20192347 권현석

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AMSE502 Phase Transformations

due Date: Mar. 23, 2021

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Problem Set #2

1. Study and summarize CSL(coincidence site lattice) boundary.

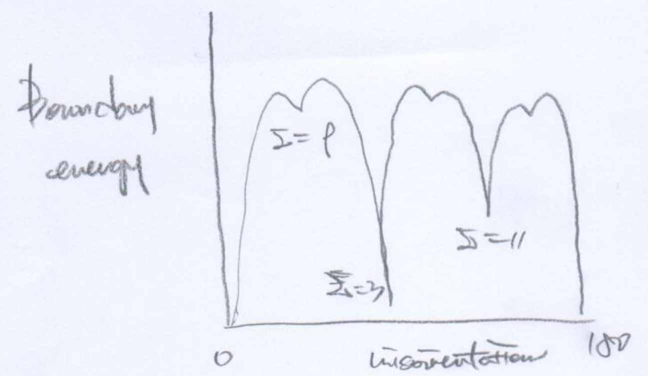
2. Assuming a one atomic layer surface phase and considering equilibrium between bulk and surface phases, one can derive the following relation between surface composition and bulk composition. (B means "bulk" and ϕ means "surface". i means arbitrary solute elements while n means solvent element)

$$\frac{X_i^\phi}{X_n^\phi} = \frac{X_i^B}{X_n^B}\, e^{-\Delta G^{seg}/RT} \qquad \text{where} \quad \Delta G^{seg} = [{}^oG_i^\phi - {}^oG_i^B] - [{}^oG_n^\phi - {}^oG_n^B] + RT\ln\frac{\gamma_i^\phi \gamma_n^B}{\gamma_n^\phi \gamma_i^B}$$

Change the above equation into the following, more general multicomponent form:

$$X_i^\phi = \frac{X_i^B e^{-\Delta G_i^{seg}/RT}}{1+\sum_{j=1}^{n-1} X_j^B (e^{-\Delta G_j^{seg}/RT} - 1)} \qquad \text{Hint: use } \sum_{i=1}^{n-1} x_i^\phi x_n^B = \sum_{j=1}^{n-1} x_j^B x_n^\phi\, e^{-\Delta G_j^{seg}/RT}$$

1. Grain boundary에서는 결정 간의 misorientation이 존재하나, 일부 격자점이 주기적으로 일치하는 경우가 생기며 이에 해당하는 점들의 집합을 CSL이라 한다. 이러한 CSL boundary에서는 boundary energy가 낮아지는 현상이 관찰된다. Lattice의 unit cell 내부의 lattice point 개수를 Σ로 나타내어지며, Σ가 작을수록 misorientation이 낮다. CSL boundary는 일치하는 격자점이 많으므로 Σ가 낮다.



2. $$\frac{X_i^{\phi}}{X_n^{\phi}} = \frac{X_i^{\beta}}{X_n^{\beta}} e^{-\frac{\Delta G^{seg}}{RT}} \quad \cdots (1).$$

$$X_i^{\phi} X_n^{\beta} = X_i^{\beta} X_n^{\phi} e^{-\frac{\Delta G^{seg}}{RT}}$$

$$\sum_{i=1}^{n-1} X_i^{\phi} X_n^{\beta} = \sum_{i=1}^{n-1} X_i^{\beta} X_n^{\phi} e^{-\frac{\Delta G^{seg}}{RT}}$$

$$X_n^{\beta}(1 - X_n^{\phi}) = X_n^{\phi} \sum_{i=1}^{n-1} X_i^{\beta} e^{-\frac{\Delta G^{seg}}{RT}} \Rightarrow \frac{X_n^{\phi}}{X_n^{\beta}} = \frac{1 - X_n^{\phi}}{\sum_{i=1}^{n-1} X_i^{\beta} e^{-\frac{\Delta G}{RT}}} \quad \cdots (2)$$

한편, $X_i^{\phi} = \frac{X_n^{\phi}}{X_n^{\beta}} X_i^{\beta} e^{-\frac{\Delta G}{RT}}$ from (1).

$$\Rightarrow X_i^{\phi} = \frac{(1 - X_n^{\phi}) X_i^{\beta} e^{-\frac{\Delta G}{RT}}}{\sum_{i=1}^{n-1} X_i^{\beta} e^{-\frac{\Delta G}{RT}}} \quad \text{from (2).}$$

$$X_i^{\phi} = \frac{X_i^{\beta} e^{-\frac{\Delta G}{RT}} - X_i^{\beta} X_n^{\phi} e^{-\frac{\Delta G}{RT}}}{\sum_{i=1}^{n-1} X_i^{\beta} e^{-\frac{\Delta G}{RT}}} = \frac{X_i^{\beta} e^{-\frac{\Delta G}{RT}} - X_i^{\phi} X_n^{\beta}}{\sum_{i=1}^{n-1} X_i^{\beta} e^{-\frac{\Delta G}{RT}}}$$

$$X_i^{\phi} \left(\sum_{i=1}^{n-1} X_i^{\beta} e^{-\frac{\Delta G}{RT}} + X_n^{\beta} \right) = X_i^{\beta} e^{-\frac{\Delta G}{RT}}$$

$$X_i^{\phi} \left(1 + \sum_{i=1}^{n-1} X_i^{\beta} \left(e^{-\frac{\Delta G_i^{seg}}{RT}} - 1 \right) \right) = X_i^{\beta} e^{-\frac{\Delta G_i^{seg}}{RT}}$$

$$\therefore X_i^{\phi} = \frac{X_i^{\beta} e^{-\frac{\Delta G_i^{seg}}{RT}}}{1 + \sum_{j=1}^{n-1} X_j^{\beta} \left(e^{-\frac{\Delta G_j^{seg}}{RT}} - 1 \right)}$$