

SPRING 2007 SEMINAR SERIES

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Room: SL 165

Everyone is invited

Multiscale Computer Simulations for Materials Science

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Abstract. Computer simulation provides great opportunities to design, characterize, and optimize materials before the expensive experimental process of synthesis, characterization, assembly, and testing. Thus, first-principles based multiscale computer simulation is a powerful approach that could accelerate, achieve, and amplify research discoveries in materials science. To illustrate the above viewpoint, I will discuss the following two examples.

(1) I have developed a first-principles based multiscale approach and further applied it to modeling single crystal plasticity of bcc Tantalum (Ta). This approach is based on dislocation mechanism and consists of a three-level modeling hierarchy: (a) derive the atomic interaction potentials for Ta, (b) predict the properties and behavior of dislocations, and (c) describe the material plasticity using a mesoscopic model. This multiscale approach captures salient features of the observed effects of temperature and strain rate on the hardening rate for high purity bcc Ta crystals.

(2) Zinc oxide (ZnO) is a unique material that has semiconducting, piezoelectric, pyroelectric, and biocompatible properties. Thus, one dimensional ZnO nanomaterials have promising applications as active components in nanoelectromechanical and biosensor systems. I propose a model that describes the size dependency of the elastic modulus of ZnO nanowires basing on the ZnO surface stresses calculated using first-principles method.

About the Speaker. Dr. Wang is a Research Assistant Professor at the University of South Carolina (Aiken campus) and a current member of USC NanoCenter. He received his Ph.D. in Materials Science with a minor degree in Computer Science from California Institute of Technology in 2002. Dr. Wang was a postdoctoral fellow at Materials Sciences Division of Lawrence Berkeley National Laboratory from 2002 to 2005. Dr. Wang has been developing and applying first-principles based multi-scale approach and novel simulation algorithms to challenging problems in a broad range of materials.