



# TMS 2011

## 140th Annual Meeting & Exhibition

February 27 to March 3, 2011

San Diego Convention Center • San Diego, California USA

### The Development of a Reference Self-Diffusion Mobility Database for the Pure Elements

Thursday, March 3, 8:30 a.m. to 4:00 p.m.

#### Overview

This workshop will focus on the development of a standard reference database for the self diffusion mobilities for the pure elements. Development of this diffusion reference database is critical for the efficient development of multicomponent diffusion mobility databases, which are essential for the modeling microstructure evolution of many industrial applications. The approach used to determine the recommended diffusion self-mobilities will be reviewed using the accepted evaluations for fcc-Al, fcc-Cu, fcc-Ni, and fcc and bcc Fe as examples. Discussions will focus on the evaluation of the Cr self-diffusion description, which was previously determined to have some anomalous behavior at low temperatures, and other well-known anomalous diffusers. Evaluation of the self-diffusivities will include experimental work, CALPHAD assessment analysis and first principles calculations. In addition, evaluation of the metastable end-member diffusivities, needed for the development of CALPHAD-based diffusion mobility database, will be discussed within the framework of published diffusion correlations and first principle calculations. For more information on previous workshops in this series see [http://www.nist.gov/mml/metallurgy/thermodynamics\\_kinetics/Diffusion-Workshop-Group.cfm](http://www.nist.gov/mml/metallurgy/thermodynamics_kinetics/Diffusion-Workshop-Group.cfm)

#### Who should attend?

This workshop is aimed at both those interested in the development and use of multicomponent diffusion mobility databases for various alloy systems and those able to provide the needed diffusion mobility quantities either by experimental or computational methods.

The organizers are seeking input from all types of users of solid state diffusion data to ensure that the needs of the community are being met when the developing a standard reference diffusion mobility database for the pure elements.

#### Topics

- Diffusion mobility databases using a CALPHAD method
- Reference diffusion mobilities for fcc-Al, fcc-Cu, fcc-Ni and fcc and bcc Fe.
- Measurement and calculations of Cr self-diffusion in bcc Cr
- Diffusion behavior in anomalous diffusers (beta-Zr, beta-Ti)
- Tracer diffusion experiments
- First-principles studies of diffusion
- Kinetic Monte Carlo simulations
- Diffusion correlations

#### Speakers

**John Ågren**, KTH - Royal Institute of Technology, Sweden  
**Sergii Divinsky**, Institute for Materials Physics, University of Münster, Germany  
**Graeme E. Murch**, The University of Newcastle, Australia  
**Nils Sandberg**, KTH, Royal Institute of Technology, Sweden  
**Anton van der Ven**, University of Michigan, USA

#### How to Register

Register by February 4, 2011 using the [online registration form](#). Cost is \$75 for members and \$100 for nonmembers.

#### For More Information

Christina Raabe Eck, *Director of Technical Support Services*  
E-mail: [raabe@tms.org](mailto:raabe@tms.org) or Telephone: (724) 776-9000, ext. 212 • (800) 759-4TMS

