Department of Materials Science and Engineering
Pohang University of Science and Technology

AMSE205 Thermodynamics I

Nov. 30, 2023

Problem Set #3

Prof. Byeong-Joo Lee
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Room 1- 311

1. The vapor pressure of solid NaF varies with temperature as

$$\ln P(atm) = \frac{-34450}{T} - 2.01\ln T + 33.74$$

and the vapor pressure of liquid NaF varies with temperature as

$$\ln P(atm) = \frac{-31090}{T} - 2.52\ln T + 34.66$$

Calculate: (20)

a) The normal boiling temperature of NaF
b) The temperature and pressure at the triple point
c) The molar heat of evaporation of NaF at its normal boiling temperature
d) The molar heat of melting of NaF at the triple point
e) The difference between the *Cp* of liquid and solid NaF

2. 반경이 r 인 spherical particle 은 표면 효과로 인해 다음 식만큼 압력을 받게 된다. (capillary pressure)

$$P = \frac{2\gamma}{r}$$

여기서 γ는 표면에너지를 의미한다.

Nano particle이나 wire는 위 효과로 인해 melting point 등 thermodynamic property가 bulk 상태일 때와는 달라지게 되는데, spherical nano particle의 melting point 강하 정도가 다음의 식으로 표현될 수 있음을 유도하시오. (10)

$$\frac{\Delta T_m}{T_m} = \frac{(\gamma_S - \gamma_L)}{\Delta H_m} \cdot \frac{2}{r} V_m$$

T_m은 bulk 상태에서의 melting point임.

ΔT_m은 melting point가 낮아진 정도이며, 낮아졌을 때 (+)값을 가짐.

γ_S, γ_L는 각각 solid와 liquid의 표면에너지,

ΔH_m은 enthalpy of melting을 나타냄.

ΔH_m와 ΔS_m은 melting point 근처에서 constant라고 가정하며,

Solid 와 liquid 의 molar volume은 V_m으로 동일하다고 가정함.

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3. 다음은 subregular solution model을 이용하여 A-B 2원 용액의 molar Gibbs energy를 표현한 것이다. (20)

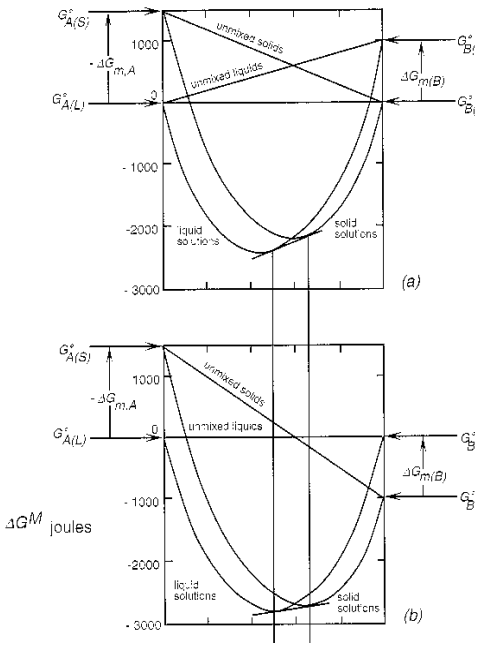
$$G_m = x_A{}^oG_A + x_B{}^oG_B + RT\{x_A \ln x_A + x_B \ln x_B\} + x_A x_B\{L_o + (x_A - x_B)L_1\}$$

a) 이 식으로부터 A, B 성분의 partial molar Gibbs energy 식을 유도하시오.

b) 위 subregular 용액 모델이, A, B 각 성분이 dilute 영역에서는 Henrian 거동을, rich 영역에서는 Raoultian 거동을 나타낸다는 실험적 사실을 재현해 냄을 보이시오.

c) 위 a)에서 유도한 A 성분의 partial molar Gibbs energy로부터 Gibbs-Duhem equation을 이용하여 B 성분의 partial molar Gibbs energy를 유도하시오.

