JOM-e: The Symposium on Computational Methods in Materials Education

Zi-Kui Liu, Long-Qing Chen, and Mark Asta

Computational methods in materials science and engineering, such as ab initio calculations, computational thermodynamics and kinetics, Monte Carlo molecular dynamics, and finite element and phase-field techniques, offer powerful tools to support decision-based selection and design of materials that meet a range of application requirements.

When supplemented with critically designed, associated experiments, these emerging modeling and simulation tools provide more efficient and robust methods to predict properties and design materials for myriad applications. Industry will continue to accelerate the use of computational methods as a primary tool in the design and selection of materials, while universities and research institutions are continuously developing new methodologies for design and new tools in computational materials science and engineering. This new paradigm of materials development can shorten the design process, lower costs, and also lead to better products.

Under such circumstances, the two-day symposium, Computational Methods in Materials Education, was held at the 2003 TMS Annual Meeting; it was organized by Zi-Kui Liu, Long-Qing Chen, and Mark Asta. Four sessions were arranged comprising 20 presentations and a panel discussion.

The first two sessions focused on improving existing traditional courses in the materials science and engineering curriculum by use of general software packages such as *MatLab* and Microsoft *Excel* as well as custom commercial packages and home-made programs. Presentations in the third session covered new computational courses and featured topics such as first-principles calculations and atomic simulations, which do not exist in the traditional materials science and engineering curriculum. The fourth session featured presentations from industry on current practices of computational approaches in industrial environments and the needs for the training of current and future workforces in the field. The panel discussion, led by Hasso Weiland from Alcoa, focused on the integration of current education methodology and needs of workforces in academia, research institutions, and industry.

To better understand these issues and to provide a representative sampling of the material presented, four papers have been adapted for inclusion in this month's *JOM-e*—the web-only supplement to the journal.

It was clear that there is great momentum toward integrating computational methods into materials science and engineering curriculum through both introducing new courses and modifying existing courses. This is because, traditionally, the field of materials science and engineering has predominantly focused on processing of materials, establishing structure-property relations, and measuring material properties. As these processes have been time-consuming and highly empirical, it takes a long time to insert new and improved materials into products. This empirical approach is increasingly shifting toward the design of materials to achieve optimal functionality, driven largely by complementary advances in computational materials science and information technology, particularly in the last few decades. Therefore, the critical needs to educate both the current and future workforces in materials science and engineering becomes evident.

Zi-Kui Liu is a member of the Materials Processing and Manufacturing Division Council. Liu is also an associate professor and Long-Qing Chen is a professor with the Department of Materials Science and Engineering at Pennsylvania State University. Mark Asta is an associate professor with the Department of Materials Science and Engineering at Northwestern University.

For more information, contact Zi-Kui Liu at Pennsylvania State University, 209 Steidle Bldg., University Park, PA 16802; (814) 865-1934; fax (814) 865-2917; e-mail liu@matse.psu.edu.

JOM-e: TEACHING COMPUTATIONAL METHODS

"An Integrated Education Program on Computational Thermodynamics, Kinetics, and Materials Design," by Zi-Kui Liu, Long-Qing Chen, Karl E. Spear, and Carlee Pollard *www.tms.org/pubs/journals/JOM/0312/LiuII/LiuII-0312.html*

"Software for Teaching Materials Processing and Diffusion," by S.E. Mohney, A.J. Miller, and G.L. Gray *www.tms.org/pubs/journals/JOM/0312/Mohney/Mohney-0312.html*

"Our Experience in Teaching Thermodynamics at the University of Wisconsin, Madison," by Y. Austin Chang and W.A. Oates *www.tms.org/pubs/journals/JOM/0312/Chang/Chang-0312.html*

"A Computational Materials Science Course for Undergraduate Majors," by J.M. Rickman and R.P. Vinci *www.tms.org/pubs/journals/JOM/0312/Rickman/Rickman-0312.html*