HW2

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1. CSL (coincidence site lattice)란 grain 간의 misorientation이 특정한 각도로 이룰 때 격자점들 중 일부가 일치하여 grain boundary energy 낮아지는 특정한 lattice를 말한다. 이 때 특정 misorientation angle은 주기성을 가져서 각도에 따라 주기적으로 에너지가 낮은 부분이 생긴다.

2.
$$^{\circ}G_i^{\phi} + RT\ln r_i^{\phi}X_i^{\phi} = \mu_i^{\phi} + 6w_i \qquad ^{\circ}G_i^{B} + RT\ln r_i^{B}X_i^{B} = \mu_i^{B}$$
$$^{\circ}G_j^{\phi} + RT\ln r_j^{\phi}X_j^{\phi} = \mu_j^{\phi} + 6w_j \qquad ^{\circ}G_j^{B} + RT\ln r_j^{B}X_j^{B} = \mu_j^{B}$$
$$\vdots$$
$$^{\circ}G_{n-1}^{\phi} + RT\ln r_{n-1}^{\phi}X_{n-1}^{\phi} = \mu_{n-1}^{\phi} + 6w_{n-1} \qquad ^{\circ}G_{n-1}^{B} + RT\ln r_{n-1}^{B}X_{n-1}^{B} = \mu_{n-1}^{B}$$

for n component ($i, j = 1, \cdots n-1$)
m

chemical potential이 같다는 점과 $w_i = w_j = \dots = w$ 라는 가정을 이용하여 식을 연립하면

$$\frac{X_j^{\phi}}{X_m^{\phi}} = \frac{X_j^{B}}{X_m^{B}} e^{-\Delta G_j^{seg}/RT} \qquad \Delta G_j^{seg} = [^{\circ}G_j^{\phi} - {^{\circ}G_j^{B}}] - [^{\circ}G_m^{\phi} - {^{\circ}G_m^{B}}] + RT\ln\frac{r_i^{\phi}r_m^{B}}{r_m^{\phi}r_i^{B}}$$

모든 식을 더하면

$$\sum_{j=1}^{n-1} X_j^{\phi} = \left(\frac{X_m^{\phi}}{X_m^{B}}\right)\sum_{k=1}^{n-1} X_k^{B} e^{-\frac{\Delta G_k^{seg}}{RT}} \longrightarrow \sum_{j=1}^{n-1} X_j^{\phi}X_m^{B} + X_m^{\phi}X_m^{B} = \sum_{k=1}^{n-1} X_k^{B}X_m^{\phi} e^{-\frac{\Delta G_k^{seg}}{RT}} + X_m^{\phi}X_m^{B}$$

$$\frac{X_m^{B}\left(\sum_{j=1}^{n-1} X_j^{\phi} + X_m^{\phi}\right)}{X_m^{\phi}\left(\sum_{k=1}^{n-1} X_k^{B} e^{-\frac{\Delta G_k^{seg}}{RT}} + X_m^{B}\right)} = 1 \qquad \frac{X_m^{B}}{X_m^{\phi}} = \sum_{k=1}^{n-1} X_k^{B} e^{-\frac{\Delta G_k^{B}}{RT}} + X_m^{B}$$

$$\left(\because \sum_{j=1}^{n-1} X_j^{\phi} + X_m^{\phi} = 1\right)$$

$$X_i^{\phi} = \frac{X_m^{\phi}}{X_m^{B}} X_i^{B} e^{-\Delta G_i^{seg}/RT} = \frac{X_i^{B} e^{-\Delta G_i^{seg}/RT}}{\sum_{k=1}^{n-1} X_k^{B} e^{-\frac{\Delta G_k^{seg}}{RT}} + X_m^{B}} = \frac{X_i^{B} e^{-\Delta G_i^{seg}/RT}}{\sum_{k=1}^{n-1} X_k^{B} e^{-\frac{\Delta G_k^{seg}}{RT}} + \left(1 - \sum_{k=1}^{n-1} X_k^{B}\right)}$$

$$X_i^{\phi} = \frac{X_i^{B} e^{-\Delta G_i^{seg}/RT}}{\sum_{k=1}^{n-1} X_k^{B}\left(e^{-\frac{\Delta G_k^{seg}}{RT}} - 1\right) + 1}$$