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）

Tue. Oct 30, 2018

Room1

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[PL3] Plenary Talk 3

Chair: William Curtin(EPFL, Switzerland)
8:30 AM - 9:20 AM Room1

[PL3] Plenary Talk 3

○David Rodney （Institut Lumière Matière, University of Lyon, France）

Wed. Oct 31, 2018

Room1

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[PL4] Plenary Talk 4

Chair: Erik Bitzek(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)
8:30 AM - 9:20 AM Room1

[PL4] Plenary Talk 4

○Yuichi Ikuhara （The University of Tokyo/Japan Fine Ceramics Center, Japan）

Thu. Nov 1, 2018

Room1

Plenary Talk | Plenary Talk

[PL5] Plenary Talk 5

Chair: Dongsheng Xu(IMR-CAS, China)
8:30 AM - 9:20 AM Room1

[PL5] Plenary Talk 5

○Rui Yang （Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China）

Fri. Nov 2, 2018

Room1

Plenary Talk | Plenary Talk

[PL6] Plenary Talk 6

Chair: Karin Dahmen(University of Illinois at Urbana Champaign, USA)

8:30 AM - 9:20 AM Room1

[PL6] Plenary Talk 6

○Muneo Hori （Earthquake Research Institute, The University of Tokyo, Japan）

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.

Plenary Talk | Plenary Talk

[PL3] Plenary Talk 3

Plasticity in crystals and glasses: from the atoms up

Chair: William Curtin(EPFL, Switzerland)

Tue. Oct 30, 2018 8:30 AM - 9:20 AM Room1

David Rodney

[PL3] Plenary Talk 3

○David Rodney （Institut Lumière Matière, University of Lyon, France）

(Tue. Oct 30, 2018 8:30 AM - 9:20 AM Room1)

[PL3] Plenary Talk 3

Plasticity in crystals and glasses: from the atoms up

○David Rodney (Institut Lumière Matière, University of Lyon, France)

Plasticity in crystalline metals is probably the most classical multiscale process, around which the Multiscale Materials Modeling community first organized at the end of the 1990s. Plasticity in glasses shares many similarities with their crystalline counterparts. In particular, in both cases, plasticity starts at the atomic scale, involving the motion of dislocation cores in crystals and shear transformation zones in glasses. In both cases also, elementary plastic events interact and organize at the mesoscale through elasticity. There are however specific challenges. In crystals, there is currently a need for quantitative and predictive data, which often require to start with a first principles description of atomic interactions. By way of contrast, in glasses, we are still in need of phenomenological information, which can be addressed with less computationally intensive models. But we are then faced with the high complexity of the configuration space and the energy landscape of disordered materials, making it difficult to characterize and predict simply even the most elementary plastic events. The aim of this talk will be to illustrate the challenges, recent progress and opportunities in the field of multiscale modeling of plasticity and to discuss through selected examples the links between atomic and mesoscopic descriptions of plasticity.

Plenary Talk | Plenary Talk

[PL4] Plenary Talk 4

Grain boundary sliding, fracture and dislocation motion in ceramics

Chair: Erik Bitzek(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)

Wed. Oct 31, 2018 8:30 AM - 9:20 AM Room1

Yuichi Ikuhara

[PL4] Plenary Talk 4

○Yuichi Ikuhara　(The University of Tokyo/Japan Fine Ceramics Center, Japan)

(Wed. Oct 31, 2018 8:30 AM - 9:20 AM Room1)

[PL4] Plenary Talk 4

Grain boundary sliding, fracture and dislocation motion in ceramics

○Yuichi Ikuhara (The University of Tokyo/Japan Fine Ceramics Center, Japan)

