



THERMODYNAMICS AND KINETICS OF MATERIALS

PROF. SASWATA BHATTACHARYA

Department of Materials Science and Metallurgical Engineering
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INTENDED AUDIENCE : Undergraduate Students and First Year PG students

INDUSTRY SUPPORT : Tata Steel, JSW, General Electric, Eaton, Kennametal India, TCS-Engineering, Hindalco, MIDHANI

,In general, all Materials and Manufacturing Industries that engage in materials processing and design

COURSE OUTLINE :

This course introduces the fundamental concepts of thermodynamics and kinetics to students of Metallurgy and Materials Engineering. Major topics covered by this course are laws of thermodynamics, thermodynamic potentials, principles of phase equilibria, theory of solutions, thermodynamics of chemical reactions, thermodynamics of surfaces, rates of reactions, principles of irreversible thermodynamics, phenomenology of diffusion and atomic mechanisms of diffusion in solids. At the end of this course, a student learns how to apply thermodynamic principles to assess the feasibility of processes, calculate phase equilibrium conditions in multicomponent, multiphase materials, construct phase diagrams, calculate thermodynamic driving force for phase change, understand the principles of kinetics of irreversible processes such as rates of reactions and diffusion processes in materials. The course also includes a virtual laboratory where the student learns to compute phase equilibria and phase diagrams of unary, binary, and ternary systems and perform simulations of diffusion using the free ThermoCalc education package and open source Pycalphad and FiPy.

ABOUT INSTRUCTOR :

Prof. Saswata Bhattacharya is an Professor in Indian Institute of Technology Hyderabad. His expertise and research interests are in the areas of phase transformations of materials, phase-field modelling of microstructures, discrete dislocation dynamics and integrated computational materials engineering (ICME). He was a guest editor for the special issue on “Phase-field Modeling” in the Journal of Indian Institute of Science. Over the past several years, he has developed and taught several undergraduate and graduate courses on thermodynamics and kinetics of materials, transport phenomena, computational materials science, and materials informatics. He also taught certificate course on Micromechanics and Modeling of Microstructures in Tata Steel, NRC-M courses on Phase-field modeling and ICME in IISc Bangalore, and interdisciplinary courses on Computational Modeling. He has done several industry-sponsored and Government-funded projects and authored more than thirty papers on computational modeling of microstructures and microstructure-property relations. Currently he is engaged in developing an open-source phase-field simulation software funded by National Supercomputing Mission, Government of India.

COURSE PLAN :

Module 1 (4 weeks):

Thermodynamic systems and variables, state of a system. Laws of thermodynamics – first law and thermodynamic processes – definitions of internal energy, enthalpy, specific heat, applications in thermochemistry; second law – reversible and irreversible processes – concept of entropy and its statistical interpretation; third law – absolute scale of temperature and absolute entropy. Reservoirs and thermodynamic potentials - Helmholtz free energy, Gibbs free energy, chemical potential. Thermodynamic relations. Maxwell's relations and their applications – relations between directly measurable and not directly measurable thermodynamic quantities

Module 2 (4 weeks):

Thermodynamic equilibrium and stability, Gibbs phase rule, Clausius-Clapeyron equation; Thermodynamics of solutions: partial molar quantities, Gibbs-Duhem relation, boiling and freezing points, ideal and non-ideal solutions, activity, quasichemical solution models, applications in clustering and ordering transformations

Module 3 (4 weeks):

Gibbs free energy-composition diagrams in binary systems; Construction of binary phase diagrams - cooling curves, x-ray diffraction method, electrical resistivity method, numerical modeling; Thermodynamics of reactions – Ellingham diagram for the formation of metal oxides; Thermodynamics of surfaces – adsorption of gases, Langmuir isotherm, Gibbs interfacial thermodynamics. Introduction to thermodynamics of irreversible processes – relation between flux and thermodynamic driving force