

NIST Diffusion/CALPHAD Data Informatics and Tools Workshop

May 14-15, 2015
Building 101, Portrait Room
NIST, Gaithersburg, MD 20899

Draft Agenda (3/12/2015)

May 14 ***CALPHAD Data Informatics and Tools***

9:00-9:30 Opening remarks

9:30-10:00 ASM Structural Data Demonstration Project on Al6061 (Larry Berardinis, ASM International)

10:00-10:30 Expansion of the Guide Data Capture and ThermoML to Metallic-based Systems (Boris Wilthan, Vladimir Diky and Kenneth Kroenlein; Thermodynamic Research Group, NIST Boulder)

10:30-11 Discussion/Break

11:00-11:30 Materials Data Curation System (Alden Dima, Sharief Youssef, and Guillaume Sousa-Amaral; NIST)

11:30-12 Using the Materials Data Curation System via the Application Programming Interface: X-ray Diffraction data (Z. Trautt, NIST)

12:00-12:30 Discussion

12:30-1:30 Lunch

1:30-2:00 Hosting Public Domain Chemicals Data Online for the Community –the Challenges of Handling Materials (Antony Williams, Royal Society of Chemistry)

2:00-2:30 RDA & Adopting RDA Infrastructure to realize MGI Goals: RDA, Data Type Registry and Metadata Efforts (Laura Bartolo, Kent State)

2:30-3:00 Application of Semantic Technology to Materials, Manufacturing and Design (Clare Paul, Air Force Research Laboratory)

3:00-3:30 Discussion/Break

3:30-4:00 NIST Materials Resource Registry (Alden Dima and Sharief Youssef, NIST)

4:00-4:15 Discussion

4:15-4:45 Development of ESPEI: free energy minimization, phase diagram calculations for multicomponent systems (Richard Otis and Zi-Kui Liu, Penn State)

4:45-5:15 A Computational Framework For Materials Design (Shengyen Li, NIST)

5:15-5:45 Discussion

6:00 Dinner TBA.

May 15, 2015

8:30-9:00 Introductions and Welcome

9:00-9:30 "Diffusion Kerf Couples for MGI Data: Design and Simulation," Nagraj Kulkarni, Robert Warmack, Irina Belova and Graeme Murch.

9:30-10:00 The Development of Thermodynamic and Diffusion Mobility Databases for Co-base Superalloys, Questek

10:00-10:30 Diffusivities in the Co-Al-W-Ni System/ Data Smoothing Methods: Do they matter? (Kil-Won Moon and William Boettinger, NIST)

10:30-11:00 Discussion/Break

11-11:00 High-Throughput Study of Diffusion and Phase Transformation Kinetics of Mg-Based Systems Mg alloy Diffusion; Wei Zhong, Ohio State University)

11:30-12:00 Phase equilibria, interdiffusion and martensitic transformations in magnetocaloric Ni-Mn-Ga alloys; Yongho Sohn , University of Central Florida

Lunch 12-1:30 pm

1:30-2:00 "Zr solute diffusion calculations: Computing diffusion in HCP materials," Dallas Trinkle, University of Illinois

2:00-2:30 Diffusivities near the Melting Temperature, Jack Douglas , NIST

2:30-3:00 Discussion

3:00 Adjourn