Ceramics have been widely used for structural applications because of their superior mechanical properties at high temperatures. It has been known that the behavior of GB sliding is strongly dependent on the GB characters such as misorientation angle between two adjacent crystals and GB plane, however, such effect has not been clarified yet. In addition, this effect in much influenced by dopant segregation at GBs. In this study, in order to clarify the atomistic mechanisms of GB sliding and its dopant effect, bicrystal studies have been performed to find the relationship between the atomic structures, chemistry and GB sliding behavior of Al2O3 ceramics. Several kinds of bicrystals including GBs with specific geometrical configuration were fabricated, and some of them were doped by rare-earth elements to enhance the GB segregation.
It has been reported that several oxides can be plastically deformed even at R.T. by dislocation slip like metals. So far, many experimental investigations have been tried for understanding the dislocation-grain boundary interaction, but these experiments were mostly carried out statically, and the fundamental processes are still not well understood yet. In this study, the nanoindentation experiments were conducted for SrTiO3 crystals their bicrystals inside TEM. Several kinds of TEM specimens for in situ nanoindentation experiments were prepared, that are single crystals and bicrystals including various types of GBs. The SrTiO3 single crystals were indented with the sharp diamond tip and successfully observed the dislocation dynamics. In the case of the GBs, the interaction between the introduced lattice dislocations and the GBs were directly observed. The dislocation-GB interaction and its dependence on the GB characters will be discussed in detail.

Plenary Talk | Plenary Talk

[PL5] Plenary Talk 5

Property optimisation of titanium alloys based on phase stability evaluation and microstructure design

Chair: Dongsheng Xu(IMR-CAS, China)

Thu. Nov 1, 2018 8:30 AM - 9:20 AM Room1

Rui Yang

[PL5] Plenary Talk 5

○Rui Yang （Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China）

(Thu. Nov 1, 2018 8:30 AM - 9:20 AM Room1)

[PL5] Plenary Talk 5

Property optimisation of titanium alloys based on phase stability evaluation and microstructure design

○Rui Yang (Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China)

Titanium alloys are extensively used in aircraft engines and have emerged as ideal materials for a wide range of biomedical implants. Applications of titanium alloys in such reliability sensitive components/devices require a thorough understanding and precise control of properties which are determined by the rich variety of phase transformations and multi scale microstructures. In many cases experimental investigations have already pointed to one or several key processes or parameters that dominate the properties and service performance of the alloys. Under such circumstances the computational and modelling tasks are relatively well defined and the results can be critical in clarifying and solving the problems. This talk will review work conducted in the past few years using such an experiment plus computation approach, taking examples from near-alpha titanium alloys and titanium aluminides for aero engine applications and from beta-type titanium alloys for biomedical use. The topics to be covered include alloying effects on the alpha phase and their relations to creep resistance and cold dwell fatigue propensity, alloying effects, phase stability and deformation mechanisms of high strength titanium aluminides, and metastable phases and stress induced transformations in beta-type titanium alloys.

Plenary Talk | Plenary Talk

[PL6] Plenary Talk 6

Integrated earthquake simulation enhanced with high performance computing

Chair: Karin Dahmen(University of Illinois at Urbana Champaign, USA)

Fri. Nov 2, 2018 8:30 AM - 9:20 AM Room1

Muneo Hori

[PL6] Plenary Talk 6

○Muneo Hori （Earthquake Research Institute, The University of Tokyo, Japan）

(Fri. Nov 2, 2018 8:30 AM - 9:20 AM Room1)

[PL6] Plenary Talk 6

Integrated earthquake simulation enhanced with high performance computing

○Muneo Hori (Earthquake Research Institute, The University of Tokyo, Japan)

Integrated earthquake simulation (IES) is a seamless simulation of earthquake hazard, disaster and disaster response for an urban area. A set of numerical analysis of Earth Science, earthquake engineering and social sciences are used to carry out this simulation, together with analysis models of the target area that are automatically constructed by using available data of undergrounds, structures, and social activities. High performance computing is essential for the simulation with higher spatial and temporal resolution and for the evaluation of uncertainties related to a possible earthquake scenario, state of structures and social activities; capability computing is used to solve a large-scale model of an urban area, and capability computing is used to solve numerous cases and analysis models for the uncertainties. This lecture presents the current state of IES that uses K computer and other supercomputers. The following topics are focused: 1) key numerical techniques that are implemented into finite element method for scalable parallel computation; 2) particle simulation for fluid and human being; ad 3) the automated model construction that take advantage of various distinct data sources. Several examples of IES that are made for actual cities in Japan are presented. Discussions are made for the future use of higher fidelity models of structures in order to make more reliable seismic response analysis.