Course code	Course Name	L-T-P - Credits	Year of Introduction
MT201	METALLURGICAL THERMODYNAMICS AND KINETICS	3-1-0-4	2016

Prerequisite : Nil

Course Objectives

- To impart the basic principles and concepts of thermodynamics, in the domain of metallurgy and materials
- To apply thermodynamic laws in metallurgical applications.

Syllabus

Thermodynamics - First law of thermodynamics - processes - Thermochemistry – Thermochemical laws and applications - Second law of thermodynamics – Entropy and its derivative, Concept of free energy, Criterion of equilibrium, Zeroth and third laws of thermodynamics, Chemical thermodynamics -Reaction Equilibrium**:** Gibbs - Helmholtz Equation - Reactions Involving Gases**:** Compressibility Factor, Law of Corresponding States, The Equilibrium Constant and ΔG°, Reactions Equilibria, Equilibria in Gaseous Systems, Reaction Extent Problems, Equilibria in Systems Containing Condensed Phases -Thermodynamics of Solutions - Thermodynamics of Binary Phase Diagrams - Free energy-composition diagram-Binary isomorphous system, Eutectic system, hypo and hyper eutectic, peritectic system, Variation of free energy with composition, Variation of free energy with temperature.

Expected Outcome.

Upon completion of the course, the student will be able to:

i. Understand the basic laws of thermodynamics
ii. Understand the multiple approaches to thermodynamics, from the bulk property point of view and from the atomistic point of view
iii. Understand concepts such as the theory of solutions, free energy, entropy, criteria for equilibrium and conditions for feasibility
iv. Understand phase equilibria and the Ellingham diagrams for oxides, sulphides, halides etc. and their applications to metallurgical processes
v. Obtain the skill to use metallurgical thermodynamic concepts and equations for understanding phase diagrams, phase transformations, theory of solutions
vi. Obtain problem solving skills in order to improve / modify industrial processes, especially in extraction metallurgy, liquid metal treatment and in heat treatment

References/Textbooks

1. David R. Gaskell, Introduction to Metallurgical Thermodynamics, McGraw Hill
2. Alain Vignes, Extractive Metallurgy, Basic thermodynamics and Kinetics, Wiley
3. Tupkary R.H., Introduction to Metallurgical Thermodynamics, TU Publishers, Nagpur
4. Upadhyaya G.S., Dube R.K., Problems in Metallurgical Thermodynamics and Kinetics, Pergamon Press.
5. Moore. J.J, Chemical Metallurgy, Butterworths
6. Darken. L.S. and Gurry. G, Physical Chemistry of Metals, Tata McGraw Hill.
7. Krishna Kant Prasad, Chemical and Metallurgical thermodynamics, New Age International Publishers
8. Sujay Kumar Dutta, Avinash B. Lele, Metallurgical Thermodynamics Kinetics and Numericals, S. Chand Publishers
9. Ghosh A, Text book of Materials & Metallurgical Thermodynamics, Prentice Hall.

Course Plan			
Module	**Contents**	**Hours**	**Sem. Exam Marks**
I	**Introduction to States of Thermodynamics** 1.1 First law of thermodynamics, 1.2 Internal energy, 1.3 Heat capacity,1.4 Specific heat and latent heat, 1.5 Enthalpy, 1.6 Isothermal and adiabatic processes, 1.7 State properties, 1.8 Heat of reaction, Heat of formation, Standard heats and Heat of transition. 1.9 Enthalpy, 1.10 Thermo-chemistry – Thermo-chemical laws and applications.	8	15%
II	**Concept of Entropy and Free energy** 2.1 Second law of thermodynamics – Entropy and its derivative; 2.2 Concept of free energy, Criterion of equilibrium, 2.3 Thermodynamic potential; 2.4 Zeroth and third law of thermodynamics; 2.5 Heat Capacity and Entropy Changes. 2.5 Sensible Heats, Heat of formation, Hess's law, Kirchoff's law equation, Transformation Heats, Reaction Heats, ΔCp, $\Delta H=f(T)$, $\Delta S=f(T)$, Adiabatic Flame Temperatures, and Heat Balances. 2.6 Problems.	10	15%
FIRST INTERNAL EXAMINATION			
III	**Reaction Equilibrium** 3.1Chemical Potential, 3.2 Maxwell equations, 3.3 Gibbs - Helmholtz Equation, 3.4 Criteria of Equilibria, 3.5 Phase Equilibria in One Component Systems , 3.6 Clausius - Claperyon Equation, 3.7 Heats of Vaporization from Vapor Pressure Data, 3.8 Shift in Transformation Temperature with Pressure. 3.9 Fugacity, activity and equilibrium constant, 3.10 Vant Hoff's isotherm, 3.11 Ellingham diagrams for oxides, sulphides, halides etc. and their applications to metallurgical processes. 3.12 Problems.	10	15%
IV	**Reactions Involving Gases** 4.1 The Behavior of Gases. 4 . 2 Compressibility Factor, Law of Corresponding States, 4 . 3 Equations of State and Fugacity. 4.4 The Equilibrium Constant and $\Delta G°$ 4.6 Reactions Equilibria - The effect of temperature and pressure on equilibrium constant. 4.7 Equilibria in Gaseous Systems 4.8 Reaction Extent Problems, 4.9 Equilibria in Systems Containing Condensed Phases, 4.10 Problems.	10	15%
SECOND INTERNAL EXAMINATION			
V	**Thermodynamics of Solutions** 5.1 Introduction to solutions, 5.2. Absolute, Partial and Integral Molar Quantities, Relative and Partial Integral Molar Quantities, 5.3 Gibb's-Duhem Equation, 5.4 Tangent Intercept Method, 5.5 Raoult's law, 5.6 Ideal Solutions, 5.7 Excess Quantities, 5.8 Actual solutions. 5.9 Regular solutions, 5.10 Henry's law, 5.11 Sievert's law, 5.12 Problems.	8	20%

VI	**Thermodynamics of Binary Phase Diagrams** 6.1 Free energy-composition diagram- Binary isomorphous system, Eutectic system, hypo and hyper eutectic, peritectic system. 6.2 Variation of free energy with composition 6.3 Variation of free energy with temperature.	10	20%
END SEMESTER EXAM			

QUESTION PAPER PATTERN:

Maximum Marks : 100 Exam Duration: 3 hours

PART A: 8 Questions from Module 1&2 (4+4). 6 questions to be answered. 6x5=30 Marks
PART B: 8 Questions from Module 3&4 (4+4). 6 questions to be answered. 6x5= 30 Marks
PART C: 6 Questions from Module 5&6 (3+3). 4 questions to be answered. 4x10=40 Marks