Multicomponent Diffusion Data and Its Impact on the Materials Design Process: Data Needed; Data Acquisition; and Data Application

NIST Diffusion Workshop Series

(Tentative Agenda as of April 19, 2012 –subject to change)

May 3-4, 2012

Building 101, Heritage Room

8:00-8:30 Introductions and Welcome

Why is Multicomponent Diffusion Data Important for Materials Design: The Need

8:30 -9:15 Design of high-strength Aluminum alloy castings – A case study on the importance of multicomponent diffusion to materials design (Abhijeet Misra, Questek Innovations)

9:15- 9:40 Integrated computational materials engineering for light metals applications (A. Luo, General Motors)

9:40-10:00 Heat Treating Industry Diffusion Data Needs Discussion (Lead by John Morral, Ohio State, and Mohammed Maniruzzaman, Caterpillar)

10:00-10:45 Routes for Rapid Synthesis of Photovoltaic Absorber Materials: The Need for Diffusion Data (T. Anderson, U Florida)

10:45-11:15 Discussion/Break

11:15-11:30 Update on Materials Simulation and the Promotion of Global Databases Activities within the World Materials Research Institute Forum (WMRIF) (A. Grische, BAM, Bundesanstalt für Materialforschung)

11:30-12:00 Data Repositories for Diffusion Data and Calculations: Will This Work? (C. Campbell, U. Kattner, B. Burton, E. Lass, NIST and L. Bartolo, Kent State)

12:00-12:15 General Discussion on Data Needs and Storage

12:15-1:30 Lunch

How Can We Get the Needed Data: *Experimental Methods*
(Yongho Sohn, UCF)

1:30-2:15 Temperature induced transitions of the grain boundary structure studied by radiotracer diffusion (S. Divinski, U. Münster)

2:15-2:45 Diffusion Studies in Mg-Al-Zn (N. Kulkarni, B. Warmack, J. Mundy, ORNL)

2:45-3:15 Thermodynamics and Correlation Effects on Diffusion in Al-Ni Melts. (A. Grische, BAM, Bundesanstalt für Materialforschung)

3:15-3:30 Break/Discussion

3:30-4:00 Oxidation and diffusion in oxides – a progress report (J. Agren, KTH)

4:30-5:00 Extracting Chemical Diffusion Coefficients from Multi-Phase Binary Diffusion Paths (Qiaofu Zhang; J-C Zhao, Ohio State Univ.)

5:00-5:30 The rms error of ternary diffusivities from one diffusion couple (John Morral, Ohio State)

5:30-6:00 Discussion

- Best practices for experimental measurements
- How and what data should be stored

6:30 Workshop Dinner: O'Donnell's Sea Grill (www.odonnellsrestaurants.com)
311 Kentlands Boulevard Gaithersburg, MD 20878

How Can We Get the Needed Data
Calculation Methods
(Session Chair: Patrice Turchi, LLNL)

8:30-9:15 High-Throughput and Ab Initio Molecular Dynamics approaches for Developing Alloy Diffusion Databases (with an Application to Radiation Induced Segregation in Ni-Cr Alloys) (D. Morgan, U. Wisconsin)

9:15-9:45 First-principles calculation of diffusion coefficients in magnetic systems: Ni, Cr, and Ni-X alloys (C. Zacherl, Penn State)

9:45-10:15 First-Principle Calculations of Diffusion of 5d transition elements in Fe (Kevin Ding, Berkeley)

10:15-10:30 Break

10:30-11:10 Understanding non-dilute diffusion within fcc: the case of Ni rich alloys (A. Van der Ven, U. Michigan)

11:10-11:50 Effect of a grain boundary structural transformation on grain boundary diffusion: A molecular dynamics study (T. Frolov, Berkeley and Y. Mishin, George Mason)

11:50-12:10 Discussion on the Limitations of the Currently Used Pseudo-Potential Approach (P. Turchi, LLNL)

12:10–12:45 Discussion

- Best Practices in using First Principles to calculate diffusion quantities;
- Can these methods be used to estimate end-member unknown quantities for CALPHAD-based diffusion mobility databases?
- Are different methods calculations consistent with one another
- How should these data/calculations be stored and retrieved?

Lunch 12:45 -1:45

What We Can Do With the Data to Meet the Materials Designer Needs

1:45-2:30 Diffusion and redistribution at moving interfaces (I. Steinbach, ICAMS)

2:30-3:15 Formation of complex interdiffusion microstructures in mulitphase diffusion couples: effect of atomic mobility (Xiaoqin Ke, John Morral and Yunzhi Wang; Ohio State U)

3:15-3:45 Discussion Workshop Wrap-Up