

SUBMIT AN ABSTRACT FOR THE FOLLOWING TMS2022 SYMPOSIUM:

MECHANICS & STRUCTURAL RELIABILITY

Grain Boundaries and Interfaces: Metastability, Disorder, and Non-Equilibrium Behavior

The interfacial regions separating different grains in polycrystalline materials, while occupying only a small fraction of total volume, largely control the system's properties, including mechanics, mass/heat transfer, radiation resistance, etc. The misorientation angle has been widely used to describe the structures of grain boundaries (GBs), but only a few types of GBs (i.e., ones with low energy and some special "coincidence number") are well understood at the current stage. In reality, given the large variety of possible metastable states, the higher disorder levels at interfaces, and their different responses to external stimuli, global equilibrium is rarely achieved in GBs of poly- or nano-crystalline materials. The large scale of non-equilibrium metastable states and the thermodynamics and kinetics therein play decisive roles in determining GB properties and their microstructural evolution.

This symposium aims to accelerate the development of new concepts and methodologies to effectively describe GBs. The role of disorder at interfaces, the broad distributions of energies and activation barriers, and their interplay with complex or extreme environments will be subjects of particular focus. Both theoretical (including modeling and simulation) and experimental studies are encouraged. The topics of interest to this symposium include, but are not limited to, the following:

- Energetics and activation barriers spectra in materials with high level of disorder (e.g., grain boundaries, amorphous states, etc.)
- Non-equilibrium thermodynamics and metastability of grain boundaries
- Novel experimental, theoretical, and data-driven techniques for microstructural characterization of interfaces
- Relationships between structure (atomic or crystallographic) and grain boundary properties
- Interactions between interfaces and extrinsic defects (e.g., dislocations, point defects, impurities, etc.) and their mechanical consequences
- Grain boundary kinetics and phase transformations at different external stimuli (e.g., mechanical loading, irradiation, thermal cycling, etc.)
- Interfaces beyond grain boundaries, such as crystalline-amorphous interfaces in hierarchical structures, precipitatematrix interfaces in multi-element alloys, etc.

ORGANIZERS

Yue Fan, University of Michigan Liang Qi, University of Michigan Jeremy K. Mason, University of California, Davis Garritt J. Tucker, Colorado School of Mines Pascal M. Bellon, University of Illinois at Urbana-Champaign Mitra L. Taheri, Johns Hopkins University Eric R. Homer, Brigham Young University Xiaofeng Qian, Texas A&M University

SYMPOSIUM SPONSORS

TMS Computational Materials Science and Engineering Committee TMS Chemistry and Physics of Materials Committee TMS Phase Transformations Committee

www.tms.org/TMS2022

QUESTIONS? Contact programming@tms.org