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AI AND SCALE BRIDGING IN DISLOCATION MECHANICS IN THE DISCRETE-CONTINUUM SCALE

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ABSTRACT

The collective motion and interaction of dislocations are the fundamental mechanisms underlying plastic deformation in crystalline materials. Capturing these processes in predictive models remains a major challenge because atomistic-scale mechanisms ultimately govern macroscopic mechanical behavior across many orders of magnitude in length and time. This challenge becomes even more pronounced in complex alloy systems and under nontrivial loading conditions. Here, multiple interacting deformation mechanisms give rise to highly coupled, high-dimensional behavior that is difficult to isolate experimentally and challenging to represent within a single modeling framework.

Developing a mechanistic understanding of this complex parameter space requires modeling approaches that span multiple length and time scales, linking dislocation-scale processes to engineering-scale material response. Addressing this need has led to a diverse range of methodologies, from physics-based homogenization and multiscale frameworks to data-driven and AI-assisted approaches, each providing unique capabilities for capturing different aspects of plastic deformation.

This symposium brings together researchers working on the modeling and simulation of dislocation-mediated plasticity, with particular emphasis on scale-bridging strategies that enhance physical understanding and enable efficient information transfer across scales. Contributions are invited from a broad range of approaches, including discrete dislocation dynamics, crystal plasticity, continuum and homogenization methods, multiscale modeling frameworks, data-driven and physics-informed methods, and machine learning or AI-based techniques for surrogate modeling, accelerated simulations, and the replacement of computationally intensive modeling components.