MANGALORE UNIVERSITY

Department of Materials Science

MSc Materials Science

MSH 404: **THERMODYNAMICS AND CHEMISTRY OF METALS** (4 Credits)

Objectives: This course aims to provide the basic concepts of heat and dynamics of a substance under various thermodynamics conditions as a sound background in thermodynamics is necessary for understanding materials. The nature of bonding, energy and structure of various metal complexes based on coordination principles are also imparted.

Expected course outcomes: The students should gain understanding of various thermodynamic processess and applications of these in heat engines. In addition to this, the idea of phase diagram of materials potentiates their logical reasoning behind selection of materials of appropriate composition to solve a particular problem in their profession.

Unit 1

Thermodynamics: Basic concepts - Thermodynamic equilibrium, thermodynamic reversibility. Laws of thermodynamics - Zeroth law, First law - Internal energy, heat, work in various systems, heat capacities, enthalpy, flow processes, second law - Carnot theorem, Clausius inequality, entropy calculations for various processes, T-S diagram, engineering applications. Thermodynamic properties of pure substances in solid, liquid and vapor phases, P-V-T behavior of simple compressible substances ideal and real gases, equation of state, compressibility factor. Free energy functions and thermodynamic potentials - Helmholtz and Gibbs free energy functions, Gibbs-Helmholtz equations. General conditions for equilibrium, thermodynamic potential functions-Maxwell relations. Applications: Tds equations, energy and heat capacity equations, Joule-Thomson coefficient, compressibilities and expansion coefficient. Phase transitions: Condition for equilibrium between phases, first, second, third and higher order phase changes with specific examples interpretations, Claperon and Clausius Claperon equation. specific heat and latent heat anomalies. 18 hours

Unit II

Phase rule-Introduction, cooling curves, phase diagrams of binary alloy systems-Mixtures, Solidsolution,Compound, Eutectic, peritectic and eutectoid reactions,Microstructural changes during cooling, Lever rule, Typical systems-Ag-Pb, Cu-Ni., Pb-Sn, Iron- Carbon, Ag-Pt, Cu-Zn, TTT and CCT diagrams, Martensitic transformation. Free energy-composition diagrams, Ternary alloy systems.

Phase transformation-Free energy changes, Nucleation and grain growth, kinetics Application - Transformation in steel, Precipitation process, solidification and crystallization, glass transition. 18 hours

Unit III

Metals-Coordinate bond and metal complexes, Valence bond theory- Formation of octahedral complex-outer and inner orbital complex-Formation of tetrahedral and square planar

complexes – Limitation of valence bond theory Crystal field theory – important features-crystal field splitting of d-orbitals in octahedral, tetrahedral, and square planar complexes applications of CFT-Distortion of octrahedral complex and Jahn – Teller theorem- Crystal field stabilisation energy and its uses – Limitations of CFT. Molecular orbital theory – comparison of different theories.

Theoretical principles of extraction of Metals – Ellingham diagram. Extraction of Iron, Preparation of steel, Effect of alloying elements. Heat treatment Processes – Annealing, Normalising, Hardening, Quenching, Tempering- Heat treatment of steel.
18 hours

References

1. Heat and thermodynamics – Mark W. Zemansky, (McGraw-Hill, 1968)
2. Thermodynamics of solids – Richard A Swalin, (John Wiley & Sons. 1972)
3. Equilibrium thermodynamics – C J Adkins (Cambridge University press, 1983)
4. Solid state phase transformation – V Raghavan (Prentice Hall, 1992)
5. Principles of Materials Science and Engineering – William F Smith (McGraw Hill 1988)
6. Chemistry in Engineering and Technology (Vol 1&2;) – J C Kuriacose and J. Rajaram (Mcgraw Hill, 1988)
7. Materials Science and Engineering – V Raghavan (Printice Hall,1995)
8. An introduction to Metallurgy – A H Cottrell (Edward Arnold,1971)
9. Materials Science and Processes – B S Narang (CBS, 1983)
10. Advanced physical chemistry – Gurdeep Raj (Goel, 1992)
11. Inorganic chemistry – Mallik, Tuli and Madan (S Chand & Co,1990)
12. Chemistry of Transition elements – Atkin & Holiday (Oxford 1985)
13. Text book of Materials Science and Metallurgy – O P Khanna (Dhanpat Rai & Sons 1984)
14. Physical Metallurgy – V Raghavan (Printice Hall,1989)
15. Engineering Chemistry – Jain & Jain (Dhanpat Rai & Sons,1993)
16. Elements of Materials Science – L H Van Vlack (Addison-Wesley, 1989)
17. Phase Rule – Gurdeep Raj (Goel pub., 1991)