SS858 ALLOY THERMODYNAMICS AND SOLID STATE PHASETRANSITIONS 3-1-0-4

Course Objectives:

1. Present a general outline of solid-state phase transitions and crystallographicdescription in materials
2. Understand how to calculate free energy of a solid using various approximationsand construct a simple phase diagram for a binary alloy
3. Description of diffusion and how to solve diffusion problems
4. Introduction to microstructural evolution using the phase field method and thecluster variation method

UNIT I: Basic introduction to crystals and crystallographic computation

The real space lattice – basis vectors and translation vectors; the four 2D crystal systems, seven 3D crystal systems, five 2D Bravais lattices and fourteen 3D Bravais lattices; Crystallographic directions and angles – real space metric tensor.

The reciprocal space – basis vectors and reciprocal lattice; Angle between planes and length of reciprocal lattice vectors – the reciprocal metric tensor.

Zones and zone axes; Relations between the direct and reciprocal space; co-ordinate transformations.

UNIT II: Thermodynamics of solid solutions

Review of basic thermodynamic functions – heat capacities, enthalpy, entropy, chemical potential, activity and activity coefficients; Statistical definition of entropy; Thermodynamics of solutions – ideal and non-ideal solutions – Henry’s law, Sieverts’s law and Raoult’s law; Approximations to the free energy function – Ideal solution, Regular solution and Sub-lattice model; the calculation of phase Diagrams (CALPHAD) technique using the sub-lattice model.

UNIT III: Thermodynamics of Binary Phase diagrams

The Gibbs phase rule; the common tangent rule; the lever rule; understanding the binary phase diagram: Binary phase diagrams of the types I, II..V; Miscibility gap; First order and second order phase transitions.

UNIT IV: Diffusion

Basic review of partial differential equations (PDEs); solution by analytical and numerical methods; Fick’s laws; Some useful solutions of the 1D Fick’s diffusion equation; Mechanisms of diffusion; Diffusion in metals, multiphase system and thermal diffusion.

UNIT V: Phase field method (PFM) and Cluster variation method (CVM)

Overview of the types of solid state phase transitions; Chemical potential, mobility and diffusion; Failure of the classical Fick’s law; Spinodal decomposition; The PFM: the Ginzburg - Landau Free energy functional - Cahn - Hillard (C-H) equation; Solution of the C-H equation using the semi-implicit Fourier spectral method; Diffusion vs. C-H model; Order-disorder transition and the Allen-Cahn (A-C) equation; Numerical solution of the A-C equation.

The CVM – Statistical thermodynamics on a discrete lattice: Internal energy and configurational entropy; Free energy in the CVM.

Reference Books:

Unit I:

1. Robert E Reed-Hill and Reza Abbaschian, *Physical metallurgy principles,* 4th Edition, SI Version, 2009. (Chapters 3-5)
2. Mark Ladd and Rex Palmer, *Structure determination by X-ray crystallography*, 5th Edition, Springer, 2014.

Unit II and Unit III:

1. David Gaskell and David Lauglin, *Introduction toThermodynamics of materials*, 5th Edition, CRC Press, 2017.
2. TaijiNishizawa, *Thermodynamics of microstructures*, ASM International, 2008.
3. Wolfgang Pfeiler, *Alloy Physics: A Comprehensive Reference*, Wiley-VCH VerlagGmbH & Co. KGaA, 2007. (Chapter 10 - S*tatistical Thermodynamics and model calculations by* Tetsuo Mohri)

Unit IV:

1. J. Crank,*Mathematics of diffusion*, 2nd Revised Edition, Oxford University Press, 1980.
2. Robert E Reed-Hill and Reza Abbaschian, *Physical metallurgy principles*, SI version, 2009.

Unit V:

1. Lecture notes.
2. Wolfgang Pfeiler, *Alloy Physics: A Comprehensive Reference*, Wiley-VCH VerlagGmbH & Co. KGaA, 2007. (Chapter 12- *Simulation techniques by* Ferdinand Haider, RafalKozubski and T.A. Abinandanan)

Course Outcomes:

On completion of this course students will be able to:

CO1. Understand the fundamental thermodynamic concepts and crystallographic Description of solids in relation to microstructure

CO2. Apply the knowledge of thermodynamics to construct a simple binary phase diagram

CO3. Understand how diffusion occurs and numerical solution of diffusion equations

CO4. Understand the principles behind the development of the Cahn-Hillard and Allan Cahn equations leading to the PFM method.

