

Multicomponent Diffusion Data and the Materials Genome

NIST Diffusion Workshop Series

April 28&29, 2014
NIST, Portrait Room

DRAFT Agenda as March 18, 2014

Monday, April 28

- 9:00-9:30 Introductions and Welcome (Coffee and Bagels will be available)
- 9:30 -10 “Short-Circuit Diffusion In Recrystallizing Microstructure: Diffusion Properties of a Recrystallization Front,” Sergiy Divinski (University of Munster)
- 10-10:30 “Magnetic Materials in Energy Systems: Applications of Diffusion Controlled Processes,” Frank Johnson (GE Global Research Center), Nagraj Kulkarni, and Robert Shull (NIST)
- 10:30-11:00 Discussion/Break
- 11:00-11:30 “Chemical Diffusivities and their Hidden Concentration Units,” John Morral (Ohio State University)
- 11:30-12:00 “Precipitation simulation of Ni-base superalloys, Fan Zhang (CompuTherm)
- 12:00-12:15 Discussion
- 12:15-1:30 Lunch (NIST Cafeteria)
- 1:30-2:00 “Diffusion and Mobility in Co-Al-based Ternary Alloys: Diffusion Couple Experiment and Assessment,” Yuwen Cu (IMDEA Materials Institute)
- 2:00-2:30 “Diffusion in Co-Al-W-Ni System: Initial Diffusion Couple Observations,” Kil-Won Moon, Eric Lass, Carrie Campbell (NIST)
- 2:30-3:00 “Mobility Database Development for Magnesium Alloys,” Michele Manuel, (University Florida)
- 3:00-3:30 Role of Solid State Diffusion Studies in Materials Selection and Process Design for Development of Low Enrichment U-Mo Metallic Nuclear Fuel Systems, Yongho Sohn (University of Central Florida)
- 3:30-4:00 Discussion/Break

4:00-4:30 “Ti-O-M interaction between oxygen and metal (M) substitution in titanium for oxygen diffusion change,” Dallas Trinkle (University of Illinois)

4:30-5:00 “Diffusion of Oxygen in Ni and Fe due to Substitutional Vacancy from DFT calculations,” Zi-Kui Liu (Penn State University)

5:00-5:30 Discussion

6:00 Workshop dinner
To Be Announced

Tuesday, April 29

NIST Diffusion Workshop

8:30-9:00 Introduction and Welcome to NIST

9:00-9:30 “Essential information to build up the diffusion genome,” John Agren (KTH)

9:30-9:45 Discussion

9:45-10:30 Update on NIST Materials Data Informatic Efforts (Campbell, Kattner, Dima, Bartolo)

10:30-11:00 Data Capture Efforts (NIST)

11:00-11:15 Data and Simulation Management Tools (NIST)

11:15-12:00 Discussion/Diffusion Workshop Wrap-up