4. A-B 2 원계에서 α, β 두 solution phase 간의 평형 조성은 두 상의 Gibbs energy vs. composition curve 에 common tangent line (공통 접선)을 그어, 두 curve 와의 접점을 찾음으로써 결정할 수 있다. 그런데, Gibbs energy curve 는 그림에서처럼 각 원소의 reference state 에 따라 달리 그려질 수 있다. 정규 용액 모델을 사용하여 α, β 두 상 간의 상평형을 나타내는 조건 식을 작성하고, 각 원소에 대해 일관된 reference state 를 사용하는 한 상평형 조성은 reference state 에 관계없이 unique 하게 결정된다는 것을 보이시오. (10)



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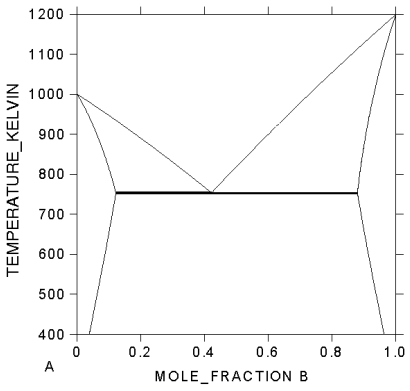
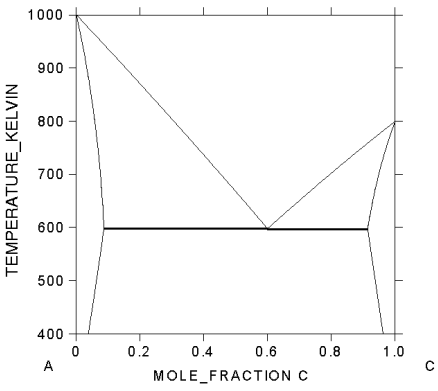
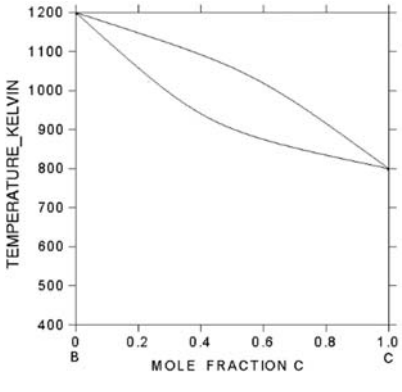
5. 1273 K, A-B 2 원계 한 고용상에서 성분 B 의 조성에 따른 activity (wrt. solid B)가 다음과 같이 측정되었다. 이 고용상의 열역학 특성을 가장 잘 나타내는 모델을 찾고 (ideal, regular, sub-regular model), 성분 B 의 activity 와 molar Gibbs energy of mixing 을 analytic 한 수식으로 표현하시오. 또, 모델 수식으로 계산한 각 조성에서의 activity 값과 실험 측정된 activity 값을 비교하여 모델의 우수성을 보이시오. (20)

x_B	a_B
0.10	0.0320
0.20	0.0800
0.30	0.1498
0.40	0.2400
0.50	0.3510
0.60	0.4782
0.70	0.6162
0.80	0.7559
0.90	0.8874
1.00	1.0000

6. The followings are binary phase diagrams among three elements A, B, C, with melting point of 1000, 1200 and 800K, respectively. Based on binary phase diagrams, sketch isothermal sections of the A-B-C ternary phase diagram at 900, 700 and 400K. (20)







화학열역학 Problem Set #3 2021.09.24 제출용

1. Solid NaF : $\ln P_s(atm) = \frac{-34450}{T} - 2.01\ln T + 33.74$

Liquid NaF : $\ln P_l(atm) = -\frac{31090}{T} - 2.52\ln T + 34.66$

(a) The normal boiling (point) temperature of NaF.

$P = 1atm$

$\ln P = 0 = -\frac{31090}{T} - 2.52\ln T + 34.66 \Rightarrow T = 2006K$ //

(b) The temperature and pressure at the triple point

① $P_s = P_l$.

