

## ADVANCES IN COMPUTATIONAL MECHANICS TO ADDRESS CHALLENGES IN DISLOCATION BASED PLASTICITY

FENGXIAN LIU<sup>\*</sup>, HAIYANG YU<sup>†</sup>, EDMUND TARLETON<sup>‡</sup>

<sup>\*</sup> Department of Materials, University of Oxford  
13 Parks Road, Oxford, UK OX1 3PH  
[fengxian.liu@materials.ox.ac.uk](mailto:fengxian.liu@materials.ox.ac.uk)

<sup>†</sup> Division of Applied Mechanics, Department of Materials Science and Engineering, Uppsala  
University, Uppsala SE-75121, Sweden  
[haiyang.yu@angstrom.uu.se](mailto:haiyang.yu@angstrom.uu.se)

<sup>‡</sup> Department of Engineering Science, University of Oxford,  
Parks Road, Oxford, OX1 3PJ  
[Edmund.tarleton@eng.ox.ac.uk](mailto:Edmund.tarleton@eng.ox.ac.uk)

### ABSTRACT

Dislocation dynamics plays a governing role in the plastic deformation of crystalline materials. The process occurs over a wide range of temporal and spatial scales, posing great challenges to the modelling of dislocation based plasticity, including the interactions between dislocation and other types of microstructural defects, such as point defects, radiation damages (e.g. microvoids and cavities), precipitates, and grain/twin boundaries. It is essential to overcome the computational bottlenecks and to bridge numerical simulation and experimental investigation at different length scales, thus establishing a multiscale framework for understanding the mechanisms of plasticity at microscale and for practical application of the theories at macroscale, etc.

This session aims to bring together scientists from different disciplines working on addressing the challenges in modelling dislocation based plasticity. The topics of interest to this invited session include, but are not limited to:

- Continuum/Discrete Dislocation dynamics and Molecular Dynamics simulations of plasticity.
- Novel computational methods and numerical techniques in the mechanics and multiscale modelling of crystalline defects.
- Interaction mechanisms among different microstructural defects, such as point defects, dislocations, precipitates, microvoids, grain boundaries and other material interfaces.
- Dislocation mechanisms in extreme environments, such as high/low temperature, hydrogen and radiation.
- Development of advanced and innovative theoretical models (thermodynamically based, stochastic, data-driven, etc);
- Continuum plasticity, phase field and other mesoscale simulation methods.