HW 1

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정규용액 모델에서,

$$G_m^s = x_A \, {}^\circ G_A^s + x_B \, {}^\circ G_B^s + RT(x_A \ln x_A + x_B \ln x_B) + x_A x_B L_{A,B}$$

$$G_m^L = x_A \, {}^\circ G_A^L + x_B \, {}^\circ G_B^L + RT(x_A \ln x_A + x_B \ln x_B) + x_A x_B L_{A,B}.$$

공통접선을 긋기 위해서는 ① 두 접선의 기울기와 ② 절편(μ, chemical potential)이 같아야 한다.

① $$\left.\frac{\partial G_m^s}{\partial x_A}\right|_{x_A = x_A^\alpha} = \left.\frac{\partial G_m^L}{\partial x_A}\right|_{x_A = x_A^\beta}$$

$$\left.\frac{\partial G_m^s}{\partial x_A}\right|_{x_A = x_A^\alpha} = G_A^s - G_B^s + RT\left(\ln \frac{x_A^\alpha}{1-x_A^\alpha} + (1-2x_A^\alpha) L_{A,B}\right)$$

$$\left.\frac{\partial G_m^L}{\partial x_A}\right|_{x_A = x_A^\beta} = G_A^L - G_B^L + RT\left(\ln \frac{x_A^\beta}{1-x_A^\beta} + (1-2x_A^\beta) L_{A,B}\right)$$

$$\left.\frac{\partial G_m^s}{\partial x_A}\right|_{x_A = x_A^\alpha} - \left.\frac{\partial G_m^L}{\partial x_A}\right|_{x_A = x_A^\beta} = (G_A^L - G_A^s) - (G_B^L - G_B^s) + RT\, f(x_A^\alpha, x_A^\beta) = 0$$

②. $$G = x_A G_A^s + x_B G_B^s + RT(x_A \ln x_A + x_B \ln x_B) + x_A x_B L_{A,B}$$
$$+ L x_A x_B (x_A + x_B)$$

$$= \quad //$$

$$= x_A(G_A^s + RT \ln x_A + L x_B^2) + x_B(G_B^s + RT \ln x_B + L x_A^2)$$

$$= \mu_A^s x_A + \mu_B^s x_B$$

$$\mu_A^s = G_A^s + RT \ln x_A^\alpha + L x_B^{\alpha\,2}$$

$$\mu_A^L = G_A^L + RT \ln x_A^\beta + L x_B^{\beta\,2},$$

$$\mu_A^s = \mu_A^L, \quad G_A^s - G_A^L + RT\left(\ln \frac{x_A^\alpha}{x_A^\beta}\right) + L(x_B^{\alpha 2} - x_B^{\beta 2}) = 0,$$

$$\mu_B^s = \mu_B^L, \quad G_B^s - G_B^L + RT\left(\ln \frac{x_B^\alpha}{x_B^\beta}\right) + L(x_A^{\alpha 2} - x_A^{\beta 2}) = 0$$

①과②의 식을 연립하면 x_A^α, x_A^β를 구할 수 있다.

이 때 ①과② 식 모두 reference state와 관련이 없는 것을 알 수 있다.

($\because$ $G_A^s - G_A^L$, $G_B^s - G_B^L$은 reference state와 관련없이 일정하므로)