$-\frac{34450}{T} - 2.01\ln T + 33.74 = -\frac{31090}{T} - 2.52\ln T + 34.66 \Rightarrow T = 1238.9K$ //

② temperature 에 triple point 대입.

$P_s = P_l = 2.289 \times 10^{-4} atm$ //

(c) The molar heat of evaporation of NaF at its normal boiling temperature.

증기(용융)에 대한 $\frac{1}{P_l}\frac{dP_l}{dT} = \frac{31090}{T^2} - 2.52\frac{1}{T} = \frac{\Delta H_l}{RT^2} \rightarrow \Delta H_l = R(31090 - 2.52T)$.

Normal boiling temperature $T = 2006K$ 대입! $\rightarrow \Delta H_l = R(31090 - 2.52 \times 2006)$

$= 216.5 kJ/mol$ //

(d) The molar heat of melting of NaF at the triple point.

$s \rightarrow g$ $\Delta H_s = R(34450 - 2.01T)$ $\rightarrow$ (c) 에서 구한 것과 동일한 방법. (용융에 대한)

$l \rightarrow g$ $\Delta H_l = R(31090 - 2.52T)$

At triple point.

$s \rightarrow g$ $\Delta H_s = R(34450 - 2.01 \times 1238.9) = 265729 J/mol$

$l \rightarrow g$ $\Delta H_l = R(31090 - 2.52 \times 1238.9) = 232539 J/mol$

$\rightarrow \Delta H_{s \rightarrow l} = \Delta H_{s \rightarrow g} - \Delta H_{l \rightarrow g}$

$= +33.2 kJ/mol$ //

(e) The difference between the Cp of liquid and solid. NaF.

$\Delta H_l - \Delta H_s = R(-3360 - 0.5T)$

$\Delta C_p = \frac{d}{dT}(\Delta H_l - \Delta H_s) = -0.5R = 4.24 J/mol \cdot K$ //

소재열역학 Problem Set #3 20210194 [illegible]

2. $P = \frac{2\gamma}{r} \Rightarrow \frac{\Delta T_m}{T_m} = \frac{(\gamma_s - \gamma_l)}{\Delta H_m} \cdot \frac{2}{r} V_m$ 유도하라

$\Delta G = \Delta H - T\Delta S$

At bulk, $\Delta G^{s \to l} = \Delta H_m - T\Delta S_m$

At nanoparticle, $\Delta G^{s \to l} = \Delta H_m - T'\Delta S_m + \int_{\frac{2\gamma_s}{r}}^{\frac{2\gamma_l}{r}} V_m dP = \Delta H_m - T'\Delta S_m + V_m \frac{2(\gamma_l - \gamma_s)}{r}$.

melting point에서

$\Delta G^{s \to l} = 0 = \Delta H_m - T_m \Delta S_m = \Delta H_m - T_m' \Delta S_m + V_m \frac{2(\gamma_l - \gamma_s)}{r}$

$-(T_m - T_m')\Delta S_m = \frac{V_m}{r} 2(\gamma_l - \gamma_s) \Rightarrow -\Delta T_m \Delta S_m = \frac{V_m}{r} 2(\gamma_l - \gamma_s)$.

$\frac{\Delta T_m}{T_m} = -\frac{2V_m}{r\Delta S_m T_m}(\gamma_l - \gamma_s) = \frac{\gamma_s - \gamma_l}{T_m \Delta S_m} \cdot \frac{2}{r} V_m = \frac{\gamma_s - \gamma_l}{\Delta H_m} \frac{2}{r} V_m$.

$dH = TdS + VdP = TdS$ (at bulk). $\rightarrow \Delta S_m = \frac{\Delta H_m}{T_m}$

소재열역학 Problem Set #3 2021[illegible]94 제보농.

