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The Hong Kong University of Science and Technology

Scientific Computation Concentration

Phase-Field Modeling of Pattern Formation and Microstructural Evolution during Solid State Processes

By

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Abstract

The phase-field approach has achieved increasing prominence in modeling pattern formation and microstructure evolution (i.e., free-boundary problems) in numerous materials science and engineering applications. Based on continuum field description of defects (i.e., microstructures), gradient thermodynamics and Green's function solution of long-range elastic interactions, the phase-field method has advantage to describe the evolution of arbitrarily complex shapes involving different types of interfaces and thermomechanical driving forces. The method can be applied at both the individual defect level (from angstroms to nanometers) and coarse-grained level (from nanometers to microns and beyond). In this presentation, the phase-field methods in modeling pattern formation and microstructural evolution during phase transformations and plastic deformation in solids will be reviewed. In particular, we will demonstrate that, when applied at the individual defect level, the microscopic phase-field model (MPF) is a superset of the Cahn–Hilliard description of chemical inhomogeneities and the Peierls description of displacive inhomogeneities. It has the ability to predict fundamental properties of individual defects such as width, structure and surface energy of homo-phase and hetero-phase interfaces, core-structure and line-energy of dislocations, and saddle-point configuration and formation energy of defect nuclei, as well as the micromechanisms of their mutual interactions, using directly ab initio calculations as model inputs. When applied at mesoscales, the coarse-grained phase-field model (CGPFM) has the ability to predict the evolution of microstructural patterns consisting of a large assembly of both chemically and mechanically interacting defects through coupled displacive and diffusional mechanisms, with user-supplied linear response rate laws, and defect energy and mobility informed by ab initio calculations, CALPHAD databases and MPF simulations. [Acta Materialia Overview 150: 58 (2010) 1212-1235].

Date: ***Tuesday, 10 April 2018***
Time: ***3:00p.m. – 4:00p.m.***
Venue: ***Room 4472, Academic Building (near Lifts 25 & 26), HKUST***

All are welcome!