SPARC Phase-III Workshop

Microstructure quantification & their mesoscale & atomistic modeling

Overview

Modern engineering applications like aerospace, automobile, electronics, bioimplants, actuators, etc., require effective structures and components with improved safety properties and reduced environmental impact. These requirements include producing specific components using (i) ultra-lightweight structural materials, (ii) advanced high-temperature and creep-resistant materials, (ii) nanostructured materials. In this regard, it is essential to have an understanding of (i) quantitative microstructure characterization of polycrystalline materials, (ii) microstructure evolution using mesoscale physics and mathematical formulation (phase-field models), and (iii) atomistic modeling via molecular dynamics and density functional theory to simulate, understand and predict the structure and properties of materials.

The workshop is in three parts. The 1st part discusses the microstructure of polycrystalline materials that determines their mechanical, electrical, magnetic and optical properties. We will focus on electron backscatter diffraction (EBSD) and scanning electron microscopy (SEM) as techniques used to quantify these complex materials' microstructure. Participants will gain an understanding of basic crystallography and diffraction theory as a foundation for how the measurement techniques work. Finally, we will discuss the analysis of the data in terms of determining quantifiable measures of the microstructure, ensuring their statistical reliability, and how these can be incorporated into models of microstructure evolution. In the 2nd part, the evolution of microstructures during processing and service will be studied using mesoscale models capable of representing moving interfaces. Mesoscale physics and mathematical formulation: continua, phase-field models. Computational implementation. The 3rd part introduces the atomistic simulation tools to model, understand and predict the structure and properties of materials. The mathematical and numerical descriptions of molecular dynamics simulations and density functional theory will be introduced. Both first principles and classical molecular simulations will be employed to establish relationships between the chemical composition, structural properties of distinct phases and ion transport characteristics.

The participants will learn these topics through lectures and hands-on tutorial sessions. There will be practice sessions on identifying lattice spacing and crystal structures using XRD, measuring bandwidth angle and d-spacing from EBSD, Calculations of microstructure and texture, case study using COMSOL Multiphysics software, structural and functional properties using Molecular dynamics simulations to stimulate research motivation of participants.

Modules	**28 hrs lecture and 8 hrs lab component 15th July – 28th July 2024 (14 days)** **Number of participants for the workshop will be limited to fifty. The selection is on a first-come, first-served basis.**
You should attend if you are	▪ Working on problems related to (i) quantitative microscopy, (ii) Crystal structure & stereographic projection, (iii) crystallographic texture, (iv) XRD, (iv) EBSD, (v) dislocations & grain boundaries, (vi) phase-field modelling, (vii) atomistic (molecular dynamics and density functional theory) simulations ▪ An engineer or researcher from the materials science and metallurgical industry (such as Tata Steel, JSW, GE) and from research centres such as BARC, IGCAR, ISRO and DMRL. ▪ Student at the post-graduate level (MTech/PhD) or early-stage researcher (post-docs and faculty) from reputed academic or technical institutions.
Fees	There are no fees
Registration	Interested researchers, faculty members, and students must register through: ..... Acceptance of the registration will be sent to you by email.

The Faculty

Dr. David P. Field is a Professor and Director at Institute of Materials Research, Washington State University, Pullman, WA, USA. He is presently the Editor-in-Chief of Materials Characterization journal. His research interests include physical and mechanical metallurgy, metal deformation and recrystallization, crystallographic texture, grain boundary structure, thin film and IC interconnect structure/properties relationships, and advanced experimental techniques.

Dr. SOMJEET BISWAS is an Associate Professor in the Dept. of Metallurgical and Materials Engineering, IIT Kharagpur, INDIA. His research domains are quantitative microscopy, crystallographic texture, grain boundary engineering, plastic deformation behavior of polycrystalline materials, fatigue and fracture behavior, and recrystallization mechanism of metals and alloys.

Dr. SINISA DJ MESAROVIC is a Professor at School of Mechanical and Materials Engineering, Washington State University, Pullman, WA, USA. His research interests are Mathematical formulation of physical processes, with particular interest in multiscale models and computational methods, as well as applications in both materials processing and service. Current focus is on mathematical and computational methods for coupled problems with moving boundaries.

Dr. SOUMIK BANERJEE is an Associate Professor at School of Mechanical and Materials Engineering, Washington State University, Pullman, WA, USA. His research interests include modeling of processing, structure and functional properties of materials and interfaces relevant to energy conversion and storage, Computational design of electrolytes for batteries, Sustainable processing and electroplating of lunar regolith using ionic liquids, Morphology of solution-processed thin perovskite films in solar cells.

Dr. SHAMPA AICH is a Professor in the Dept. of Metallurgical and Materials Engineering, IIT Kharagpur, INDIA. Her research interests are materials and microstructure characterization and correlation with functional properties such as magnetic and shape memory effects. Atomic migration and diffusion between multi-layer bi-metallic thin films.

