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: $g = 9.81\ m/sec^2$

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" ia 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}	**Δh (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:
$h = -7283 + 23.465\ T + 0.004889\ T^2 - 43914\ T^{-1}$ J/mol
and $s^o_{298.15} = 64.785$ 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:
$g^E = \omega_{AB}X_AX_B + \omega_{BC}X_BX_C + \omega_{CA}X_CX_A$
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^E_A.

Question 6 (4 points)

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

$$2Fe(liq) + SiO_2(liq) = 2FeO(liq) + Si(liq)$$

(b) A liquid Fe-Si alloy solution is at equilibrium with a liquid slag solution $FeO\text{-}SiO_2$ at 1873 K. The composition of the slag is $X_{FeO} = X_{SiO_2} = 0.5$. Calculate the composition of the metallic solution as well as the equilibrium oxygen pressure. Use the data supplied below.

Data:			
	$Fe(liq) + \frac{1}{2}O_2 =$	$FeO(liq)$	$\Delta G^o_{1873} = -155348$ J
	$Si(liq) + O_2 =$	$SiO_2(sol)$	$\Delta G^o_{1873} = -576159$ J
	$SiO_2(sol) =$	$SiO_2(liq)$	$\Delta G^o_{1873} = 545$ J

$FeO\text{-}SiO_2$ 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^E_{Si} (J/mol)	g^E_{Fe} (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:

$$h = h^o + X_v h_v$$
$$s^{non\text{-}config} = s^o + X_v s_v$$

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

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.