



Symposia Summary

Computational Thermodynamics and Kinetics

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After ten years, this symposium keeps going strong, with close to 90 papers presented, including nearly 20 invited talks, 50 contributed talks, and more than 20 posters distributed among eight sessions and spanning the entire week of the conference. The symposium was organized around several themes: thermodynamics and kinetics of defects, energy materials, thermodynamics and phase transformations; microstructural evolution and thermodynamics; and, for the first time, microstructural evolution in soft matter systems.

Computational and experimental experts shared their most recent contributions to the understanding of thermodynamics and kinetics of materials, using a wide range of theoretical, modeling and experimental techniques. Simulation techniques ranged from atomistic methods (classical molecular dynamics, density functional theory) to continuum approaches based on the phase-field method. Experimental results used a wide range of state-of-the-art characterization techniques, ranging from the latest 3-D atom probe tools to advanced studies using neutron scattering and other related techniques. Materials discussed ran the gamut from conventional structural materials to advanced multi-functional materials. In the inaugural soft matter session, phase transformation phenomena were explored, both experimentally and computationally, in lipid bilayer membrane systems.

Besides these thematically-arranged sessions, this symposium hosted two special sessions honoring Brent Fultz, California Institute of Technology, who was awarded the 2010 TMS Electronic, Magnetic & Photonic Materials Division Distinguished Scientist Award for his outstanding contribution to fundamental understanding of thermodynamics in materials using inelastic neutron scattering. The sessions were held jointly with the symposium on Neutron and X-ray Studies of Advanced Materials and featured presentations on topics of vibrational entropy and scattering, with several talks by Fultz's former students, colleagues, and friends. The speakers also took the opportunity to share interesting stories of working with Fultz.

"I was delighted by the quality of the talks at the symposium," said Fultz. "What was so interesting to me is that our thinking about how alloy phase stability is affected by vibrational entropy has broadened out so much, and so quickly. All the talks went well beyond the original tests of harmonic models at low temperatures. Especially for high temperature behavior, branches of work have grown into effects of electrons, spins, other phonons, and even nonlinear chaotic behavior. Some of this still needs sorting out, but useful predictions about alloy thermodynamics are already starting to emerge."

Sponsored by the TMS Chemistry and Physics of Materials Committee and co-sponsored by several other TMS and ASM technical committees, the symposium continues to attract some of the most important scientists in the field of thermodynamics and kinetics of materials. With the support of TMS and the continued interest of the community, we are confident that this series will continue well into the following decade.

—Submitted by Raymundo Arroyave