SS859 INTRODUCTION TO POLYMER SCIENCE AND TECHNOLOGY

3-1-0-4

Course Objectives:

This course is aimed at imparting basic knowledge to students about polymers and structure-property correlation in polymers and polymer composites. Students will be able to understand various applications of polymers, polymer blends and polymer composites in membrane separations, biomedical applications, fuel cells, paints etc.

Unit 1: Introductory Polymer Science

Classification of polymers, Molecular weight distribution, Molecular weight averages, Poly dispersity index, Polymer synthesis: Step growth and Chain growth polymerization, Different polymerization techniques, Thermodynamics of polymer solutions- Flory-Huggins theory, Measurement of molecular weight by gel permeation chromatography, Intrinsic viscosity measurements, Light scattering methods.

Unit 2: Physical and Mechanical Properties of Polymers

The amorphous state, the glass transition, factors affecting glass transition temperature, Thermodynamics of glass transition, Secondary relaxation processes, Crystalline state of polymer chains, Melting, Crystallization kinetics, Determination of melting and crystallization temperature, Structure-property correlation, Mechanical properties and testing, Viscoelasticity

Unit 3: Natural, Synthetic Polymers and Polymer Blends

Biopolymers- Proteins, Polysaccharides, Naturally occurring elastomers, Commodity thermoplastics- Polyolefins, Vinyl polymers, Thermoplastic polyesters, Thermoplastic elastomers, Thermosets such as epoxy, unsaturated polyesters, Engineering Polymers: Polyamides, ABS, Polycarbonates, Polysulfones, Polyphenylenesulfide, Specialty Polymers: Polyimides, Ionic polymers, Liquid crystalline polymers, Additives and polymer blends, polymer composites/nanocomposites

Unit 4: Polymer Processing and Rheology

Basic processing operations such as extrusion, molding, calendaring, Introduction to polymer rheology- Newtonian and non-Newtonian fluids, Constitutive equations, Elastic properties of polymeric fluids, Melt instabilities, Rheometry.

Unit 5: Applications of Polymers and Polymer Composites for Advanced Technologies

Membrane separations, Biomedical engineering and drug delivery, Light emitting diodes, Fuel cells, Solar cells, EMI shielding, Anticorrosion coatings, Paints.

Reference Books

1. Joel R Fried, *Polymer Science & Technology*, 2nd Ed., PHI learning Pvt.Ltd., 2009.
2. J. Brydson, *Plastic Materials*, 7th Ed., CBS publishers and Distributors, 2005.
3. G. Odien, *Principles of Polymerization*, 3rd Ed., Wiley Interscience Publications, 1991.
4. F. W. Billmeyer, *Textbook of Polymer Science*, 1st Ed., Wiley – India Pvt. Ltd., 2012.
5. G. Pritchard, *Plastics Additives*, *An A – Z reference*, Springer – VerlagGmbh, 1997.

6. L. A. Utracki (Ed.), *Polymer Blends Handbook* (Part – 1 & 2), Springer, 2003.

Course Outcomes:

On completion of this course students will be able to:

CO1. Acquire knowledge on polymer classification and molecular weight determination of polymers
CO2. Understand physical and mechanical properties of polymers
CO3. Understand basic polymer processing operations and rheology
CO4. Apply the basic ideas acquired related to polymers and polymer composites to tailor make the properties for different applications

SS860 X-RAY AND ELECTRON DIFFRACTION TECHNIQUES

3-1-0-4

Course Objectives:

1. Introduce the concept of diffraction with X-rays and electrons to the student
2. Briefly describe the use of X-rays to determine crystal structures, constructphase diagrams and analyse phase transitions and particle agglomeration in materials;a topic on refinement methods is also introduced
3. Introduce the student to conventional transmission electron microscopy (TEM)and its utility to analysecrystal structures, analyse line and planar defectsand grain boundaries in materials
4. Qualitative treatment of phase contrast (High Resolution) TEM

UNIT I: Properties of X-rays and description of crystals

Production and detection of X-rays; Directions and intensities of diffracted beams; Detectors and measuring intensities of X-rays; Methods of X-ray diffraction; Penetration of X-rays; Grain size, particle size and crystal perfection and orientation.

