

Fall 2017 Joint Colloquium

Materials Department & Materials Research Laboratory

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University of California, Berkeley
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Friday, December 8th, 2017
11:00 am, ESB 1001

Insights into Deformation Mechanisms in Metals from Computational Simulations: The Case of Deformation Behavior in Titanium Alloys

The past decade has witnessed a rapid increase in the use of first-principles calculations and classical atomistic simulations to guide the discovery and design of materials for applications across a broad range of technologies. For structural materials, this type of modeling can be used to provide unique insights into the atomic mechanisms underlying mechanical deformation behavior. In this talk I will illustrate insights gained from atomic-scale modeling in this context, focusing on recent investigations of the dramatic effect of solutes on the deformation behavior of hcp-structured titanium solid solutions. I will focus specifically on the origin of experimentally observed changes in deformation microstructures associated with solute content for both Ti-Al and Ti-O alloys. For both systems, experiments observe transitions to planar slip that are associated with increasing solute content. First-principles and atomistic modeling suggest that this behavior stems from two different origins in these two systems, associated with short-range-order softening in the case of substitutional Ti-Al, and a novel slip-induced restructuring in interstitial Ti-O systems. The relevance of these insights to alloy design will be discussed.

Bio

Mark Asta is a professor and department chair of Materials Science and Engineering at the University of California, Berkeley. His research interests include the development and application of atomic-scale computational modeling for the prediction of equilibrium and kinetic properties of materials, and for computationally aided materials discovery and design. His work has included numerous contributions to the science of crystalline interfaces in materials, as well as the modeling of disordered materials. Professor Asta received his PhD in an interdisciplinary Materials Physics program at UC Berkeley in 1993. He was a postdoc and then staff member at Sandia National Laboratories, Livermore from 1993-2000. He moved to Northwestern to join the faculty of Materials Science and Engineering at Northwestern in 2000, returning to California as a faculty member at UC Davis in 2005. He moved to UC Berkeley in 2010, becoming Department Chair in 2012. He currently holds the Arthur C. and Phyllis G. Oppenheimer Endowed Chair for Advanced Materials Analysis at UCB. He is also a Fellow of the American Physical Society, a recipient of the ASM Silver Medal and the 2019 recipient of the TMS William Hume-Rothery award.

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Hosted by Anton Van der Ven.