Carnegie Mellon

Materials Science and Engineering Seminar Series

Dr. Yunzhi Wang

Ohio State University

"Microscopic Phase-Field Modeling of Shear-Dominated Process During Phase Transformation and Plastic Deformation"

Friday, January 27, 2006
10:30 A.M. Refreshments, 11:00 A.M. Seminar
Singleton Room, Roberts Engineering Hall (REH)

Based on gradient thermodynamics of non-uniform systems, Green's function solution of long-range interactions, and field representation of microstructures, the phase-field method has been used widely in describing microstructures consisting of various types of extended defects. Typical examples include homo- and hetero-phase interfaces, ferromagnetic and ferroelectric domain walls, and dislocations. Although the method has enjoyed remarkable success in recent years, it is limited to microstructural features at the mesoscopic length scales. In this presentation, we discuss the most recent development of the method in capturing microstructural features at the microscopic length scales that control the micromechanisms of shear dominated processes during phase transformation and plastic deformation. Three examples are chosen to illustrate the new capabilities of the method at the microscopic level: (a) structure and energy of small angle grain boundaries consisting of regular dislocation networks, (b) initiation and growth of martensite, and (c) shearing of γ' precipitates in Ni-base superalloys and slip transmission across α/β interfaces in Ti alloys during creep deformations. In particular, we employ *ab initio* calculations of the generalized stacking fault (GSF) energy as the input and show quantitatively that the microscopic phase-field model is a 3D generalization of the Peierls model that has been the cornerstone of modern nanomechanics.

Yunzhi Wang received a M.S. in 1992 and a Ph.D. in 1995 in Materials Science and Engineering from Rutgers University. He joined the Department of Materials Science and Engineering at The Ohio State University (OSU) in 1996 as an assistant professor. He is now a professor working in the field of computational materials science and engineering. His major research interests include (a) microstructural evolution and microstructure--dislocation interactions in high-temperature structural materials, (b) microstructure development in advanced multi-domain magnetic materials under applied fields, (c) interdiffusion microstructure and diffusion path in multi-component and multiphase coatings and multi-layers and (d) grain growth and texture development in anisotropic media and migration of interfaces and dislocations with segregating defects and precipitates. His work is part of a greater effort in developing microstructure- and micromechanisms-based modeling tools at the Center for Accelerated Maturation of Materials (CAMM) at OSU.