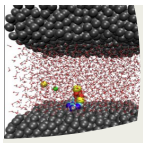
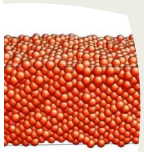
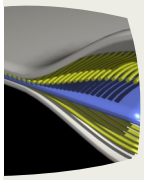

UCI Samueli School of Engineering

Department of Civil and Environmental Engineering

Presented By:
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Specialty Metals Branch
Weapons & Materials Research Directorate

Civil Engineering Seminar Series

Thursday, April 28th, 2016
MDEA
4:00PM to 4:50PM

Virtual Diffraction Characterization of Atomistic Stimulations

Virtual diffraction is advancing the synergy between experimental studies and computational modeling by offering greater means for model validation and by providing insights to complex phenomena that are observed during material characterization. Specifically, virtual diffraction techniques developed by Coleman et al. can create x-ray, electron, and Kikuchi diffraction patterns directly from large-scale atomistic simulation data. To create these patterns, these techniques use a highly parallelized algorithm to compute kinematic diffraction intensities across a three-dimensional mesh of reciprocal space. These algorithms have been fully integrated into the LAMMPS molecular dynamics simulator enabling the efficient computation of diffraction patterns from multimillion atom simulations as they evolve through space and time. The virtual diffraction methods account for different atom species within a multicomponent system and do not require any assumptions of the modeled crystal structure, which enables the exploration of a multitude of materials classes. This presentation will introduce the framework for computing virtual x-ray, electron, and Kikuchi diffraction patterns within LAMMPS atomistic simulations as well as showcase its applications. First, virtual diffraction is used to explore the effects of pre-twinning and texture during nanocrystalline deformation. Virtual x-ray and electron diffraction patterns computed from these simulations at different stages of tension and compression show unique peak splitting and peak rotation as a function of their initial twin content and texture, respectively. Second, virtual x-ray and Kikuchi diffraction patterns are used as a metric for validating select empirical interatomic potentials developed for boron based ceramics. The simulated diffraction patterns are used to quantify the deviation between the predicted energy minimized structures using the empirical potentials and DFT. These virtual diffraction patterns are also compared directly to experimental patterns to help identify the fundamental polytypes present within the experiment.

Dr. Shawn P. Coleman is a postdoctoral researcher at the U.S. Army Research Laboratory in the Lightweight and Specialty Metals Branch of the Weapons and Materials Research Directorate. He completed his Ph.D. in Mechanical Engineering from the University of Arkansas in 2014, where he investigated the structure and properties of ceramic interfaces using atomistic simulations and virtual diffraction characterization. His advancements to virtual diffraction characterization as a route to connect simulations with experiments were recognized by the Materials Research Society (MRS) through the 2014 Graduate Student Silver Award. The blend of material science and high performance computing was highlighted by the National Center for Supercomputing Application (NCSA) as well as recognized by the Extreme Science and Engineering Discovery Environment (XSEDE) 2014 Best Paper Award. Dr. Coleman's current research interests at the U.S. Army Research Laboratories include the development of automated characterization techniques using materials simulation and the creation of material property databases to foster the intelligent design of lightweight materials.