SS866 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.