3. $G_m = x_A {}^\circ G_A + x_B {}^\circ G_B + RT\{x_A \ln x_A + x_B \ln x_B\} + x_A x_B \{L_0 + (x_A - x_B) L_1\}$

(a) A, B 성분의 partial molar Gibbs energy 식을 유도.

$Q = x_A \overline{Q_A} + x_B \overline{Q_B}$

$dQ = \overline{Q_A} dx_A + \overline{Q_B} dx_B \rightsquigarrow \frac{dQ}{dx_B} = -\overline{Q_A} + \overline{Q_B} \quad \because x_A = 1 - x_B$

$x_A \frac{dQ}{dx_B} = -x_A \overline{Q_A} + x_A \overline{Q_B} \Rightarrow Q + (1 - x_B) \frac{dQ}{dx_B} = x_A \overline{Q_A} + x_B \overline{Q_B} - x_A \overline{Q_A} + x_A \overline{Q_B} = \overline{Q_B}$

$\therefore \overline{Q_B} = Q + (1 - x_B) \frac{dQ}{dx_B}$

* $\overline{G_A} = G_m + (1 - x_A) \frac{dG_m}{dx_A}$

$\frac{dG_m}{dx_A} = {}^\circ G_A - {}^\circ G_B + RT(\ln x_A - \ln x_B) + (1 - 2x_A)(L_0 + (x_A - x_B)L_1) + x_A x_B 2L_1$

$\overline{G_A} = x_A {}^\circ G_A + x_B {}^\circ G_B + RT(x_A \ln x_A + x_B \ln x_B) + x_A x_B (L_0 + (x_A - x_B)L_1)$
$+ x_B {}^\circ G_A - x_B {}^\circ G_B + RT(x_B \ln x_A - x_B \ln x_B) + (1 - 2x_A) x_B (L_0 + (x_A - x_B)L_1) + 2x_A x_B^2 L_1$
$= {}^\circ G_A + RT \ln x_A + x_B(L_0 + (x_A - x_B)L_1) - x_A x_B (L_0 + (x_A - x_B)L_1) + 2x_A x_B^2 L_1$
$= {}^\circ G_A + RT \ln x_A + x_B^2 L_0 + x_A x_B L_1 - x_B^2 L_1 - x_A^2 x_B L_1 + x_A x_B^2 L_1 + 2x_A x_B^2 L_1$
$= {}^\circ G_A + RT \ln x_A + x_B^2 L_0 + 3x_A x_B^2 L_1 + x_B L_1 - 2x_B^2 L_1 - x_A^2 x_B L_1$
$= {}^\circ G_A + RT \ln x_A + x_B^2 L_0 + L_1(3x_A x_B^2 + x_B - 2x_B^2 - (1 - x_B)^2 x_B)$
$= {}^\circ G_A + RT \ln x_A + x_B^2 L_0 + L_1(3x_A x_B^2 - x_B^3) = {}^\circ G_A + RT \ln x_A + x_B^2 L_0 - (x_B^3 - 3x_A x_B^2) L_1$

* $\overline{G_B} = G_m + (1 - x_B) \frac{dG_m}{dx_B}$ → 부호 달라 + A,B 뒤바뀜.

$\frac{dG_m}{dx_B} = {}^\circ G_B - {}^\circ G_A + RT(\ln x_B - \ln x_A) + (1 - 2x_B)(L_0 + (x_A - x_B)L_1) - 2x_A x_B L_1$

$\overline{G_B} = x_A {}^\circ G_A + x_B {}^\circ G_B + RT(x_A \ln x_A + x_B \ln x_B) + x_A x_B (L_0 + (x_A - x_B)L_1)$
$+ x_A {}^\circ G_B - x_A {}^\circ G_A + RT(x_A \ln x_B - x_A \ln x_A) + x_A (1 - 2x_B)(L_0 + (x_A - x_B)L_1) - 2x_A^2 x_B L_1$
$= {}^\circ G_B + RT \ln x_B + x_A^2 L_0 + (x_A^3 - 3x_A^2 x_B) L_1$

위 $\overline{G_A}$ 풀었던 동일한 방법으로 계산.
A, B 뒤바뀐 부분 + 아래와 부호 달라짐.

