

Master of Technology In Nanoscience & Technology
1st year '1st Semester, Examination 2024
Thermodynamics of Materials

Answer any five questions

Marks

1. a) State the first law of thermodynamics. 2+8
 Consider a system of water and water vapor at a uniform temperature, contained in a cylinder fitted with a friction less piston. This cylinder is placed in thermal contact with a heat reservoir at temperature T. The water vapor pressure in the cylinder is p_{H_2O} which is the saturated vapor pressure of water at temperature T. Calculate the change in the entropy of the combined system of water and heat reservoir when one mole of water is allowed to evaporate (i) reversibly, (ii) irreversibly.
- b) At a pressure of 1 atm the equilibrium melting temperature of lead is 600K. At this temperature the latent heat of melting of lead is 4810 J/mole. Calculate the entropy produced when 1 mole of supercooled liquid lead spontaneously freezes at 590K and 1 atm pressure. The constant pressure molar heat capacity of liquid lead as a function of temperature, at 1 atm pressure is given by $c_{p(l)} = 32.4 - 3.1 \times 10^{-3} T$ J/K and for solid lead $c_{p(s)} = 23.6 - 9.75 \times 10^{-3} T$ J/K 10
2. a) Discuss the criteria of equilibrium of a closed system under going change of state by the following processes - 7 + 7
 (i) Constant volume, constant temperature process, when the system does not perform any P-V work.
 (ii) Constant pressure, constant temperature process, when the system performs no form of work other than P - V work.
- b) Define chemical potential of a species in a particular phase. 2 + 4
 Show that $dG = -SdT + VdP + \sum \mu_i dn_i$
3. a) State and derive Gibb's phase rule. 6
 Consider the cracking of gaseous ammonia according to the reaction 14
 $2NH_3(g) = N_2(g) + 3H_2(g)$
 under constant total pressure of 1 atm. and at 400°C. Calculate the equilibrium partial pressure of all the component of the system.
 Given: $\Delta G^\circ = 87030 - 25.8 \ln T - 31.7 T$ J
4. $2C (gr) + O_2 (g) = 2CO (g)$
 $\Delta G^\circ = -223400 - 175.3T$ J
 $2Ni (s) + O_2 = 2NiO (s)$
 $\Delta G^\circ = -471200 + 162T$ J
 a) Draw the Ellingham diagrams of the two oxidation reactions given above. 6
 b) Calculate the temperature at which all the phases will be stable in the system. 4
 c) Is it possible to reduce NiO (s) by graphite at 900°C? Explain the answer with reason. 4
 d) Discuss the effect of phase transformation of the reactant and the product in the Ellingham diagram. 3 + 3

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5. a) Draw the phase stability diagram of a carbon saturated Si - N - O system at 1350°C, indicating the stable zones for the phases SiO_2 (s), SiC (s) and Si_3N_4 (s). Take p_{N_2} and p_{O_2} as the two independent variables. Given: $\text{SiC (s)} = \text{Si (s)} + \text{C (s)} \quad \Delta G^\circ = 17460 - 1.83T \text{ cal}$ $\text{SiO}_2 \text{ (s)} = \text{Si (s)} + \text{O}_2 \text{ (g)} \quad \Delta G^\circ = 216800 - 42.00T \text{ cal}$ $\text{Si}_3\text{N}_4 \text{ (s)} = 3\text{Si (s)} + 2\text{N}_2 \text{ (g)} \quad \Delta G^\circ = 173000 - 75.3T \text{ cal.}$	20
6. a) Consider a binary A – B solution at a fixed temperature and pressure. Show that $\sum X_A dQ_A = 0$ where Q is any extensive molar property and X_A is the mole fraction of A.	6
b) Show that in a binary solution of A and B the molar Gibbs free energy of mixing is given by $\Delta G^M = RT (X_A \ln a_A + X_B \ln a_B)$.	7
c) Define activity coefficient of a solution. How does it varies with heat of reaction of a solution.	3 + 4
7. a) Define partial molar quantities of a thermodynamic property. For a binary A - B solution at a fixed temperature and pressure, show that the partial molar Gibbs free energy of the component A is given by $G_A = G + X_B (dG / dX_A)$	10
b) From the first law of thermodynamics, find out the expression for heat absorbed or rejected and work done by a system moving from state 1 to state 2 (i) for constant pressure process and (ii) constant volume process.	5 + 5
8. a) Discuss the basic postulate of statistical mechanics. Discuss the classical and quantum mechanical description of states.	2 + 3 + 3
b) Define activity quotient. Show that the criteria for reaction equilibrium of a system containing components in condensed solution is given by $\Delta G^\circ = -RT \ln Q^{eq}$ When the symbols have got their usual meaning.	2 + 10