Atomistic modelling for microstructural evolution

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Overview

The modelling of atomistic and microstructural evolution is an important academic problem of scientific interest as well as an important practical problem of great industrial importance. The models of microstructural evolution can be broadly classified into atomistic models and continuum models. The continuum models themselves can be classified into mesoscale and macroscale models.

In the atomistic models, both molecular dynamics and Monte Carlo models are extensively used to study and understand microstructural evolution. Specifically, these models and their extensions can be used to both understand microstructural evolution and to generate parameters which are hard to evaluate experimentally but are needed in meso-scale continuum models.

In this course, we will give a hands on training on modelling microstructural evolution using atomistic models as well as indicate their statistical basis. We will make the students use existing open source codes as well as write some simple codes and scripts, and familiarize them with both the basic underlying concepts as well as the practical implementation and use. This also includes to learn about limitations inherent to these tools.

The primary objectives of the course are as follows: i) To teach the fundamentals of atomisitic models (with hands on sessions), ii) To explain the statistical basis of atomistic models, iii) To expose the students to some of the open source codes that are available, and iv) To apply atomistic models and their extensions to problems such as ordering, precipitation, grain growth, and deformation induced microstructural evolution.

Modules	**MD and MC : September 19 - September 30, 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 Dr Ferdinand Haider is in the faculty of Department of Physics at the University of Augsburg, Germany. His research interests include Metallic alloys, phase transformations in alloys, phase separation, precipitation reactions, extreme plastic deformation, recrystallization of deformed metals, electron microscopy of metals, computer simulation in materials science, corrosion of metals, high temperature corrosion, and, friction stir welding

Professor M P Gururajan is in the faculty of Department of Metallurgical 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

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