(c) If

$x_A \to 1$ (Rich) $\Rightarrow \overline{G_A} = {}^{\circ}G_A + RT\ln x_A + 0$ ⇒ ideal solution과 동일한 거동 $a_i = x_i$ ∴ Raoultian

$x_B \to 0$ (dilute) $\Rightarrow \overline{G_B} = {}^{\circ}G_B + \boxed{RT\ln x_B + L_0 + L_1} \to RT\ln k x_i$

↳ constant

↳ $a_i = k x_i$ 형태의 거동 ∴ Henrian 거동

$x_A \to 0$ (dilute) $\Rightarrow \overline{G_A} = {}^{\circ}G_A + RT\ln x_A + \underbrace{\boxed{L_0 - L_1}}_{\text{constant}}$ ⇒ Henrian 거동

$x_B \to 1$ (Rich) $\Rightarrow \overline{G_B} = {}^{\circ}G_B + RT\ln x_B + 0$ ⇒ Raoultian 거동.

↳ constant ×

(d) Gibbs-duhem equation,

$$x_A d\overline{G_A} + x_B d\overline{G_B} = 0$$

$$x_A \frac{d\overline{G_A}}{dx_A} = -x_B \frac{d\overline{G_B}}{dx_A} \rightarrow \frac{d\overline{G_A}}{dx_A} = -\frac{x_B}{x_A}\frac{d\overline{G_B}}{dx_A}, \quad \frac{d\overline{G_B}}{dx_A} = -\frac{x_A}{x_B}\frac{d\overline{G_A}}{dx_A}$$

$$\frac{d\overline{G_A}}{dx_A} = RT\frac{1}{x_A} - 2(1-x_A)L_0 + 3(1-x_A)^2 L_1 + 3(1-x_A)^2 L_1 - 6x_A(1-x_A)L_1$$

$$= RT\frac{1}{x_A} - 2(1-x_A)L_0 + 6(1-x_A)^2 L_1 - 6x_A(1-x_A)L_1$$

$$-\frac{x_A}{x_B}\frac{d\overline{G_A}}{dx_A} = -\frac{RT}{x_B} + 2\frac{x_A}{x_B}(1-x_A)L_0 - \frac{6x_A}{x_B}(1-x_A)^2 L_1 + \frac{6x_A^2}{x_B}(1-x_A)L_1 = \frac{d\overline{G_B}}{dx_A}$$

$$-RT\frac{1}{1-x_A} + 2x_A L_0 - 6x_A(1-x_A)L_1 + 6x_A^2 L_1 = \frac{d\overline{G_B}}{dx_A}$$

$$\int \frac{d\overline{G_B}}{dx_A} dx_A = RT\ln(1-x_A) + L_0 x_A^2 - 3L_1 x_A^2 + 2L_1 x_A^3 + 2L_1 x_A^3 + C.$$

$$= RT\ln x_B + x_A^2 L_0 + (4x_A^3 - 3x_A^2)L_1 + C$$

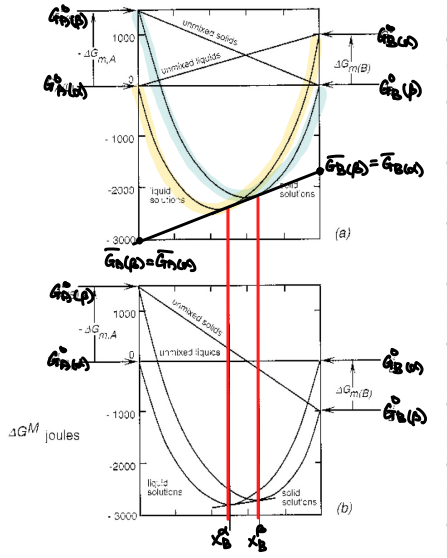
$$= RT\ln x_B + x_A^2 L_0 + (x_A^3 - 3x_A^2 x_B)L_1 + C$$

↳ ${}^{\circ}G_B$

(a)에서 구한 $\overline{G_B} = {}^{\circ}G_B + RT\ln x_B + x_A^2 L_0 + (x_A^3 - 3x_A^2 x_B)L_1$ 과 동일한 결과 구함.

