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

Agenda

Tuesday April 14		
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	Diffusion Impacts on Hot Cracking Predictions	Qiaofu Zhang, University of Alabama
10:45-11:15	Break	
11:15-11:45	Diffusion in alloys and intercalation compounds used as electrodes of Li and Na batteries	Anton van der Ven, University of California, Santa Barbara
11:45-12:15	On a universal relationship between grain boundary diffusion, grain boundary free energy, and grain boundary segregation	Yuri Mishin, George Mason
12:15-12:30 pm	Discussion	
12:30- 1:30 pm	Lunch	
2:00-2:30 pm	The Improvements of Diffusion Mobility Parameters in the FCC Co-Cr-Ni-Re System	Kil-won Moon, NIST
2:30-3:00 pm	Predicting Gibbs Free Energies of Complex Solid Solutions and Oxides Using AI/ML	Dongwon Shin, ORNL
3:00-3:30	Break	
3:30-4:00	Surface Diffusion on Glasses	John Perepezko, University Wisconsin
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	Discussion on data needs for grain boundary diffused magnets	Industry/NIST Discussion
4:45-5:00 pm	nMat Overview	Johnathan Seppala, NIST
5:15 pm	Adjourn	

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Wednesday April 15		
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	
10:30-10:45	Identifying best practices for calculating the ionic current of aqueous electrolyte solutions	Kathleen Schwarz, NIST
10:45-11:30	Discussion on data and model needs for improved corrosion predictions.	Industry/NIST Discussion
11:30-11:45	Discussion/Closing remarks	
12:00-1:00 pm	Lunch	
Tours of NIST Labs for those who are interested		