UNIT II: X-ray analysis

Determination of phase diagrams; Order-disorder phase transitions; Chemical analysis by diffraction - Hanawalt method, directcomparison and internal standard methods; Chemical analysis by fluorescence and absorption.

UNIT III: Precise lattice parameter measurements - Rietveld refinement methods

General methods of precise lattice parameter measurement: Least Squares method, Cohen’s method, Calibration method; Hugo Rietveld’s method of full pattern refinement; Introduction and practice of refinement using the FullProof software (open source).

UNIT IV: Transmission Electron Microscopy

Comparison of scattering by electrons and X-rays; Elastic and Inelastic electron scattering; Basic instrumentation and imaging modes in the TEM; Obtaining and indexing parallel beam electron diffraction patterns; the Kikuchi lines and use of Convergent Beam Electron Diffraction (CBED) techniques.

UNIT V: Phase Contrast Imaging and HR-TEM

Different contrast mechanisms in the TEM - Amplitude, Mass-thickness, Z-contrast, STEM diffraction contrast; Analysing defects - two beam condition, weak beam dark field imaging, thickness and bending effects, planar defects, strain field imaging; High resolution TEM.

Reference Books:

1. B. D. Cullity and S.R. Stock, *Elements of X-ray Diffraction*, 3rd Edition,Pearson Education India, 2014.
2. VitalijPecharsky and Peter Zavalij, *Fundamentals of powder diffraction and structural characterization of materials*, 2nd Edition, Springer, 2005.
3. David B. Williams and C. Barry Carter, *Transmission Electron Microscopy – A textbook for Materials Science*, 2nd Edition, Springer, 2011.

Course Outcomes:

On completion of this course students will be able to:

CO1. Understand fundamental concepts of X-ray diffraction

CO2. Apply diffraction techniques to study materials

CO3. Understand electron diffraction and the instrumentation of the TEM

CO4. Understand how to index 2D electron diffraction patterns.

SS861 CLASSICAL FIELD THEORY 3-1-0-4

Course objectives:

The course introduces the concepts and calculations involved in classical field theory. It extensively explains the theory of hydrodynamics and classical field theory of Gravitation.

UNIT 1: Continuum Mechanics

Review of Classical Mechanics:Lagrangian and Hamiltonian formalisms, Liouville's theorem,Transformation theory, Action-Angle variables, Hamilton-Jacobi equations.Lagrangian and symmetries: Energy-Momentum tensor, Noether's theorem and applications

UNIT 2: Hydrodynamics

The velocity and density fields. Continuity equation, Pascal's Law and the stress tensor, Bernoullis principle, Euler equations. Gravity waves, Viscosity, Navier-Stokes equations. Boundary conditions, examples of flow, low Reynolds number flows, Stokes limit. Relativistic Hydrodynamics.

UNIT 3: Maxwell's theory as a Classical Field Theory

Lorentz transformation,The electromagnetic field tensor, covariant charge density and current, action formalism for electrodynamics, Maxwell's equations and relativistic covariance, Lagrangian and Hamiltonian formalism, Symmetries and covariance, Gauge invariance.

UNIT 4: Classical Field Theory of Gravitation

Principle of equivalence, curvilinear coordinates, metric, connection, curvature tensor, energy-momentum tensor, Einstein field equations and its Newtonian limit.

Reference Books:

1. L. D. Landau and E. M. Lifshitz, *The Classical Theory of Fields*, Pergamon Press, 4th Edition, 1980.
2. G. Giachetta, L. Mangiarotti and G. Sardanashvily, *Advanced Classical Field Theory*, World Scientific, 2009.
3. Florian Scheck, *Classical FieldTheory- On Electrodynamics, Non-Abelian Gauge Theories and Gravitation*, Springer, 2012.