소재열역학 Problem Set #3 2020194 계홍준

4



$$G^{\circ}_{A(\beta)} - G^{\circ}_{A(\alpha)} = -\Delta G_{m,A}$$

$$G^{\circ}_{B(\alpha)} - G^{\circ}_{B(\beta)} = \Delta G_{m,B}.$$

$$G^{\alpha}_m = x_A G^{\circ}_{A(\alpha)} + x_B G^{\circ}_{B(\alpha)} + RT(x_A \ln x_A + x_B \ln x_B) + x_A x_B L^{\alpha}_{AB}$$

$$G^{\beta}_m = x_A G^{\circ}_{A(\beta)} + x_B G^{\circ}_{B(\beta)} + RT(x_A \ln x_A + x_B \ln x_B) + x_A x_B L^{\beta}_{AB}$$

* common tangent line (공통접선)

① slope (기울기) 동일

$$\left.\frac{\partial G^{\alpha}_m}{\partial x_B}\right|_{x_B = x_B^{\alpha}} = \left.\frac{\partial G^{\beta}_m}{\partial x_B}\right|_{x_B = x_B^{\beta}}$$

$$G^{\alpha}_m = (1-x_B) G^{\circ}_{A(\alpha)} + x_B G^{\circ}_{B(\alpha)} + RT\{(1-x_B)\ln(1-x_B) + x_B \ln x_B\} + (1-x_B) x_B L^{\alpha}_{AB}$$

$$G^{\beta}_m = (1-x_B) G^{\circ}_{A(\beta)} + x_B G^{\circ}_{B(\beta)} + RT\{(1-x_B)\ln(1-x_B) + x_B \ln x_B\} + (1-x_B) x_B L^{\beta}_{AB}$$

$$\left.\frac{\partial G^{\alpha}_m}{\partial x_B}\right|_{x_B = x_B^{\alpha}} = -G^{\circ}_{A(\alpha)} + G^{\circ}_{B(\alpha)} + RT(-\ln(1-x_B^{\alpha}) + \ln x_B^{\alpha}) + (1-2x_B^{\alpha}) L^{\alpha}_{AB}$$

$$\left.\frac{\partial G^{\beta}_m}{\partial x_B}\right|_{x_B = x_B^{\beta}} = -G^{\circ}_{A(\beta)} + G^{\circ}_{B(\beta)} + RT(-\ln(1-x_B^{\beta}) + \ln x_B^{\beta}) + (1-2x_B^{\beta}) L^{\beta}_{AB}$$

$$(G^{\circ}_{A(\beta)} - G^{\circ}_{A(\alpha)}) + (G^{\circ}_{B(\alpha)} - G^{\circ}_{B(\beta)}) + RT\left(\ln\frac{1-x_B^{\alpha}}{1-x_B^{\beta}} + \ln\frac{x_B^{\alpha}}{x_B^{\beta}}\right) + (1-2x_B^{\alpha}) L^{\alpha}_{AB} - (1-2x_B^{\beta}) L^{\beta}_{AB} = 0$$

* reference 계산

$G^{\circ}_{A(\beta)} - G^{\circ}_{A(\alpha)} = -\Delta G_{m,A} \rightarrow \Delta G^{\circ\, ref\to\beta}_{A} - \Delta G^{\circ\, ref\to\alpha}_{A} = \Delta^{\circ} G^{\alpha\to\beta}_{A} = -\Delta G_{m,A}$

