NIST Diffusion Workshop March 25-26, 2009

Tentative Agenda
(Revised 3/13/09)

Highlighting Diffusion Challenges Associated with Sustainable Energy Applications

Wednesday, March 25 Bldg. 101. Lecture Room C

8:30-9:00 Introductions and Welcome

Diffusion Challenges for Developing Materials for Sustainable Energy Applications

9:00-9:30 "Interplay of diffusion and dissociation mechanisms during hydrogen absorption in metals"(A. Borgschulte, EPMA)

9:30-9:45 Discussion

9:45-10:00 "Diffusion Challenges in Photovoltaic Processing" (L. Eldada, HelioVolt)

10:00-10:30 "Routes for Rapid Synthesis of $CuGa_xIn_{1-x}Se$ Absorbers," (T. Anderson, U. Florida)

10:30-11:00 "Development of a Diffusion Mobility Database for Cu-In-Se," (C. Campbell, NIST)

11:00-11:15 Discussion

Grain Boundary Diffusion

11:15-11:45 "Modeling of diffusion along grain boundaries and triple junctions" (Y. Mishin, George Mason)

11:45-12:15 "Grain boundary motion" (W. J. Boettinger, NIST)

12:30 – 2:00 Lunch

Diffusion Modeling and Applications

2:00-2:30 "Update on Diffusion Mobilities in Oxide Systems" (J. Ågren, KTH)

2:30-3:00 "Diffusion simulations of internal oxidation" (A. Madeshia and John Morral, OSU)

3:00-3:30 Discussion/Break

3:30-4:00 “Diffusion modeling in the Al-Fe-Ni” (Y. Du, Central South University)

4:00-4:30 “ Simulating interdiffusion in NiAl/Ni-base superalloy substrates” (Anders Engström, Thermo-Calc AB)

4:30-5:00 “Modeling and Experimentation of ThermoTransport in Multicomponent-Multiphase Alloys,” (Y. Sohn, U. Central Florida)

6:00 Workshop Dinner

Café Mileto
18056 Mateny Road
Germantown, MD 20874
(301) 515-9378

Thursday, March 26th Bldg. 101. Lecture Room C

Development of Standard Reference Diffusion Mobilities

8:15-8:30 Welcome

8:30-9:00 “Insights into the development of Standard Reference Databases” (A. Dinsdale, NPL)

9:00-9:30 “Challenges in Creating a Pure Element Tracer Diffusion Database” (Nagraj Kulkarni, ORNL)

9:30-9:45 Discussion

9:45-10:15 “Review of First Principles Comparisons to Pure Elements,” (Z-K. Liu, Penn State)

10:15-10:45 “ First Principles Calculations of Diffusion Coefficients in Non-Dilute Alloys” (Anton Van der Ven, U. Michigan)

10:45-11:15 “Molecular Dynamics Study of Self-Diffusion in Zr” (Mikhail Mendelev, Ames Lab)

11:15-11:45 “First-principles calculations of solute-vacancy binding in Mg.” (Dongwon Shin, Northwestern)

11:45-12:15 Discussion/Action Items

12:30 Adjourn

12:30 Lunch meeting of sub-group meeting on Reference Self –Diffusion Mobilities