Course Outcomes:

After the completion of the course student is expected to:

CO1. Have a deep understanding of the concepts and physical ideas of classical field theory and perform calculations in field theory, with special application to electromagnetism.

CO2. Study and analyse classical theory of hydrodynamics in depth

CO3. Understand the Electromagnetism and Gravitation as a classical relativistic field theory

SS862 GENERAL THEORY OF RELATIVITY 3-1-0-4

Course objectives:

The aim of the course is to have a comprehensive physical idea and mathematical understanding of General theory of Relativity and its applications in fields like Cosmology and Astrophysics.

UNIT 1: Introduction

Special Theory of Relativity, Four vectors, Minkowskispace time, Relativistic Dynamics, Action for the relativistic free particle. The principle of equivalence, Principle of General covariance, Prelude to General Theory of Relativity – historical developments.

UNIT 2: Tensor Analysis

Riemannian space, Curvilinear coordinates, Tensors, Affine connection, Covariant derivative, Geodesics, Riemann-Christoffel curvature tensor, Bianchi identities, Ricci Tensor, Curvature Scalar.

UNIT 3: Einstein Field Equations

Gravity and Geometry,Energy-momentum tensor, Bianchi identities, Einstein tensor, The vacuum Einstein equations, Einstein-Hilbert Action. Motion in Gravitational Field, Weak Gravitational Field.

UNIT 4:Schwartzchild Solution and Tests of General Theory of Relativity

Centrally symmetric Gravitational Field,Static spherically symmetric space-time, Schwartzchild Solutions, Radial Freefall, Lighcones.

Tests of General Theory of Relativity:Perihelion of Mercury, Deflection of light.

UNIT 5: Black Holes and Cosmology

Relativistic Stellar star structure, Gravitational Collapse, Black Holes.

Cosmology: Homogeneity and Isotropy of the Universe, Friedmann– Robertson–Walker metric, Cosmological solutions.

Text Books:

1. Ashok Das, *Lectures on Gravitation,* World Scientific, 2013.
2. Steven Weinberg, *Gravitation and Cosmology: Principles and Applications of theGeneral Theory of Relativity,* Wiley India, 2008.
3. ØyvindGrøn, SigbjornHervik,*Einstein's general theory of relativity: with modern applications in cosmology,* Springer,2002.

Reference Books:

1. Landau &Lifshitz, *Classical Field Theory*, University Science Books, 1E, 2004
2. C. W. Misner, K. S. Thorne and J. A. Wheeler,*Gravitation*, Princeton Univ Press, 2017.
3. A. Einstein, *Relativity: The Special and the General Theory*, General Press, 2013.

Course Outcomes:

After the completion of the course student is expected to:

CO1: Use differential geometry to describe the properties of a curved space and demonstrate specialised analytical skills and techniques necessary to carry out the study of special theory of relativity using tensor calculus.

CO2: Understand Einstein's field equations, account for the physical interpretation of its components, and prove that Newton's theory of gravity is recovered in the non-relativistic limit.

CO3: Study of solution of Einstein field equation in the case of static, spherically symmetric gravitational field. Study of particle trajectories and tests of GTR.

CO4: Apply the mathematical and physical ideas of the theory of general relativity for the study of various systems in astrophysics and cosmology

SS863 ADVANCED PARTICLE PHYSICS 3-1-0-4

Course Objectives:

The course introduces the different scattering process, symmetries of high energy particles. It also details the standard theoretical models employed in particle physics.

UNIT 1: Scattering Processes

Relativistic kinematics, phase space, Mandelstam variables, Feynman rules, lifetimes and cross-sections, Golden rule; scattering of a spinless charged particle by electromagnetic field, scattering of electrons by electromagnetic field,$e-\mu$ scattering, Moller scattering, electron-proton scattering and form factors, higher order corrections, vacuum polarization, charge renormalization, Lamb shift,$g-2$

UNIT 2: Symmetries and Quarks

Discrete symmetries, isospin-SU(2), G-parity, SU(3)-classification of mesons and baryons, mass formula, magnetic moments, motivation for colour as an internal symmetry.

