MECHANICAL ENGINEERING COLLOQUIUM: SPRING 2016

Special MIE Seminar

Friday, February 26, 2016
*******10:30 A.M. in room GITC 3710*******

Multiscale Modeling of Ultrafine-Scaled Materials

-Bottom-up Interface Engineering-

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Abstract

Future advancements in energy technologies demand novel materials that tolerate extreme environments that exceed the capability of even the most advanced materials to date. For centuries, improvements in structural materials are largely based on enhancing the microstructures and properties of the constituents. In the recent years, with the discovery of various classes of ultrafine-scaled (UFS) materials (such as nano-multilayered composites, nano-crystalline materials, nano-twinned materials), materials science is entering a revolutionary era. Now, specific properties of the UFS materials can be attained through "interface engineering", where the architecture/structure of the interfaces are carefully controlled. Interfaces are important in materials of any microstructural size scale, because they can act as sources, sinks, barriers, and storage sites for defects - including dislocations, which are the main carrier of plastic deformation. In nanostructured materials, interfaces dominate material's mechanical response and can engender properties superior to those of their coarse-grained counterparts. However, the "interface engineering" of the UFS materials is hindered by the lack of an accurate, efficient materials model that incorporates the important role of the interfaces. The conventional materials models follow the 'constituent-dominated paradigm' and are unable to capture the physics of unit mechanisms at interfaces. Among the modern models, atomistic modeling can elucidate the unit processes occurring within/at/across interfaces but cannot predict macroscopic properties. Dislocation Dynamics (DD) models have the unique advantage of exploring the dislocation activity in single crystal, but typically do not incorporate the role of interfaces in mechanical deformation. Therefore, to achieve efficient "interface engineering", my research takes a bottom-up multiscale approach which combines the advantages of the atomistic modeling and DD models. The focuses are: (1) to understand the interface's structures and the role of interface in material's deformation using atomic-scale study; (2) to develop a multiscale materials modeling tool by advancing the current DD models and incorporating interface physics characterized at atomic scale to predict mechanical performance of materials at meso-scale.

Biosketch

Shuai Shao is currently a Postdoctoral Research Associate at Center for Advanced Vehicular Systems (CAVS), Mississippi State University. His main research interest is the multiscale modeling of ultra-fine scaled materials. Dr. Shao received his Ph.D in Mechanical Engineering from Washington State University in May 2012. His thesis focused on the atomistic studies of deformation mechanisms in nanoscale multilayered metallic composites. After graduation, he continued to work at WSU on the statistical quantification of plastic deformation in small volumes. He joined the Materials Science and Technology Division of Los Alamos National Laboratory in November 2012. In February 2016, he joined CAVS. He has authored/co-authored over 23 articles in peer-reviewed journals and has given 20 invited/regular presentations.