

The 9th International Conference on  
**Multiscale Materials Modeling**

Toward the next twenty years, opening new era in Multiscale Materials Modeling

Oct. 28-Nov. 2, 2018, Osaka, Japan



Symposium C

**Crystal plasticity: from electrons to dislocation microstructure**

Predicting dislocation mediated crystal plasticity is an inherent multiscale modeling process that ranges in length scale from the atomic scale of the dislocation cores to the micrometer scale of dislocation substructures, and the intermediate mesoscopic scale of elastic interactions between defects. Modeling crystal plasticity also requires capturing events that span multiple time scales, including fast events driven by dislocation glide and slower thermally-activated events like dislocation nucleation, cross-slip and climb, obstacle bypass or solute drag. Significant progress has been made over the past years in the development of multiscale methods that couple these different scales into a single framework or through upscaling strategies. There is also an increased interest in developing physically based coarse-graining procedures, leading to crystal plasticity laws relying on the elementary mechanisms controlling the evolution of the dislocation microstructure.

To highlight such achievements, this symposium will focus on recent advances in dislocation-based modeling of plasticity, from the atomic to the continuum scale. Owing to the multiscale nature of crystal plasticity, contributions are solicited both on fundamental modeling of dislocation properties and on microstructural-based modeling of mechanical systems closer to the technological applications with incorporation of alloying effects, elastic anisotropy, thermally activated events, interactions with other structural defects, etc. Topics of interest include, but are not limited to:

- Dislocation core properties from atomistic simulations, including electronic structure calculations, with a special emphasis on the effects of solute elements and the description of thermally activated processes.
- Fundamental dislocation properties, such as activation energies and rates for dislocation nucleation, glide, cross-slip, climb etc.
- Discrete dislocation dynamics simulations and other coarse-grained mesoscopic modeling of the dislocation microstructure evolution.
- Interactions of dislocations with other defects, including, twin and grain boundaries, precipitates, etc.
- Continuum descriptions of the dislocation microstructure leading to physically based crystal plasticity simulations.
- Multiscale bridging methods or upscaling strategies linking different length and/or time scales in crystal plasticity.
- Microstructural-based modeling of engineering and technological systems, with incorporation of alloying effects, elastic anisotropy, thermally activated events, interactions with other structural defects etc.

Invited speakers:

Amit Acharya, Carnegie Mellon University, USA  
Irene Beyerlein, Univ. California Santa Barbara, USA  
Vasily Bulatov, Lawrence Livermore National Lab., USA  
Daryl Chrzan, Univ. California Berkeley, USA  
Jaafar El-Awady, Johns Hopkins University, USA  
Jaime Marian, Univ. California Los Angeles, USA  
Giacomo Po, Univ. California Los Angeles, USA  
Stefan Sandfeld, TU Bergakademie Freiberg, Germany  
François Willaime, CEA Saclay, France

Organizers

Emmanuel Clouet, CEA Saclay, France.  
Nikhil Chandra Admal, Univ. California Los Angeles, USA  
Yinan Cui, Univ. California Los Angeles, USA  
Dan Mordehai, Technion - Israel Institute of Technology, Haifa, Israel  
David Rodney, Univ. Claude Bernard Lyon 1, France.  
Tomohito Tsuru, Japan Atomic Energy Agency, Japan

Abstract submission deadline: March 31<sup>st</sup>, 2018

Web site: [http://mmm2018.jp/symposia/symposia\\_c.html](http://mmm2018.jp/symposia/symposia_c.html)