UNIT 3:Parton Model and QCD

Deep inelastic scattering (DIS) of electrons on nucleons, structure functions and scale invariance, Bjorken scaling, parton model; quantum chromodynamics:Lagrangian, symmetries.

Beta-decay, μ-decay, parity violation,$V-A$ theory of weak interactions, conserved vector current (CVC) hypothesis.

UNIT 4: Standard Model and Neutrino Physics

Glashow-Salam-Weinberg model, neutral current, physics of W, Z and Higgs, CKM mixing, C,P,T transformations, CP violation.

Neutrino Physics: neutrino oscillations.

Reference Books:

1. T. D. Lee, *Particle Physics and Field Theory*, Harwood, 1981.
2. T Cheng and L. Li,Gauge *Theory of Elementary Particles*, Oxford University Press, 1984.
3. I.J.R. Aitchison and A.J.G. Hey, *Gauge Theories in Particle Physics*, Vol. 1: From Relativistic Quantum Mechanics to QED, 3rd Edition, Taylor & Francis,2002.
4. J.D. Bjorken and S.D. Drell, *Relativistic Quantum Fields*, McGraw-Hill, 1965

Course Outcomes:
After the completion of the course student is expected to:

CO1: Be familiar with main theoretical concepts and experimental techniques used in elementary particle physics
CO2: Be able to make quantitative estimates of cross-sections etc. of basic elementary particle processes
CO3: Have a basic understanding of the Standard Model and of theoretical methods employed in particle physics

SS864 QUANTUM FIELD THEORY 3-1-0-4

Course Objectives:

The main objective of this course is to learn the basic concepts and techniques of quantum field theory, with applications to elementary particle physics, with special emphasis to Quantum Electrodynamics (QED).

UNIT 1: Non-relativistic quantum field theory

Quantum mechanics of many particle systems; second quantisation; Schrodinger equation as a classical field equation and its quantisation; inclusion of inter-particle interactions in the first and second quantised formalism

UNIT 2: Canonical quantization of free fields

Real and complex scalar fields, Dirac field, electromagnetic field, Bilinearcovariants, Projection operators, Charge conjugation and Parity on scalar, Dirac and electromagnetic fields.

UNIT 3:Interacting fields

Interaction picture, Interacting Klein-Gordon field, Covariant perturbation theory, S-matrix and its computation from n-point Green functions, Wick’s theorem, Feynman diagrams.

UNIT 4: QED

Feynman rules, Example of actual calculations: Rutherford, Bhabha, Moeller, Compton etc. Decay and scattering kinematics. Mandelstam variables and use of crossing symmetry, coupling Dirac field to electromagnetic field, Feynman rules for computing Green functions, symmetries and Ward identity.

UNIT 5: Higher order corrections and Gauge theories:

One-loop diagrams. Basic idea of regularization and renormalization, Landau pole. Degree of divergence, Calculation of self-energy of scalar in φ4 theory using cut-off or dimensional regularization, Path integrals for scalar and fermionic fields.

Gauge theories:Gauge invariance in QED, non-abelian gauge theories(classical theory, quantization), QCD (introduction), Asymptotic freedom, Spontaneous symmetry breaking, Goldstone theorem, Higgs mechanism,Yang-Mills theory.

Reference Books:

1. M. E. Peskin and D. V. Schroeder,*An Introduction to Quantum Field Theory*, Addison-Wesley, New York, 1995.
2. Steven Weinberg, *Quantum Theory of Fields, Vols. I and II,* Cambridge University Press, 1996.
3. I.J.R. Aitchison and A.J.G. Hey, *Gauge Theories in Particle Physics, Vol. 1: From Relativistic Quantum Mechanics to QED*, 3rd Edition, Taylor &Francis, 2002.

4. Lahiri and Pal, *A First Book of Quantum Field Theory*, Narosa, 2007.
5. J.D. Bjorken and S.D. Drell, *Relativistic Quantum Fields*, McGraw-Hill, 1965

Course Outcomes:

After the completion of the course student is expected to:

CO1: Have an understanding of field quantisation and the expansion of the scattering matrix
CO2: Apply Feynman rules to calculate probabilities for basic electromagnetic processes with particles (decay and scattering)
CO3: Understand the basics of quantum electrodynamicsand introduction to QCD
CO4: Familiarity with the concept of Higher order corrections, re-normalization and Gauge theories

SS865 SEMICONDUCTING MATERIALS AND DEVICES 3-1-0-4

Course Objective:

This course is intended to familiarize the research students about the theory behind the functioning of semiconductor devices. It also provide research students the insight useful for understanding new semiconductor devices and technologies.

