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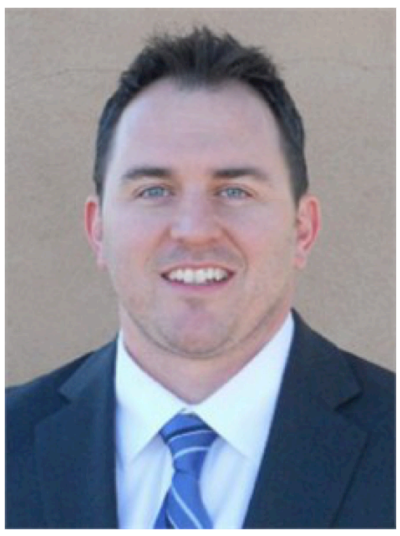

Professor Garritt Tucker
Drexel University, Philadelphia, Pennsylvania

Atomistic Methods to Quantify Nanoscale Strain and Deformation Mechanisms in Nanostructured Materials

Thursday, August 27, 2015
3:00 - 4:00pm
MSL Auditorium (TA-03, Bldg. 1698, Room A103)

Abstract: As the theoretical physicist, Sir Frederick Charles Franck, said, 'Crystals are like people: it is the defects in them that make them interesting.' Fundamental research in Materials Science and Engineering focuses on linking structure and behavior, and elucidating the influence of defects on material behavior. 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 nanoscale materials modeling, using various atomistic simulation techniques, aimed at uncovering the influence of defects (i.e., dislocations, excess free volume, and grain boundaries) on the structure, evolution, and deformation of nanostructured metallic materials.

Large-scale parallel molecular dynamics simulations have proven capable of providing unprecedented insight into key deformation processes underlying microstructure evolution. We not only show that the cooperation of various deformation mechanisms is responsible for the observed enhancement in nanocrystalline bulk behavior and structural evolution, but also for the first-time provide quantitative evidence for a transition to interfacial-mediated strain accommodation near maximum strength in nanocrystalline copper. Our approach uses novel microscale kinematic metrics derived from continuum mechanics theory to compute non-local behavior. These metrics are formulated specifically to potentially translate information into larger-scaled computational models from atomistics and thereby capture underlying nanoscale behavior. We also study rate-dependent grain growth and twinning processes in textured metals using the metrics and high-performance computing algorithms. Finally, I will discuss the broader impact of these studies, possible extensions of this work for structural applications, and investigations into the structure and evolution of microstructures in extreme environments on the scientific community.

Bio: Prof. Tucker is an Assistant Professor in the Department of Materials Science and Engineering at Drexel University. He heads the Computational Materials Science and Design Research Group at Drexel where he employs a myriad of computing/numerical/theoretical techniques to research both the fundamental physics and properties of materials and new avenues for tailoring advantageous functional properties in nanostructure materials. He earned his Ph.D in 2011 from the School of Materials Science and Engineering at the Georgia Institute of Technology in the Mechanics of Materials group and was nominated for the Sigma Xi award. Prior to starting at Drexel in 2013, he spent two years as a postdoctoral research appointee at Sandia National Laboratories in Albuquerque, NM in the Computational Materials and Data Science group. Since joining the faculty at Drexel University, his work has been featured at both domestic and international conferences, and he has recently been awarded the Most Outstanding Teacher Award in 2015.

If you would like to meet with Prof. Tucker, please contact Nathan Mara at namara@lanl.gov, or 667-8665

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