Multicomponent Diffusion Data and the Materials Genome

NIST Diffusion Workshop Series

May 9-10, 2013

Thursday May 9

8:30-9:00 Introductions and Welcome (Coffee and Bagels will be available)

9:00 -9:30 The Materials Genome Initiative at NIST (James Warren, NIST)

9:30- 10:00 Interdiffusion and Phase Growth Kinetics in the Magnesium-Aluminum Binary System (A. Luo, General Motors)

10:00-10:30 "Diffusion Investigations in Selected Binary System of Mg," (Yongho Sohn, University of Central Florida)

10:30-10:45 Break

10:45-11:15 Derived Uncertainties and the Evaluation of Multicomponent Interdiffusion Data, (J. LaCombe, University of Nevada, Reno)

11:15-11:45 Stress-induced anisotropic diffusion in alloys: Complex Si solute flow near a dislocation core in Ni (D. Trinkle, University of Illinois)

11:45-12:15 First Principles Data Use in Data Repositories (TBA)

12:15-1:30 Lunch

1:30-2:00 ESPEI and Diffusion, (Richard Otis, Penn State)

2:00-2:45 Development of File and Data Repositories (NIST, Kent State)

2:45-3:15 Hands on Demos of Tools

3:15-3:45 Break-Discussion

3:45-4:15 Materials Data from the Software Developers Perspective (Discussion with various software/industry users)

4:15 – 4:45 Small Group Discussion on Data Schemas (Experimental, CALPHAD use, First Principles etc.)

4:45-5:30 Group Discussion

6:00 Workshop dinner

Friday May 10

9:00 – 9:30 Tracer Diffusivity Data Collection and Reporting; Examples from the Mg-based systems," (Kulkarni, ORNL)

9:30-10:00 Update on the Development of a Self-Diffusion Reference Databases (Campbell, NIST)

10:00-10:15 Break

10:15 – 11:00 Small group discussions on the development of various data schemas (experimental and computational data)

11:00 -11:30 Review of group discussions

11:30-12:00 Workshop wrap-up