Unit 1: Band structure and Electronic properties of Semiconductors

Semiconductor Statistics: Energy distribution functions, Density of states, Density of carriers in Intrinsic and Extrinsic semiconductors, Compensation in semiconductors, Heavy doping - Bandtail states, Effective mass, Hall Effect. Carrier Generation and Recombination, Characteristics of Excess Carriers: continuity equations, time-dependent diffusion equations. Excess - carrier lifetime: Effect of traps and defects,Surface effects.

Concept of band gap: Direct and indirect bands in semiconductor, Bandstructure of selected Semiconductors: Si,Ge, GaAs, GaN, ZnO, Chalcopyrites, Delafossites, Perovskites. Semiconductor alloys, Lattice-mismatched and pseudomorphic materials, variation of Energy bands with alloy composition, Amorphous Semiconductors.

Unit 2: *p-n* junctions

p-n junction formation, Electrostatics of the *p-n* junction: Contact potential and Space Charge. Current - Voltage relationship, Quasi- Fermi levels and High- level injection, Graded Junctions, Junction Breakdown, Tunnel Diode.

Unit 3: Metal-Semiconductor and Semiconductor Heterojunctions

Schottky Barriers: Ideal junction properties, Non-ideal Effects on the Barrier Height, Current-Voltage Relationship, Capacitance-Voltage. Ohmic Contacts: Ideal Non-rectifying Barriers, Tunneling Barrier, Specific contact resistance: Multiple -Contact Two-Terminal Methods. Heterojunctions: Heterojunction Materials, Energy-Band Diagrams, Two-Dimensional Electron Gas, Current-Voltage Characteristics, Band Offsets, Heterojunction Band Lineups - Types.

Unit 4: Metal Oxide Semiconductor Field Effect Transistor (MOSFET)

Review of Bipolar junction transistors (BJT) and Junction Field Effect Transistors (JFET). Introduction to Metal Oxide Semiconductor Capacitor (MOS), Capacitance - Voltage Characteristics of MOS structure, MOSFET Operation: Current -Voltage Characteristics, Substrate Bias Effects, Depletion and Enhancement MOSFETs. Challenges in Real MOSFETS: Subthreshold Conduction, Mobility Variation with Gate Bias, Important Effects in Short-Channel MOSFETs. Heterojunction FET: High electron mobility transistors (HEMT), Thin film transistors (TFT).

Unit 5: Optoelectronic Devices

Optical absorption: Photon absorption coefficient, electron-hole pair Generation rate. Solar cells: *p-n* junction solar cell, Conversion efficiency and solar concentration, Nonuniform absorption effects, Heterojunction solar cells. Photodetectors: Photodiode, *p-i-n* photodiode, Phototransistors.

Reference Books:

1. Donald Neamen and Dhrubes Biswas, Semiconductor *Physics and Devices*, 4th edition, McGraw Hill Education, 2017.

2. Umesh K Mishra and Jasprit Singh, *Semiconductor Device Physics and Design*, Springer,2008.

3. Marius Grundmann, *The Physics of Semiconductors - An Introduction IncludingDevices and Nanophysics,* Springer, 2006.

4. Simon Sze and Kwok Ng, *Physics of Semiconductor Devices*, 3rd edition, Wiley, 2008.

5. Pallab Bhattacharya, *Semiconductor Optoelectronic Devices*, 2nd edition, Pearson, 2017.

Course Outcomes:

On successful completion of the course, the student will able to

CO1: Understand and analyse the density of carriers and carrier transport in semiconductors
CO2: Gain deep knowledge on the physics of semiconductor junctions, metal-semiconductor junctions and heterojunctions.
CO3: Understand the working of the field effect transistors.
CO4: Describe the functioning of the optoelectronic devices.

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