$G^{\circ}_{B(\alpha)} - G^{\circ}_{B(\beta)} = \Delta G_{m,B} \rightarrow \Delta G^{\circ\, ref\to\alpha}_{B} - \Delta G^{\circ\, ref\to\beta}_{B} = \Delta^{\circ} G^{\beta\to\alpha}_{A} = \Delta G_{m,B}.$

constant.

$$-\Delta G_{m,A} + \Delta G_{m,B} + RT\left(\ln\frac{1-x_B^{\alpha}}{1-x_B^{\beta}} + \ln\frac{x_B^{\alpha}}{x_B^{\beta}}\right) + (1-2x_B^{\alpha}) L^{\alpha}_{AB} - (1-2x_B^{\beta}) L^{\beta}_{AB} = 0$$

constant.

③ 양쪽의 chemical potential 동일 → 평형조건

$\overline{G_A^\alpha} = \overline{G_A^\beta}$ $\overline{G_B^\alpha} = \overline{G_B^\beta}$

$\overline{G_A^\alpha} = G_{A(\alpha)}^\circ + RT\ln a_A^\alpha = G_{A(\alpha)}^\circ + RT\ln\gamma_A^\alpha x_A^\alpha = G_{A(\alpha)}^\circ + RT\ln x_A^\alpha + L_{AB}^\alpha x_B^{\alpha 2}$

$\overline{G_A^\beta} = G_{A(\beta)}^\circ + RT\ln a_A^\beta = G_{A(\beta)}^\circ + RT\ln x_A^\beta + L_{AB}^\beta x_B^{\beta 2}$

$\overline{G_B^\alpha} = G_{B(\alpha)}^\circ + RT\ln a_B^\alpha = G_{B(\alpha)}^\circ + RT\ln x_B^\alpha + L_{AB}^\alpha x_A^{\alpha 2}$

$\overline{G_B^\beta} = G_{B(\beta)}^\circ + RT\ln a_B^\beta = G_{B(\beta)}^\circ + RT\ln x_B^\beta + L_{AB}^\beta x_A^{\beta 2}$

$\overline{G_A^\alpha} = \overline{G_A^\beta} \Rightarrow \underbrace{G_{A(\beta)}^\circ - G_{A(\alpha)}^\circ}_{\Delta G_{m,A}} + RT\ln\left(\frac{x_A^\beta}{x_A^\alpha}\right) + L_{AB}^\alpha x_B^{\alpha 2} - L_{AB}^\beta x_B^{\beta 2} = 0$

$\overline{G_B^\alpha} = \overline{G_B^\beta} \Rightarrow \underbrace{G_{B(\alpha)}^\circ - G_{B(\beta)}^\circ}_{\Delta G_{m,B}} + RT\ln\left(\frac{x_B^\alpha}{x_B^\beta}\right) + L_{AB}^\alpha x_A^{\alpha 2} - L_{AB}^\beta x_A^{\beta 2} = 0$

이 두식을 연립하여 풀면 x_A^α x_B^α 등 평형조성을 reference state와 관계없이 일정한 값이 나온다. (unique 하게 결정)

$\Delta G_{m,A}$, $\Delta G_{m,B}$, L_{AB}^α, L_{AB}^β 는 일정한 온도에서 상수값,

$\Delta G_{m,A}$, $\Delta G_{m,B}$ 에서 reference 를 정하는 것이다. (중요)

신재료열역학 Problem Set #3 2021.09.14 제출용.

5. ① Ideal solution

Ideal solution은 입자간의 상호작용 $\times \rightarrow a_T = x_T$

실제에서 주어진 데이터는 $a_T \neq x_T$ 이므로 Ideal solution이 아니다.

② Regular solution model

$\Delta G^M = RT(x_A \ln a_A + x_B \ln a_B) = RT(x_A \ln x_A + x_B \ln x_B + x_A \ln \gamma_A + x_B \ln \gamma_B)$

$= RT(x_A \ln x_A + x_B \ln x_B) + x_A x_B \Omega_{AB}$

$\therefore RT \ln \gamma_B = \alpha' x_B^2 = \Omega_{AB} x_B^2$ → Hildebrand.

