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TMS 2018

147th Annual Meeting & Exhibition

MARCH 11 – 15, 2018

PHOENIX, ARIZONA

SUBMIT AN ABSTRACT TO:

PHYSICAL METALLURGY

HUME-ROTHERY AWARD SYMPOSIUM: COMPUTATIONAL THERMODYNAMICS AND ITS IMPLICATIONS TO KINETICS, PROPERTIES, AND MATERIALS DESIGN

Thermodynamics is a science concerning the state of a system when interacting with the surroundings. Computational thermodynamics enables quantitative calculations of thermodynamic properties as a function of both external conditions and internal configurations and empowers the new materials research paradigm of integrated computational prediction and experimental validation approaches. The central constituent of computational thermodynamics is the modeling of the thermodynamic description of individual phases in the complete space of external and internal degrees of freedom. Over the past 40 years, the CALPHAD modeling of thermodynamics has proven to be a successful approach applicable to complex multicomponent materials. Integration with first-principles calculations based on density functional theory, which is capable of predicting electronic structures of atomic interactions, have further significantly enhanced the efficiency and robustness of thermodynamic modeling. Computational thermodynamics plays a central role in materials design, integrated computational materials engineering (ICME), and the Materials Genome Initiative (MGI). Two important contributions of computational thermodynamics are to predict the phase stability of a system under given conditions and provide driving forces for internal processes in a system so the evolution of such internal processes can be quantitatively simulated. Furthermore, as first and second derivatives of the free energy with respect to system variables, many physical properties can be calculated such as thermal expansion and elastic properties. Additionally, through the mapping of the energy landscape in the framework of computational thermodynamics, a broad range of properties can be predicted and modeled such as diffusion coefficients, interfacial energy, and dislocation mobility. Applications of these new capabilities include improvements in the understanding of atomic interactions and the role of alloy elements and trace additions on phase stability and phase transformation behavior; improvement of existing materials for enhanced performance; and the design and development of new materials for an optimal combination of properties.

The focus of this symposium is to assess the state of the art in computational thermodynamics for predictions and modeling capabilities and to identify the key steps needed to make further progress. Abstracts are invited which contribute to the above themes with critical appraisals of the strengths and weaknesses of various approaches for specific properties and applications. Case studies involving the use of computational thermodynamics to study practical problems are welcomed, along with studies involving both advanced experimental work and state-of-the-art modeling approaches.

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