NIST Diffusion Workshop March 23-24, 2010

(Agenda as of 3/15/10)

Highlighting Diffusion Challenges Associated with Sustainable Energy Applications

Tuesday, March 23 Bldg. 101. Lecture Room A

8:15-8:45 Introductions and Welcome
Brief updates from past topics

Diffusion Challenges for Developing Materials for Sustainable Energy Applications

Photovoltaics

8:45-9:15 Routes for Rapid Synthesis of $CuGa_xIn_{1-x}Se_2$ Absorbers (T. Anderson, U. Florida)

9:15-9:45 Modeling Cu migration in CdTe Devices (G. Teeter, NREL)

9:45- 10:00 Cu_2ZnSnS_4: Evaluation of a new potential photovoltaic absorber material (G. Teeter, NREL)

10:00-10:30 Characterizing 3-D Photovoltaics (D. Josell, NIST)

10:30-10:45 Break/Discussion

Ni-base Superalloys and modeling other topics

10:45-11:15 Microstructure Modeling of 3rd Generation Disk Alloys (A. Misra, QuesTek Innovations)

11:15- 11:45 Diffusion in temperature gradients (J. Agren, KTH)

11:45-12:15 DICTRA simulations of type 3 boundaries using the homogenization model (Ke and Morral, Ohio State)

12:30-1:30 Lunch

Phase-Fielding Modeling of Diffusion Controlled Processes

1:30-2:00 Phase Field Simulations of Nanostructure Formation (P. Voorhees, Northwestern)

2:00-2:30 Simulation of Diffusion Using the Smoothed Boundary Method Coupled with Phase Field Models (K. Thornton, U. Michigan)

2:30-3:00 Phase-field simulation of diffusion couples (L. Zhang, ICAMS, U. Bochum)

3:00-3:15 Update on the NIST Interatomic Potentials Repository and Atomistic Simulations for Industrial Applications (C. Becker, NIST)

3:15-3:45 Break /Discussion

3:45-4:15 Phase Field Modeling of Diffusion Controlled Defect Processes (Y. Wang, Ohio State)

4:15-4:45 Phase Modeling of coupled diffusion in ionic crystals (L-Q Chen, Penn State)

4:45-5:15 Phase –field modeling of Reactive Wetting (J. Warren, NIST)

5:15-5:30 Phase-field modeling of Line Edge Roughness in Block Copolymer Resists (A. Bosse, NIST)

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

Cash Bar 6:00 – 7:00 pm
Dinner 7:00

Wednesday, March 24th Bldg. 101. Lecture Room A

Development of Standard Reference Diffusion Mobilities

8:30-9:00 Grain boundary diffusion and segregation in copper: radiotracer measurements on poly- and bi-crystals (S. Divinski, U. Münster)

9:00-9:30 Atomic mobility and diffusivity in Al alloys (Y. Du, Central South University, China)

9:30-10:00 Computer simulation of self-diffusion in bcc Fe (M. Mendelev, Ames Lab)

10:00-10:30 Self-Diffusivities in Liquid Alloys, (Z-K Liu, Penn State)

10:30-10:45 Break/Discussion

10:45-11:30 Review of Draft Recommendations for the Self-Diffusion Mobilities of Ni, Al, Cu, Cr and Fe

11:30-12:00 Wrap/Action Items

12:30-1:30 Lunch

1:30- 4:00 pm Sub-group meeting on Reference Self-Diffusion Mobilities (Lect Rm A)