



Department of Sustainable Energy Engineering Indian Institute of Technology Kanpur

Proposal for New Course

Course Title	: Structure, Interfaces, and Phase Stability in Functional Materials
Credits (L-T-P [C])	: 3-0-0-9
Duration of Course	: Full Semester
Proposing Department/IDP	: Sustainable Energy Engineering (SEE)
Other Departments/IDPs which may be interested in the proposed course	: MSE, MSP, PHY, EE, ME, CHE, CHM
Other faculty members interested in teaching the proposed course	: Ashish Garg (SEE), Vivek Verma (SEE), Shikhar Misra (MSE)
Proposing Instructor(s)	: Sudarshan Narayanan, Srinivas Karthik Yadavalli
Offered for	: PG students of SEE and other departments or programs (MSE, MSP, PHY, EE, ME, CHE, CHM), 3/4 th year UG students
Status of the course	: DE / OE (PG and UG)
Prerequisite(s) for the course	: None Preferred: SEE-602 or any basic course on solid-state physics or energy materials

Course Objectives

This course provides an integrated understanding of how structure, interfaces, and phase stability govern the behaviour of modern functional materials used in energy applications. Comparing and contrasting traditional metallurgy-centric treatments, the course emphasizes multiphase, heterogeneous, and composite systems, where interfaces and defects play a critical role in enabling functionality. Students will develop a rigorous foundation in crystallography, diffraction, and defects, alongside thermodynamics, phase equilibria, and transformation kinetics, and learn to interpret phase diagrams in the context of both equilibrium and processing-driven (metastable) materials. Special emphasis is placed on distinguishing classical mixtures from engineered composites, and on understanding how structural complexity and interfacial phenomena influence performance in systems such as photovoltaics, batteries, fuel cells, and catalytic materials.

Expected Learning Outcomes

Students will be able to analyze and describe the crystal structure and phase constitution of functional materials. They will develop the ability to apply thermodynamic principles and phase diagrams to assess phase stability under equilibrium and non-equilibrium conditions. Students will understand the critical role of defects, interfaces, and heterogeneous architectures in governing transport, reactivity, and device performance. They will also distinguish between classical mixtures and engineered composites, and evaluate how processing and kinetics influence their formation and stability. Finally, students will be equipped to connect fundamental materials concepts to practical applications in energy and electronic systems.

Short summary for inclusion in the Courses of Study Booklet

The course “Structure, Interfaces, and Phase Stability in Functional Materials” examines the role of structure, interfaces, and phase stability in determining the behaviour of functional materials. It covers key concepts in crystallography, defects, thermodynamics, phase diagrams, and transformation

kinetics, with emphasis on multiphase and heterogeneous systems, while drawing a distinction between classical mixtures and engineered composites. By drawing applications from energy and electronic materials, including batteries, fuel cells, and photovoltaics, the course will help assess the structure-property-function paradigm in functional materials.



Course Contents

S. No.	Broad Title	Topics	No. of lectures
1.	Introduction	<ul style="list-style-type: none"> • Overview of functional materials: classical (metallurgical) and functional materials, mixtures and composites, interfaces • Structure-property-function relationships: coupling between structure, defects, and performance 	2
2.	Structure of solids	<ul style="list-style-type: none"> • Advanced crystallography topics: crystal symmetry, point groups and space groups, crystal packing, crystalline and non-crystalline materials • Crystal structures in functional materials: Rock salt, perovskites, spinels, layered structures, common non-ferrous oxides and sulfides; polymorphism, allotropy, and anisotropy • Basic and advanced diffractometry: Neutron and electron diffraction, SAXS, WAXS; phase identification in mixtures, <i>in situ</i> and <i>operando</i> techniques for energy materials 	5
3.	Crystal defects and disorder	<ul style="list-style-type: none"> • Defects: Types, thermodynamics, dislocations, grain boundaries, interfaces; Order, disorder, and distortion • Defect-property correlation: ionic and electronic conductivity, defect engineering • Examples/applications: Crystalline-polycrystalline-amorphous Si, oxygen vacancy transport 	5
4.	Thermodynamics of Materials	<ul style="list-style-type: none"> • Basic concepts: Energy, enthalpy, entropy, free energy • Chemical potential & phase equilibria/stability: multicomponent systems, ideality of solutions/mixtures; Ellingham, Pourbaix diagrams • Thermodynamics of defects: configurational entropy, defect formation energy • Thermodynamics in functional systems: reactions involving solids, liquids, gases, and ions – batteries, fuel cells, catalytic systems • Examples/applications: Assess stability of metal species in solution for synthesis and recovery of critical metals/minerals 	5
5.	Phase diagrams	<ul style="list-style-type: none"> • Fundamentals: Unary and binary systems, Gibbs phase rule; ordered and intermediate phases; equilibrium in heterogeneous systems • Binary phase diagrams: Eutectic, peritectic systems; interpretation in ceramics, alloys, and polymer solutions and blends; influence of interfaces • Multicomponent phase diagrams: Ternary systems • Phase stability in functional materials, engineered composites: Under operating conditions; electrochemical phase diagrams, spinodal decomposition • Examples/applications: Lithiation-induced structural and phase transformations in electrodes, degradation in perovskites; NMC cathode and slag-forming oxides as ternary systems. 	5
6.	Phase transformations	<ul style="list-style-type: none"> • Diffusion fundamentals: Fick's laws, diffusion mechanisms (atomic, ionic, vacancy) • Nucleation theory: Homogeneous and heterogeneous nucleation, 	5

		<p>energy barriers</p> <ul style="list-style-type: none"> • Growth/transformation kinetics: Interface-controlled vs. diffusion-controlled, microstructure evolution; phase separation, precipitation • Transformations in functional materials: Order-disorder transformations; phase changes in PV and battery materials • Examples/applications: Precipitation from solution in critical mineral recovery 	
--	--	--	--

Textbooks, reference books, suggested readings, and any other references:

- D.A. Porter & K.E. Easterling, Phase Transformations in Metals and Alloys, Nelson Thornes
- David R. Gaskell, Introduction to the Thermodynamics of Materials, Taylor & Francis
- B.D. Cullity and S. R. Stock, Elements of X-ray Diffraction, Pearson
- W.D. Callister & D.G. Rethwisch, Materials Science and Engineering: An Introduction, Wiley
- L.V. Azaroff, Introduction to Solids, Tata McGraw Hill
- A.R. West, Solid State Chemistry and its Applications, Wiley
- M. Ohring, Materials Science of Thin Films, Elsevier
- F. Habashi, Principles of Extractive Metallurgy (Vols. 1-2), Gordon & Breach
- M. Pourbaix, Atlas of Electrochemical Equilibria in Aqueous Solutions, NACE International.
- Reviews and journal articles

Course Proposer(s)	Recommended / Not recommended	This course is approved / Not approved
 (Sudarshan Narayanan)		
 (Srinivas Karthik Yadavalli)	Convenor, DPGC (SEE)	Chairman, SPGC
Dated: 22 / 06 / 2026	Dated:	Dated: