Phase Field Modeling of Nano and Microstructural Evolution

Thursday, March 6, 2014, 3:30P.M.

Lower Level Auditorium, Geddes Hall

Refreshments served at 3:00 p.m. in the Geddes Hall Coffee House

Predicting and controlling nano/microstructure-property-processing relations in materials play important roles in design and manufacturing of engineering parts and structures. With recent progress in supercomputing, computational modeling and simulations have become commanding modules in studying nano and microstructures of materials in different engineering and science disciplines. Along this path, diffusive-interface or phase field modeling methodology has recently emerged as a powerful computational tool to study nano and microstructural evolutions towards predicting nano/microstructure-property-processing relations in materials. A broad spectrum of moving boundary problems in engineering and physics, such as those in solidification, grain growth, multi-phase fluid flow, and solid state phase transformation, can be successfully simulated with phase field models.

In this seminar, a Cahn–Hilliard* phase field model will be presented for diffusion-controlled solid state phase transformation in binary alloys, coupled with elasticity of the solid phases. A new Galerkin finite element formulation will be introduced with mixed-order interpolation functions to simultaneously solve the fourth and second order partial differential equations governing the phase-field and elasticity, respectively. Some other phase field–finite element models will be presented, including those for solidification microstructures of pure and multi-component lightweight metals, and oxidation, solid state martensitic phase transformation and hydride precipitation in nuclear fuel cladding materials. Finally, a new phase field model connected to density functional theory and molecular dynamics simulations will be presented, which naturally incorporates elasticity, plasticity, and nucleation and evolution of dislocations.

*J.W. Cahn and J.E. Hilliard, Free energy of a nonuniform system. I. Interfacial free energy, J. Chem. Phys. 28 (1958) 258–267.

Dr. Mohsen Asle Zaeem
Materials Science and Engineering
Missouri University of Science and Technology

If you are interested in meeting individually with Dr. Zaeem, please contact Linda at 631-5431.