

## NIST Diffusion Workshop May 12-13, 2008

*Highlighting Diffusion Challenges Associated with Sustainable Energy Applications*

### **Monday, May 12 Bldg. 101. Lecture Room A**

8:30-9:00 Introductions and Welcome

#### ***Diffusion Challenges for Developing Materials for Sustainable Energy Applications***

9:00-9:15 Brief review of previous workshops (C. Campbell)

9:15-9:45 “H Diffusion in Pd and Pd Alloy Membranes. The Role of Non-ideality” (T. Flanagan, U. Vermont)

9:45-10:15 “Hydrogen Diffusion in Steels” (Z. Feng and L. Anovitz, ORNL)

10:15-10:45 Diffusion in CIGS ( $\alpha$ -CuIn<sub>x</sub>Ga<sub>1-x</sub>Se<sub>2</sub>) Photovoltaics (W. Kim, Institute of Energy Conversion, U. Delaware)

10:45-11:15 Discussion/ Break

11:15-11:45 “U-Mo/Al Alloys Diffusion Couples : Fuel/Cladding Interactions” (Y.Sohn, UCF)

11:45-12:15 “Uncertainties in Multicomponent Diffusivities and the Determination of Long-Term Diffusivities at Low Temperatures” (J. LaCombe, U. Nevada-Reno)

Lunch 12:30-1:30

#### ***First –Principles***

1:30-2:00 “ Diffusion of Transition Metal Solutes in Nickel” (R. Reed, U. Birmingham, UK)

2:00-2:30 “First-Principles Calculations of Diffusion Coefficients in fcc, bcc and hcp” (Z. Liu, Penn State)

2:30-3:00 “Diffusion coefficients from first principles: from intercalation compounds to complex alloys” (A. van der Ven, U. Michigan)

3:00-3:30 “Diffusion of Substitutional Impurities in bcc Fe: First-Principles Modeling” (M. Asta, U. California – Davis)

3:30-3:45 “Atomistic Simulations in Industrial Research: Workshop Summary” (C. Becker, NIST)

3:45-4:00 Break

***Modeling Applications***

4:00-4:30 "Modeling of Diffusion-induced transformations in Ni superalloys (A. Mirsa, QuesTek)

4:30-5:00 "Apply Phase Field Modeling to Real Systems by Integrating with PanEngine" (K. Wu, CompuTherm)

5:00-5:30 "TC-PRISMA" (P. Mason, Thermo-Calc AB)

**6:30 Dinner**

Café Mileto

Cloppers Mill Village

18056 Mateny Road

Germantown, MD 20874

**Tuesday, May 13 Bldg 223, Rm B307**

8:45-9:00 Welcome

9:00-9:30 "Update on Diffusion Mobilities in Oxide Systems" (J. Ågren, KTH)

9:30-9:45 "Diffusion Mobilities in the Cu-In-Se system" (C. Campbell, NIST)

9:45-10:15 Discussion/ Break

10:15-10:45 Single-Phase Layer Formation in Two-Phase Diffusion Couples (J. Morral, OSU)

10:45-11:15 "Phase field Simulation of Thermotransport" (Sohn, UCF)

11:15-11:45 "Singularities in Diffusion Paths" (J. Li, U. Penn, OSU)

11:45-12:30 Discussion/Action Items

12:30 Adjourn/Lunch