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[PL1]Plenary Talk 1

Amorphous materials on the meso-scale: achieving experimental length and timescales
Chair: Ju Li(MIT, USA)
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Christopher A. Schuh

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Amorphous materials on the meso-scale: achieving experimental length and timescales
○Christopher A. Schuh (Department of Materials Science and Engineering, MIT, USA)

The defining characteristic of metallic glass is disorder, with the fundamental unit of metallic glass plasticity being the Shear Transformation Zone (STZ), a local cluster of 20-100 atoms rearranging to accommodate shear strain. While the energy scales of STZs are well understood, deterministic relationships between disordered atomic structures and their respective mechanical responses have proven elusive (in stark contrast to, for example, the predictable response of a dislocation to a stress field). In lieu of such detailed deterministic relationships, we turn to stochastic modeling based on the energetics of STZ activation. This talk will review the development and current status of the class of meso-scale models referred to as Shear Transformation Zone Dynamics. These models calculate STZ activation rates by transition state theory with energy barriers modeled using Eshelby’ s continuum solutions for isotropic inclusions. In these models individual STZs interact through their elastic fields, which are evaluated by the finite element method, and the sample is evolved under the control of a kinetic Monte Carlo algorithm. We particularly review our most recent developments incorporating dynamic structural state variables and improved numerical methods into a new generation of STZ dynamics simulations. With these advances, STZ dynamics simulations are now approaching the level where they can be compared one-to-one (both in terms of length and time scales) with physical nanomechanical experiments.