NIST Diffusion Workshop: Data and Model Needs for Efficient Critical Material Usage and Recovery

DRAFT Agenda

Tuesday April 14		
Time (ET)	**Presentation/Activity**	**Speaker**
8:30-9:00	Arrival/Check-in	
9:00-9:15	Welcome/Introductory Remarks	Carelyn Campbell, NIST
9:15-9:45	Holistic integration of computational and experimental diffusion data	J-C Zhao, University of Connecticut
9:45-10:15	Understanding microstructure evolution in additively manufactured alloys during heat treatment	Wei Xiong, University of Pittsburgh
10:15-10:45	Break	
10:45-11:15	Diffusion in alloys and intercalation compounds used as electrodes of Li and Na batteries	Anton van der Ven, University of California, Santa Barbara
11:15-11:45	On a universal relationship between grain boundary diffusion, grain boundary free energy, and grain boundary segregation	Yuri Mishin, George Mason
11:45-12 pm	Discussion	
12:00- 1:30 pm	Lunch	
1:30-2:00 pm	The Improvements of Diffusion Mobility Parameters in the FCC Co-Cr-Ni-Re System	Kil-won Moon, NIST
2:00-2:30 pm	Predicting Gibbs Free Energies of Complex Solid Solutions and Oxides Using AI/ML	Dongwon Shin, ORNL
2:30-3:00	Break	
3:00-3:20	Surface Diffusion mechanisms	John Perepezko, University Wisconsin
3:20-4:00 pm	Discussion on data needs for grain boundary diffused magnets	
4:00-4:30 pm	Beyond the Lattice: Diffusion Challenges That Push the Boundaries of CALPHAD-Based Tools	Paul Mason, Thermo-Calc
4:30-4:45 pm	nMat Overview	Johnathan Seppala, NIST
5:00 pm	Adjourn	

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Wednesday April 15		
Time (ET)	**Presentation/Activity**	**Speaker**
8:45-9:00	Arrival/check-in	
9:00-9:30	Augmented tracer-interdiffusion couple method: a high-throughput approach for consistent measurements of the tracer diffusion coefficients	Sergiy Divinski, University of Münster
9:30-10:00	Simplified treatment of diffusion in ionic systems and molten slags	John Ågren, KTH
10:00-10:30	Break	
10:30-11:00	TBA	Kathleen Schwarz, NIST
11:00-11:30	Discussion on data and model needs for improved corrosion predictions	
11:30-11:45	Discussion/Closing remarks	
12:00-1:00 pm	Lunch	