THE WORLD COMES HERE.

TMS2025

154th Annual Meeting & Exhibition

March 23–27, 2025
MGM Grand Las Vegas
Hotel & Casino
Las Vegas, Nevada, USA
#TMSAnnualMeeting

SUBMIT AN ABSTRACT FOR THE FOLLOWING TMS2025 SYMPOSIUM:

DATA-DRIVEN AND COMPUTATIONAL MATERIALS DESIGN

Local Chemical Ordering and Its Impact on Mechanical Behaviors, Radiation Damage, and Corrosion

Recent developments in the field of compositionally complex materials have sparked thought-provoking speculations regarding the role of local chemical ordering (LCO) in various chemistry–microstructure relationships. The practical motivation is clear: LCO could present a new dimension for tuning and designing the behavior of structural and functional materials. Meanwhile, from a fundamental perspective, the ubiquity of LCO suggests that it might be an indispensable component of predictive physical models of compositionally complex materials. A comprehensive thermodynamic and kinetic framework of LCO and its connections to microstructural evolution and phase stability is still lacking. This absence speaks to a considerable challenge in working with the staggering chemical complexity of LCO, which lies just beyond the capability of current experimental and computational approaches.

In this symposium we will explore emerging trends on computational and experimental efforts in understanding LCO and its impact on materials properties. Our goal is to deepen our understanding of novel concepts and highlight methodological challenges hindering the quantitative characterization of LCO.

Specific topics include:

- LCO impact on defects and microstructural evolution, spanning from atomistic to the mesoscale
- LCO during early stages of ordering, leading to precipitation of long-range ordered phases (e.g., L12 and B2)
- Nonequilibrium dynamics and kinetics of LCO under extreme driving conditions, including high strain rate, high/cryogenic temperatures, radiation, and corrosion
- Experimental characterization of LCO, including electrical resistivity measurements, calorimetry, electron microscopy, and x-ray
- Simulation and modeling approaches, including first-principles methods, atomistic simulations, thermodynamic modeling, machine learning, and data-science approaches

ORGANIZERS

Rodrigo Freitas, Massachusetts Institute of Technology**; Sriswaroop Dasari,** Idaho National Laboratory**; Penghui Cao,** University of California, Irvine**; Yang Yang,** Pennsylvania State University**; Mitra Taheri,** Johns Hopkins University**; Megan McCarthy,** Sandia National Laboratories**; Irene Beyerlein,** University of California, Santa Barbara**; Rajarshi Banerjee,** University of North Texas**; Srinivasan Srivilliputhur,** University of North Texas

SYMPOSIUM SPONSORS

TMS Structural Materials Division, TMS Materials Processing & Manufacturing Division, TMS Chemistry and Physics of Materials Committee, TMS Computational Materials Science and Engineering Committee, TMS Corrosion and Environmental Effects Committee, TMS Nuclear Materials Committee, TMS Phase Transformations Committee

www.tms.org/TMS2025

QUESTIONS?
Contact programming@tms.org