Venue

Department of Metallurgical and Materials Engineering, Indian Institute of Technology Kharagpur – 721 302, West Bengal, INDIA

Contact

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Level: U.G. 4th Year and P.G. 1st Year

Discipline: Metallurgical and Materials Engineering/Mechanical Engineering/Materials Science

Prerequisites: Basic knowledge of materials characterization, mechanical and physical metallurgy, continuum mechanics, thermodynamics, basic finite elements, computing, transport phenomena.

Contents *(# of lecture hours)*

Topics	Brief Description	# of hours
Part-I: Microstructure and texture of materials		
Crystallography and microstructure	Lattice constants, Interplanar spacing, Interplanar angles, Structure factor.	**2**
Texture	Pole figures, Inverse pole figures, Euler space, Rodrigues vectors.	**2**
Diffraction principles	Bragg's law and diffraction theory, application of Bragg's law to EBSD measurements, features of EBSD patterns that can be used in analysis of structure.	**2**
Electron Microscopy	SEM basic operation, electron gun, electron optics, imaging strategies.	**2**
Texture Calculations	Texture calculations, generalized spherical harmonics method, pole figure inversion, differences between X-ray and electron-based diffraction data and the resultant differences in calculation techniques.	**2**
Identifying texture Components	Identification of various texture components, discussion of how texture develops and evolves, what to look for in pole figures and Euler space plots to properly identify fiber textures and individual components.	**2**
Part-II: Mesoscale modelling of evolving microstructures		
Introduction and fundamentals	Physical and micromechanical foundations of mesoscale continua. Weak and strong form of a boundary value problem. Thermodynamics. Mathematical foundations of the finite element method	**2**
Phase field models	Thermodynamics of surfaces. Sharp and diffuse interface formulations.	**2**
Phase field models in solids	Thermodynamics of solids. Phase transformations. Diffusion and creep. Sintering. Finite element formulation.	**2**
Part-III: Atomistic modelling of structure and functional properties		
Introduction and fundamentals	Materials/Interfaces, Introduction of key materials, Structural properties and correlation with ion transport	**2**
Statistical mechanics as a tool to evaluate properties	Introduction to ensembles, partition functions, thermodynamic properties, and fluctuation-dissipation theorem.	**2**
Molecular dynamics simulations	Mathematical and numerical description, First-principles, Technical aspects, Case studies, Applications and Performance.	**2**
Density functional theory	Mathematical and numerical description, First-principles, Technical aspects, Case studies, Applications and Performance	**2**
Monte Carlo approach	Scaling up from atomistic simulations. Introduce kinetic Monte Carlo as a stochastic tool to model deposition, growth and evolution of structure.	**2**

Lab component *(if relevant)*

Experiment	Brief Description	# of hours
XRD vs. EBSD	Use data from XRD measurements to calculate lattice spacing and identify crystal structures. Use EBSD patterns to measure bandwidth angle and show how d-spacing measurements could be done.	**2**
Calculations of microstructure and texture	From the EBSD scanned data, identify and quantify (i) different microstructural features and (ii) texture using (a) Pole figure, (b) Inverse pole figure and (c) Euler space. Use data to pull out specific features that help to identify processed structures.	**2**
COMSOL Multiphysics software	A case study using computational tool	**2**
Molecular dynamics simulations – structural and functional properties	Use data from MD simulations to calculate (a) pair distribution functions and compare with XRD and Neutron scattering data, and (b) functional properties such as diffusion coefficient based on data from pre-run simulations.	**2**

References:

Books

- A.J. Schwartz, M. Kumar, B.L. Adamas, D.P. Field, Electron Backscatter Diffraction in Materials Science, Springer Link (2009).
- U.F. Kocks C.N. Tome, H.-R. Wenk. Texture and Anisotropy, Cambridge University Press (2000)
- V. Randle and O. Engler, Introduction to Texture Analysis, Taylor and Fransis (2009).
- R.E. Sonntag, G.J. Van Wylen, Fundamentals of Statistical Thermodynamics, John Wiley & Sons Inc. (1968).
- J.M. Haile, Molecular Dynamics Simulation: Elementary Methods, John Wiley & Sons, Inc. (1992).
- T.J.R. Hughes, *The finite element method,* Dover publications (2000).
- L.E. Malvern, *Introduction to the mechanics of a continuous medium*. Prentice Hall (1969).
- S.Dj. Mesarovic, S. Forest, H.M. Zbib, Eds. *Mesoscale models: From micro-physics to macro-interpretation*, CISM International Centre for Mechanical Sciences book series, Springer (2019).
- N. Provatas, P.Elder, *Phase-field methods in materials science and engineering*, Wiley (2010).

Online material:

- B. Beausir, J.J. Fundenberger, Analysis tools for electron and X-ray diffraction, ATEX - software (2017).
- COMSOL Multiphysics User manual.