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1. CSL에 대하여

CSL (coincidence site lattice) 언급하기에 앞서 grain boundary란?

grain과 grain간의 interface를 의미한다. 일반적으로 다른 두 grain 방향으로 인해 misorientation이 발생한다. 이는 높은 energy를 가지고 있고 2D-defect로 취급된다. 하지만 특정 misorientation angle에서 일부 lattice points들이 일치하는 경우가 발생하는데 이를 coincidence site lattice (CSL)이라고 한다. 이럴 경우 다른 misorientation angle에 비해 grain boundary energy가 매우 낮아진다. twin boundary도 여기에 해당된다. 이를 표현하는데 있어 Σ를 사용하는데 Σ는 항상 홀수값을 가지며 값이 낮을수록 misorientation이 작다. Σ1는 perfect crystal을 의미한다.

2.

∘ $\frac{x_i^\phi}{x_n^\phi} = \frac{x_i^B}{x_n^B} \cdot e^{-\Delta G^{seg}/RT}$, $\Delta G^{seg} = [{}^\circ G_i^\phi - {}^\circ G_i^B] - [{}^\circ G_n^\phi - {}^\circ G_n^B] + RT \ln \frac{\gamma_i^\phi \gamma_n^B}{\gamma_n^\phi \gamma_i^B}$

$(\mu_i^\phi = \mu_i^B)$ $\qquad = w^\circ \sigma_i - w^\circ \sigma_n + [\Delta^{xs}\bar{G}_i^\phi - \Delta^{xs}\bar{G}_n^\phi] - [\Delta^{xs}\bar{G}_i^B - \Delta^{xs}\bar{G}_n^B]$

↓

∘ $\sigma w_i = [{}^\circ G_i^\phi - {}^\circ G_i^B] + RT \ln \frac{\gamma_i^\phi}{\gamma_i^B} + RT \ln \frac{x_i^\phi}{x_i^B}$

$\sigma = \frac{1}{w_i}[{}^\circ G_i^\phi - {}^\circ G_i^B] + \frac{1}{w_i}[\Delta^{xs}\bar{G}_i^\phi - \Delta^{xs}\bar{G}_i^B] + \frac{RT}{w_i}\ln(x_i^\phi / x_i^B)$

$= \cdots$

$= \frac{1}{w_n}[{}^\circ G_n^\phi - {}^\circ G_n^B] + \frac{1}{w_n}[\Delta^{xs}\bar{G}_n^\phi - \Delta^{xs}\bar{G}_n^B] + \frac{RT}{w_n}\ln(x_n^\phi / x_n^B)$

∘ $-\left\{ \frac{1}{w_i}[{}^\circ G_i^\phi - {}^\circ G_i^B] - \frac{1}{w_n}[{}^\circ G_n^\phi - {}^\circ G_n^B] + \frac{1}{w_i}[\Delta^{xs}\bar{G}_i^\phi - \Delta^{xs}\bar{G}_i^B] - \frac{1}{w_n}[\Delta^{xs}\bar{G}_n^\phi - \Delta^{xs}\bar{G}_n^B] \right\}$ $\simeq \Delta G_i^{seg}$

$= \frac{RT}{w_i}\ln(x_i^\phi / x_i^B) - \frac{RT}{w_n}\ln(x_n^\phi / x_n^B)$

∘ $\ln\left[(x_i^\phi / x_i^B)^{\frac{1}{w_i}} / (x_n^\phi / x_n^B)^{\frac{1}{w_n}}\right] = -\Delta G_i^{seg}/RT$

$\Rightarrow \frac{x_i^\phi}{x_i^B} = \left(\frac{x_n^\phi}{x_n^B}\right)^{(\frac{w_i}{w_n}=1)} \cdot e^{-\Delta G_i^{seg}/RT}$ $\quad (\frac{w_i}{w_n}=1)$

∘ $x_i^\phi = \left(\frac{x_n^\phi}{x_n^B}\right) \cdot x_i^B \cdot e^{-\Delta G_i^{seg}/RT} = \left(\frac{\sum_{j=1}^{n-1} x_j^\phi}{\sum_{j=1}^{n-1} x_j^B e^{-\Delta G_j^{seg}/RT}}\right) \cdot x_i^B \cdot e^{-\Delta G_i^{seg}/RT}$ $\quad \left(\sum_{j=1}^{n-1} x_j^\phi x_n^B = \sum_{j=1}^{n-1} x_j^B x_n^\phi \cdot e^{-\Delta G_j^{seg}/RT}\right)$

↳ $= \frac{1 - x_n^\phi}{\sum_{j=1}^{n-1} x_j^B e^{-\Delta G_j^{seg}/RT}}$ $\quad \left(\sum_{j=1}^{n-1} x_j^\phi = (x_1^\phi + x_2^\phi + \cdots + x_{n-1}^\phi + x_n^\phi) - x_n^\phi\right)$

$= \frac{(1 - x_n^\phi) \cdot x_i^B \cdot e^{-\Delta G_i^{seg}/RT}}{\sum_{j=1}^{n-1} x_j^B e^{-\Delta G_j^{seg}/RT}}$

$= \frac{x_i^B \cdot e^{-\Delta G_i^{seg}/RT} - x_n^\phi \cdot x_i^B \cdot e^{-\Delta G_i^{seg}/RT}}{\quad} = \frac{x_i^B \cdot e^{-\Delta G_i^{seg}/RT} - x_i^\phi \cdot x_n^B}{\quad}$

∘ $x_i^\phi \left(\sum_{j=1}^{n-1} x_j^B e^{-\Delta G_j^{seg}/RT} + x_n^B\right) = x_i^B \cdot e^{-\Delta G_i^{seg}/RT}$, $\left(x_n^B = 1 - \sum_{j=1}^{n-1} x_j^B\right)$

∴ $x_i^\phi = \frac{x_i^B \cdot e^{-\Delta G_i^{seg}/RT}}{1 + \sum_{j=1}^{n-1} x_j^B \left(e^{-\Delta G_j^{seg}/RT} - 1\right)}$