

ÉCOLE POLYTECHNIQUE
Département de génie chimique
Programme de matériaux

MET 6208
ÉNERGÉTIQUE DES SOLUTIONS

CONTRÔLE I

Jeudi, le 29 octobre 2009

9h30 - 12h30

NOTES:

- All documentation permitted***
- There are 7 questions***

Le professeur : Arthur D. Pelton

Question 1 (3 points)

In a binary solution A-B,

$$h^E = \omega X_A X_B$$

$$s^E = \eta X_A X_B$$

where ω and η are constants and X_A and X_B are the mole fractions.

Write an expression for the activity of component A, a_A , as a function of X_A , X_B and T.

Question 2 (2 points)

The system is a rock with a mass of 1.0 kg. In its initial state the rock is suspended 1.0 m above the ground. The rock is released and allowed to fall. Calculate the entropy change of the system, ΔS , and of the surroundings, ΔS_{surr} :

- (i) at the moment just before the rock strikes the ground,
- (ii) after the rock has struck the ground and come to rest.

Assume that the initial and final temperature of the rock and the surroundings is 298.15K.

Data: $g = 9.81 \text{ m/sec}^2$

Question 3 (2 points)

The integral molar enthalpy of mixing of Li-Mg liquid alloys at 1000K is given as a function of composition in the following table.

“Solution A” is a pre-mixed solution containing 2.0 moles of Mg and 8.0 moles of Li.

“Solution B” is a pre-mixed solution containing 8.0 moles of Mg and 2.0 moles of Li.

Calculate the enthalpy change when solution A and solution B are mixed at 1000K to form 20.0 moles of a final solution containing 10.0 mol Mg and 10.0 mol Li at 1000K.

X_{Mg}	$\Delta h \text{ (J/mol)}$
0	0
0.1	-1092
0.2	-2343
0.3	-3586
0.4	-4653
0.5	-5368
0.6	-5384
0.7	-4611
0.8	-3205
0.9	-1519
1.0	0

Question 4 (3 points)

For Pb solid:

$$h = -7283 + 23.465 T + 0.004889 T^2 - 43914 T^{-1} \text{ J/mol}$$

$$\text{and } s_{298.15}^{\circ} = 64.785 \text{ J/mol. K}$$

Calculate the entropy of solid Pb at 600K.

Question 5 (3 points)

In a regular ternary solution with components A-B-C:

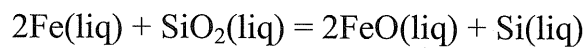
$$g^E = \omega_{AB} X_A X_B + \omega_{BC} X_B X_C + \omega_{CA} X_C X_A$$

where the ω_{ij} are constants and the X_i are the mole fractions.

Calculate an expression for the partial molar excess Gibbs energy of component A, g_A^E .

Question 6 (4 points)

(a) From the data supplied below, calculate the equilibrium constant of the following reaction at 1873 K:



(b) A liquid Fe-Si alloy solution is at equilibrium with a liquid slag solution FeO-SiO₂ at 1873 K. The composition of the slag is $X_{\text{FeO}} = X_{\text{SiO}_2} = 0.5$. Calculate the composition of the metallic solution as well as the equilibrium oxygen pressure. Use the data supplied below.

Data:	$\text{Fe}(\text{liq}) + \frac{1}{2}\text{O}_2 =$	$\text{FeO}(\text{liq})$	$\Delta G_{1873}^{\circ} =$	-155348 J
	$\text{Si}(\text{liq}) + \text{O}_2 =$	$\text{SiO}_2(\text{sol})$	$\Delta G_{1873}^{\circ} =$	-576159 J
	$\text{SiO}_2(\text{sol}) =$	$\text{SiO}_2(\text{liq})$	$\Delta G_{1873}^{\circ} =$	545 J

FeO-SiO₂ liquid solutions at 1873 K
activity coefficients

X_{SiO_2}	γ_{FeO}	γ_{SiO_2}
0.7	0.920	1.575
0.6	0.834	1.908
0.5	0.856	1.856
0.4	0.959	1.694
0.3	1.202	1.504

Fe-Si liquid alloys at 1873 K

X_{Si}	g_{Si}^E (J/mol)	g_{Fe}^E (J/mol)
0	-103260	0
0.1	-90630	-720
0.2	-72520	-3950
0.3	-49900	-11560

Question 7 (3 points)

- (a) Calculate the configurational multiplicity, t^{config} , of one mole of a pure metal which contains X_v vacancies distributed randomly on the lattice sites. Using Boltzmann's equation and Stirling's approximation, calculate an expression for the molar configurational entropy s^{config} . (Note that X_v is very small.).
- (b) Since X_v is very small, the "solution" of vacancies in the metal can be considered to be a very dilute Henrian solution. That is the molar enthalpy and non-configurational entropy are very nearly linear functions of the vacancy content:

$$h = h^0 + X_v h_v$$

$$s^{\text{non-config}} = s^0 + X_v s_v$$

where h^0 and s^0 are the molar enthalpy and non-configurational entropy of vacancy-free metal, and h_v and s_v are constants where $(h_v - Ts_v) \gg 0$.

Write an expression for the molar Gibbs energy g of the solution. By minimizing g with respect to X_v , derive an expression for the number of vacancies at equilibrium as a function of T , h_v and s_v .