Mon. Oct 29, 2018

Room1

Plenary Talk | Plenary Talk

[PL1] Plenary Talk 1

Chair: Ju Li(MIT, USA)
10:10 AM - 11:00 AM Room1

[PL1] Plenary Talk 1

○Christopher A. Schuh （Department of Materials Science and Engineering, MIT, USA）

Plenary Talk | Plenary Talk

[PL2] Plenary Talk 2

Chair: Alexey Lyulin(Technische Universiteit Eindhoven, The Netherlands)
11:00 AM - 11:50 AM Room1

[PL2] Plenary Talk 2

○Maenghyo Cho （School of Mechanical and Aerospace Engineering, Seoul National University, Korea）

Plenary Talk | Plenary Talk

[PL1] Plenary Talk 1

Amorphous materials on the meso-scale: achieving experimental length and timescales

Chair: Ju Li(MIT, USA)

Mon. Oct 29, 2018 10:10 AM - 11:00 AM Room1

Christopher A. Schuh

[PL1] Plenary Talk 1

○Christopher A. Schuh （Department of Materials Science and Engineering, MIT, USA）

(Mon. Oct 29, 2018 10:10 AM - 11:00 AM Room1)

[PL1] Plenary Talk 1

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.

Plenary Talk | Plenary Talk

[PL2] Plenary Talk 2

Multiscale modeling and realization of photo-responsive polymers

Chair: Alexey Lyulin(Technische Universiteit Eindhoven, The Netherlands)

Mon. Oct 29, 2018 11:00 AM - 11:50 AM Room1

Maenghyo Cho

[PL2] Plenary Talk 2

○Maenghyo Cho （School of Mechanical and Aerospace Engineering, Seoul National University, Korea）

(Mon. Oct 29, 2018 11:00 AM - 11:50 AM Room1)

[PL2] Plenary Talk 2

Multiscale modeling and realization of photo-responsive polymers

○Maenghyo Cho (School of Mechanical and Aerospace Engineering, Seoul National University, Korea)

Liquid crystalline polymers which contain photochromic chromophores can show macroscopic mechanical deformation under light irradiations. The light-induced shape change of the photo-responsive polymers (PRPs) comes from the trans-to-cis, or cis-to-trans isomerization of the mesogens, and it can be utilized to the microscale opto-mechanical actuation device. However, it is difficult to analyze and precisely predict the deformation because the theoretical approach requires a comprehensive knowledge of broad, interdisciplinary physical regimes that range from photochemical reaction kinetics to manipulating continuum scale deformations. Here, we develop a new multiscale model which integrates light input conditions, mesogen alignment, and continuum polymer deformations through sequential multiscale framework combining the DFT(density functional theory), MD(molecular dynamics), and continuum FE(finite element) method. In addition, the multiscale approach is applied to design the photo-mechanical behavior of the PRP nanocomposites with the consideration of the opto-mechanical coupling effect and microscopic interaction between the PRP matrix and fillers. This integrated framework can help to design the PRP and its composites.