MAE Seminar May 15th, 2015, - 10:30am - 11:30am, Location: MDEA, #311 on the UCI Campus Map

Hosted by: Professor Tim Rupert (trupert@uci.edu)

Computational Methods for Quantifying Plasticity in Nanostructured Materials

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ABSTRACT: As the theoretical physicist, Sir Frederick Charles Franck, said, 'Crystals are like people: it is the defects in them that make them interesting.' Although material functionality is ultimately realized on the macroscale, processes at the atomic-scale inherently govern bulk properties. In this talk, I will discuss our recent research in the area of materials modeling of nanoscale plasticity, using various atomistic simulation techniques, aimed at uncovering the influence of defects (i.e., dislocations and interfaces) on the structure, evolution, and deformation of nanostructured metallic materials for emerging technologies.

In particular, massively-parallel molecular dynamics simulations on high-performance computational platforms have proven capable of providing unprecedented insight into key deformation processes underlying the mechanics of materials and structures. We not only show that the cooperation of various nanoscale mechanisms are responsible for the observed enhancement in nanocrystalline bulk behavior, but also for the first-time, provide quantitative evidence for a transition to interfacial-mediated plasticity near maximum strength. Our approach leverages novel microscale kinematic metrics derived from continuum mechanics theory to compute non-local fields. These metrics are formulated specifically to translate information into microscale computational models from atomistics theory, and thereby capture underlying nanoscale physics. Our work suggests various avenues for improving the mechanical strength and stability of engineered hierarchical materials through a computer-aided design approach, and illustrates opportunities to tune the functional properties of nanostructured materials.

BIO: Dr. Garritt Tucker is an Assistant Professor in the Department of Materials Science and Engineering at Drexel University. He received a B.S. degree in Physics and Mathematics from Westminster College, followed by a Ph.D. in Materials Science and Engineering from the Georgia Institute of Technology in 2011. Professor Tucker performed his postdoctoral research at Sandia National Laboratories with Dr. Stephen Foiles, before joining Drexel in 2013. His research group focuses on computational materials science, with an emphasis on nanoscale structure-property relationships, microstructural evolution, defect/interface interactions, and the development of synergistic tools to connect computational and experimental methods.