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ME/ISE SEMINAR: Yue Fan, Ph.D.

Mechanics of Structural Materials under Non-equilibrium Processing: a Tale of Two Solids by Energy Landscape-based Atomistic Modeling

Monday, March 14 | 3:30 PM | MEB 246

An improved fundamental understanding of materials performance at complex processing environments away from equilibrium has become a compelling need in many important applications, ranging from sustainable energy system to advanced manufacturing. I will introduce the behaviors of two different materials systems (crystals and glasses) under complex environments. I will demonstrate the seemingly different systems can be understood within the same framework by combining the transition state theory and potential energy landscape (PEL)-based atomistic modeling. In addition, by tuning surrounding environments, it is possible to alter the PEL structure, manipulate the kinetics, and thus control the materials behaviors.

In particular the first part of this talk concerns the mechanisms of interactions between dislocations and obstacles in nuclear fuel cladding materials, under very wide range of thermo-mechanical processing conditions (*i.e.* strain rate from $10^{-6}s^{-1}$—$10^{7}s^{-1}$), which was never possible to address explicitly before. It is demonstrated that, due to a non-linear coupling behavior between thermal activation and strain rate, dislocation channeling mechanism is dominant at high temperatures and low strain rates; while defects recovery prevails at low temperatures and high strain rates. The boundary differentiating the two mechanisms is further quantified, and the hereby predicted mechanism map is validated against available experiments and simulations. In the second part of the presentation, I will discuss the performance of ZrCu-based metallic glasses at different non-equilibrium meta-stable states. It is demonstrated that deformation modes (localized *vs* cascade) depend on the density of local minima of the materials underlying PEL: higher density would enable more efficient energy dissipation and yield better ductility. The implications of these examples, as well as the broad impacts on other important problems and future research plans, are also discussed.

Yue Fan is a Eugene P. Wigner Fellow at Oak Ridge National Laboratory, working in the Materials Science and Technology Division. He received his Ph.D. degree from Massachusetts Institute of Technology in 2013. He has received several honors, including “Young Scientist Award for Best Oral Presentation” (by 2010 Nuclear Materials Conference), “Aneesur Rahman Postdoctoral Fellowship” (2012, by Argonne National Laboratory), and “Eugene P. Wigner Fellow” (2013, by Oak Ridge National Laboratory). His primary research interest is to provide a substantive knowledge on mechanics and microstructural evolution in complex systems via predictive modeling, and thus facilitate the development of new science-based high performance materials with novel functions and unprecedented strength, durability, and resistance to traditional degradation and failure.