

Metallurgical Thermodynamics

Credits: 4

Unit-I: Objectives and limitations to thermodynamics, concepts of system and state, heterogeneous and homogeneous systems, extensive and intensive properties of system, thermodynamic variables, thermodynamic equilibrium, Reversible and irreversible processes, First Law of thermodynamics, Nature of first law, relationship between heat and work, internal energy and the first law of thermodynamics, calculations of work, constant capacity, reversible adiabatic processes, reversible isothermal pressure or volume changes of an ideal gas, enthalpy change with temperature, Kirchhoff's equation.

Unit-II: Second law of thermodynamics: Efficiency of a cyclic process, Carnot cycle, carnot theorem, second law of thermodynamics, concept of entropy, entropy and quantification of irreversibility, reversible processes, Third law of thermodynamics: Background of third law deductions from third law, applications of third law, and other methods of obtaining ΔS^0 for a reaction.

Unit-III: Free energy functions: Purposes of the new functions, definition of Helmholtz and Gibbs free energy change, meaning of thermodynamically possible process, determination of ΔG from thermal data useful relationships between free energies and other thermodynamic functions, Maxwell's equation and Gibbs-Helmholtz equation, Fugacity, activity and equilibrium constant: Concepts of fugacity, activity and equilibrium constant variation of the equilibrium constant with temperature.

Unit-IV: Tabular methods of recording thermodynamic data, sigma functions, Claussius – Clapeyron equation: Introduction, derivation of the Claussius – Clapeyron equation for single substance, Duhring's rule for the estimation of the vapour pressure of an element, Integration of Claussius – Clapeyron equation. DIFFUSION: Fick's law of diffusion and its application, Kirkendal effect. Self-diffusion in pure metals, Temperature dependence of the diffusion coefficient, diffusion along the grain boundaries and surfaces.

Unit-V: ELLINGHAM DIAGRAMS: Introduction, calculation of equilibrium constants from standard free energy changes, general description of Ellingham diagrams, Interpretation of two or more free energy change Vs. temperature lines taken together, derivation and uses of the oxygen, nomographic scale in Richardson's diagrams.

Unit-VI: SOLUTIONS: Composition, partial molar quantities, ideal solutions, Raoult's Law, actual (Nonideal) solutions, Sieverts law, Gibb's - Duhem equation, integration of Gibb's - Duhem equation, Excess thermodynamics quantities, Kinetics: Kinetics of chemical process, Molecularity and order of a reaction, zero order reactions, first order, second order reactions, Determination of order of reaction, collision theory, theory of absolute reaction rates, consecutives and simultaneous reactions, catalysis in chemical reactions.

Resources:

Text Books:

1. Introduction to the thermodynamics of materials – D.R. Gaskell
2. Textbook of materials and metallurgical thermodynamics: Ahindra Ghosh

References:

1. Physical chemistry for metallurgists – J. Mackowiak
2. Thermodynamics of solids-R. S. Swalin
3. Physical chemistry of metals-L. S. Darken & Robert W. Gurry
5. Fundamentals of thermodynamics- Claus Borgnakke & Richard E. Sonntag
6. An introduction to thermodynamics-Y. V. C. Rao
7. Fundamentals of engineering thermodynamics- M. J. Moran & H. N. Shapiro.