$$\left.\begin{aligned} -\Delta G_{m,A} &= G^{\circ}_{A,\beta} - G^{\circ}_{A,\alpha} \\ \Delta G_{m,B} &= G^{\circ}_{B,\alpha} - G^{\circ}_{B,\beta} \end{aligned}\right) \quad 1$$

Regular Solution.

$$\Delta G^{\alpha} = X_A\,{}^{\circ}G_A^{\alpha} + X_B\,{}^{\circ}G_B^{\alpha} + RT\,(X_A \ln X_A + X_B \ln X_B) + L\,X_A X_B$$

$$\Delta G^{\beta} = X_A\,{}^{\circ}G_A^{\beta} + X_B\,{}^{\circ}G_B^{\beta} + RT\,(X_A \ln X_A + X_B \ln X_B) + L\,(X_A X_B)$$

$$(X_A + X_B = 1)$$

$$\Delta G^{\alpha} = (1-X_B)\,{}^{\circ}G_A^{\alpha} + X_B\,{}^{\circ}G_B^{\alpha} + RT\big((1-X_B)\ln(1-X_B) + X_B \ln X_B\big) + L\,(1-X_B)X_B$$

$$\Delta G^{\beta} = (1-X_B)\,{}^{\circ}G_A^{\beta} + X_B\,{}^{\circ}G_B^{\alpha} + RT\big((1-X_B)\ln X_B + X_B \ln X_B\big) + L\,(1-X_B)X_B$$

Common tangent line $\left(\dfrac{d\Delta G^{\alpha}}{dX_B} = \dfrac{d\Delta G^{\beta}}{dX_B} \right)$

$$\frac{d\Delta G^{\alpha}}{dX_B} = -G_A^{\alpha} + G_B^{\alpha} + RT\big(-\ln(1-X_B) + \cancel{(-1)} + \ln X_B + \cancel{1}\big) + (1-2X_B)L$$

$$= -G_A^{\alpha} + G_B^{\alpha} + RT \ln \frac{X_B}{1-X_B} + (1-2X_B)L$$

$$\rightarrow \left.\frac{d\Delta G^{\alpha}}{dX_B}\right|_{X=X_B} = \left.\frac{d\Delta G^{\beta}}{dX_B}\right|_{X=X_B}$$

$$-G_A^{\alpha} + G_B^{\alpha} + RT \ln \frac{X_B^{\alpha}}{1-X_B^{\alpha}} + (1-2X_B^{\alpha})L = -G_A^{\beta} + G_B^{\beta} + RT \ln \frac{X_B^{\beta}}{1-X_B^{\beta}} + (1-2X_B^{\beta})L$$

$$(G_A^{\beta} - G_A^{\alpha}) + (G_B^{\alpha} - G_B^{\beta}) + RT \ln\left(\frac{X_B^{\alpha}}{X_B^{\beta}} \cdot \frac{1-X_B^{\beta}}{1-X_B^{\alpha}} \right) + (1-2X_B^{\alpha})L^{\alpha} - (1-2X_B^{\beta})L^{\beta}$$

$$= 0$$

According to eq. ① ...

$$-\Delta G_{m,A} + \Delta G_{m,B} + RT \ln\left(\frac{X_B^{\alpha}}{X_B^{\beta}} \cdot \frac{1-X_B^{\beta}}{1-X_B^{\alpha}}\right) + (1-2X_B^{\alpha})L^{\alpha} - (1-2X_B^{\beta})L^{\beta}$$

→ reference state와 independent 하다.,

(Temperature & ${}^{\circ}G$ difference 에 영향)

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

AMSE502 Phase Transformations

due Date: Mar. 11, 2021 — Prof. Byeong-Joo Lee

Problem Set#1 calphad@postech.ac.kr
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[상평형 기초] 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.