METALLURGICAL THERMODYNAMICS AND KINETICS OF MATERIALS(4-0)

Module-I (14 Hours)

General principles: first and second law, mathematical formalism for the thermodynamic description of closed systems with constant composition. Mathematical formalism for the thermodynamic description of systems with variable composition. The chemical potential. Partial properties. -- Relation between integral and partial molar properties. Chemical potential of ideal gases (pure and mixtures) and non-ideal gases (pure and mixtures). Chemical potential of pure liquids and solids and of components in liquid and solid solutions. The activity concept.Standard states and activities. Ideal solutions and non-ideal solutions. Activity coefficients. Properties of solutions. Simple solution models.

Module-II (14 Hours)

Introductory concepts of statistical thermodynamics. The regular solution model.Phase stability and phase diagrams Reaction equilibrium, oxidation and reduction, Ellingham diagrams.Thermodynamics vs. kinetics, homogeneous and heterogeneous reactions; Chemical Reaction Control-rate equation, reaction rate constant, reaction order, non-elementary reactions; Basic concepts of reaction steps, rate of reactions, Order of reaction, Determination of order of reactions. Arrhenius equation in reaction kinetics, Mechanism of reaction and rate controlling steps, Activated complex and its thermodynamic and kinetic aspects, Effect of concentration and temperature on reaction kinetics. Kinetics of heterogeneous reactions.

Module-III (14 Hours)

Solid State Diffusion -Fick's Law, mechanism of diffusion, uphill diffusion, Kirkendall effect, steady and transient diffusion;External Mass Transfer -fluid flow and its relevance to mass transfer, general mass transport equation, concept of mass transfer coefficient, models of mass transfer -film theory and Higbie's penetration theory; Internal Mass Transfer-Ordinary and Knudsen diffusion, Mass transfer with reaction; Adsorption -physical adsorption vs. chemisorption, adsorption isotherms; Langmuir, BET, adsorption as the rate limiting step; gasification of C by CO2, dissolution of N2 in molten steel, porous solids, specific surface area and pore size distribution;

Applications in extractive metallurgy, e.g. iron and steel making, copper making

Applications in physical metallurgy, e.g. solid phase transformations and equilibria in metallic alloys, cemented carbides etc

Books for reference:

1. Gaskell D.R., Metallurgical Thermodynamics.

2. Darken and Gurry, Physical Chemistry of Metals

3. Ragone, David V. Thermodynamics of Materials. Vol. 1. New York, NY: Wiley,

4. Porter, David A., and K. E. Easterling. Phase Transformations in Metals and Alloys. 2nd ed. New York, NY: Chapman & Hall,

5. Balluffi, Robert W., Samuel M. Allen, and W. Craig Carter. Kinetics of Materials. Hoboken, NJ: J. Wiley & Sons,