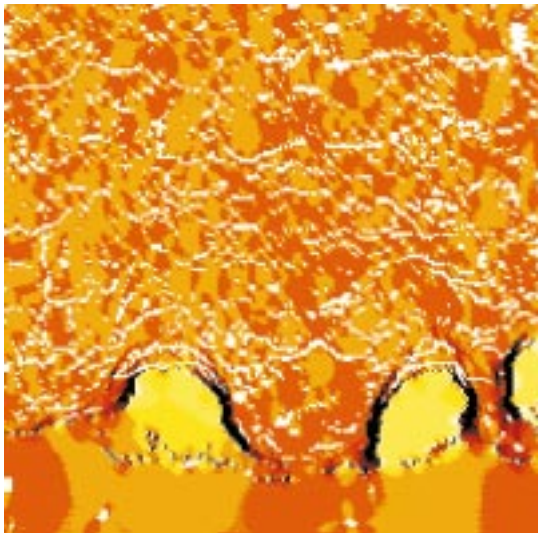

Figure 4. An OOF **calculation of a component of the stresses found in a thermal barrier coating upon cooling due to the different coefficients of thermal expansion in the coating (top), substrate (bottom), and interfacial region. The initial microstructure was imported into** oof **from a scanned micrograph using** ppm2oof. **The yellow regions are at the maximum tension, and the black regions are at maximum compression. (Figure courtesy of Edwin R. Fuller and Steven A. Langer.)**

Sharon C. Glotzer is a cofounder and the former director of the NIST Center for Theoretical and Computational Materials Science. She is now an associate professor in the departments of chemical engineering, materials science, and physics at the University of Michigan, Ann Arbor. Her technical interests include molecular and mesoscale simulation of soft materials, complex fluids, self- and guided assembly of nanostructured materials, and supercooled liquids and glasses. She belongs to the American Physical Society, Materials Research Society, American Institute of Chemical Engineers, American Chemical Society, and the American Association for the Advancement of Science. Contact her at sharon.glotzer@nist.gov.

James A. Warren is a theoretical physicist in NIST's Metallurgy Division and cofounder and acting director of the Center for Theoretical and Computational Materials Science. His technical interests include pattern formation in materials, microstructure evolution, dendritic growth, grain growth, dislocation dynamics, and solidification. He belongs to the Materials Research Society, American Physical Society, Metals Minerals and Materials Society, and the American Association for the Advancement of Science. Contact him at the Center for Theoretical and Computational Materials Science, Nat'l Inst. of Standards and Technology, Gaithersburg, MD 20899; jwarren@nist.gov.