Phase Field Crystal Modelling and its applications

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Overview

The processing of materials leads to changes in microstructures of the materials which in turn decide the properties. Thus, microstructures form the bridge between processing and material properties. Hence, the formation and evolution of microstructures is a problem of both academic and industrial importance.

Typically, microstructural evolution is studied using phase field models. Phase field models are continuum models and hence smear out or average out the information at the atomistic scale. On the other hand, atomistic models such as molecular dynamics and Monte Carlo simulations can be used to study microstructural evolution at the atomistic scale. But, the time scales that molecular dynamics simulations can reach is rather limited. Thus, for cases in which the atomistic structure plays a crucial role in the evolution of microstructures, there is a need for developing a model that bridges scales. Phase Field Crystal (PFC) is one such model which can be considered as the time averaged molecular dynamics model and hence, resolves the structures of materials atomistically on the spatial scale but can reach up to diffusional time scales.

PFC models have been emerging as an efficient atomistic computational tool to study materials science problems at the atomistic length scale. The continuum description of atoms in the PFC model naturally gives rise to lattice structures, elasticity, and defect structures, which are crucial in describing material phenomena at the atomistic scale.

The primary objectives of the course are as follows: i) To teach the fundamentals of PFC (with hands on sessions), ii) To connect the PFC modelling to classical density functional theories, iii) To indicate the current advances in terms of multi-modal and multi-phase PFC approaches, and, iv) To apply PFC to problems such as solid-melt interfacial anisotropy, dislocation dynamics, grain boundary grooving in nanoparticles, and grain boundary stability.

Modules	**PFC modelling : October 10 - October 21, 2022**
You Should Attend If...	▪ You are an Engineer and/or Researcher from materials and manufacturing industry, government and industrial R&D laboratories. ▪ You are a faculty or student: students at all levels (BTech/MSc/MTech/PhD) or Faculty from academic institutions and technical institutions.
Fees	The participation fees for taking the course is as follows: **Participants from abroad : US $500** **Industry/ Research Organizations: 30000** **Academic Institutions: 10000** The above fee include all instructional materials, computer use for tutorials and assignments, laboratory equipment usage charges, 24 hr free internet facility. The participants will be provided with accommodation on payment basis.

The Faculty

Professor Kuo-An Wu is in the faculty of Department of Physics at the National Tsing Hua University, Taiwan. His research interests include Condensed Matter, Pattern Formation, Computational Materials Science at the Nanoscale, Mathematical Biology - Synchronization and Population Dynamics, and, Polymer Physics.

Professor M P Gururajan is in the faculty of Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai, India. His research and teaching interests include phase field modelling, molecular dynamcis and Monte Carlo modelling, modelling microstructural evolution, mechanics and thermodynamics of materials, data analysis and interpretation, diffusion and kinetics, simulation and optimization, and modelling.

Course Co-ordinator

Prof. M P Gururajan
Phone: 0912225767631
E-mail: guru.mp@iitb.ac.in

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