$RT \ln \gamma_B = \alpha' x_A^2 = \Omega_{AB} x_A^2$

$RT(x_A \ln \gamma_A + x_B \ln \gamma_B) = (x_A + x_B) x_A x_B \Omega_{AB} = x_A x_B \Omega_{AB}$

$x_A x_B \Omega_{AB} + RT \ln \gamma_B = (x_A + x_B) x_A \Omega_{AB} = x_A \Omega_{AB}$

$\Omega_{AB} \cdot x_A(1-x_B) = RT \ln \gamma_B \rightarrow \Omega_{AB} = \frac{RT \ln \gamma_B}{(1-x_B)^2}$

constant in regular solution

* $\Delta G_m^{xs} = \Delta H^M = x_A x_B \Omega_{AB}$

$\Delta \bar{H}_B = \bar{G}_B^{xs}$

$(1-x_B)^2 \Omega_{AB} = RT \ln \gamma_B$

$\Omega_{AB} = \frac{RT \ln \gamma_B}{(1-x_B)^2}$

* $x_B \gamma_B = a_B$

x_B	a_B	γ_B	Ω_{AB}
0.1	0.032	0.3200	−14888
0.2	0.0800	0.4000	−15153
0.3	0.1498	0.4993	−15000
0.4	0.2400	0.6000	−15018
0.5	0.3510	0.7020	−14979
0.6	0.4782	0.7970	−15009
0.7	0.6162	0.8803	−14995
0.8	0.7559	0.9449	−15003
0.9	0.8804	0.9860	−14922
1.0	1.0000	1.000	—

모든 표에서 일부 값들의 Ω_{AB} 값이 안정한 값 (약 −15000)을 가지고 있음을 확인할 수 있다.

따라서, Regular solution model이 적합하다.

$RT \ln \gamma_B = \Omega_{AB} x_A^2$

$\gamma_B = \exp(\Omega_{AB} x_A^2 / RT)$

$a_B = x_B \exp(x_A^2 \Omega_{AB} / RT)$ → $a_B = \gamma_B x_B$

$\Delta G^M = RT(x_A \ln x_A + x_B \ln x_B) + x_A x_B \Omega_{AB}$

$= RT((1-x_B)\ln(1-x_B) + x_B \ln x_B) + x_B x_B \frac{RT \ln \gamma_B}{(1-x_B)^2}$

$\Delta \bar{G}_B^M = \Delta \bar{H}_B^M - T\Delta \bar{S}_B^M = \Omega_{AB} x_A^2 + RT \ln x_B$

$= (1-x_B)^2 \Omega_{AB} + RT \ln x_B$

③ subregular solution model

→ 조성에 따라 Ω_{AB}가 변화해야함

$\Omega_{AB} = a + bX_B$

$G^{xs} = X_A X_B (a + bX_B)$

위에서 구한 결과처럼 Ω_{AB} 값이 일정하기 때문에 subregular solution model은 적절하지 않다.

④ 우수성

$a_B = X_B \exp\left(\frac{X_A^2}{RT}\Omega_{AB}\right)$, & $\Omega_{AB} = -14996.3$ (average value).

a_B (실험 측정)	a_B (수식으로 계산)	오차율(%)
0.0320	0.0317	0.9
0.0800	0.0808	1
0.1498	0.1498	0
0.2400	0.2402	0.08
0.3518	0.3509	0.03
0.4182	0.4183	0.02
0.6162	0.6162	0
0.7559	0.7559	0
0.8824	0.8813	0.01
1.0000	1.0000	0

오차율이 무척 작은 것을 확인할 수 있다.

따라서,

우수한 regular solution model이다.

6. The followings are binary phase diagrams among three elements A, B, C, with melting point of 1000, 1200 and 800K, respectively. Based on binary phase diagrams, sketch isothermal sections of the A-B-C ternary phase diagram at 900, 700 and 400K. (20)