상변태론 HW #2 신소재공학과 20222389 김창훈

Q1.

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

$$\rightarrow 1 = \left(\frac{x_i^B}{x_i^\phi}\right)\cdot\left(\frac{x_n^\phi}{x_n^B}\right)\cdot e^{-\Delta G^{seg}/RT} \qquad \left(x_1^\phi + x_2^\phi + \cdots + x_n^\phi = 1 = \sum_{i=1}^{n-1} x_i^\phi + x_n^\phi\right)$$

$$\rightarrow \left(\sum_{i=1}^{n-1} x_i^\phi\right) + x_n^\phi = \left(\frac{x_i^B}{x_i^\phi}\right)\left(\frac{x_n^\phi}{x_n^B}\right) \cdot e^{-\Delta G^{seg}/RT}$$

— 빼고 이항.

$$\rightarrow \left(x_i^\phi \cdot x_n^B\right) \cdot \left(1 + \sum_{i=1}^{n-1} \left(x_i^\phi / x_n^\phi\right)\right) = x_i^B \cdot e^{-\Delta G^{seg}/RT}$$

$$\rightarrow x_i^\phi \cdot x_n^B + \left(\frac{x_i^\phi}{x_n^\phi} \cdot \boxed{x_n^B \cdot \sum_{i=1}^{n-1} x_i^\phi}\right) = x_i^B \cdot e^{-\Delta G^{seg}/RT}$$

using Hint $\left(\sum_{i=1}^{n-1} x_i^\phi \cdot x_n^B = \sum_{j=1}^{n-1} x_j^B \cdot x_n^\phi \cdot e^{-\Delta G_j^{seg}/RT}\right)$

$$\rightarrow x_i^\phi \cdot x_n^B + \frac{x_i^\phi}{\cancel{x_n^\phi}} \cdot \sum_{j=1}^{n-1} x_j^B \cdot \cancel{x_n^\phi} \cdot e^{-\Delta G_j^{seg}/RT} = x_i^B \cdot e^{-\Delta G^{seg}/RT}$$

$$\left(x_1^B + \cdots + x_n^B = 1 \rightarrow x_n^B = 1 - \sum_{j=1}^{n-1} x_j^B\right)$$

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

multi component eq로 변환 완료.

Question2. study and summarize CSL boundary

- 결정구조에서 다양한 defects가 존재함. Grain scale 에서 다른 방위를 가지는 2-D defects (planar)인 Grain boundary가 형성됨.
- Grain boundary는 5가지의 degree of freedom 이 존재함.

[Rotation part : 회전축 2개 $(\vec{o})$, 각도 1개 (θ)
[translation part : 방위 2개 $(\vec{n})$ (GB plane)]

$\vec{o} \perp \vec{n}$ = tilt
$\vec{o} \parallel \vec{n}$ = twist

↳ 하나의 Grain 의 atomic site가 다른 grain의 site와 degree of freedom 내 일치하면 Coincidence-site lattice (CSL) GB 라고 한다.

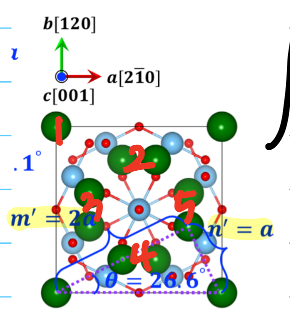
- 전산재료 연구 관점에서 CSL gb를 이용하면 computational cost가 확연히 줄어 이를 기반으로 다양한 modeling 이 가능함.
  ↳ periodic boundary size 감소, 구조 단순화 속도↑

- $\Sigma a[\vec{o}]/(\vec{c})$ 로 묘사되며 $\vec{o}$ 는 rotation axis, $\vec{c}$는 gb plane의 miller index를 의미한다.

$$\Sigma = \frac{\text{Coincidence unit cell volume}}{\text{Rotated unit cell volume} \times (u^2+v^2+w^2)} = \text{coincidence lattice 내부의 격자 sites 개수}$$

<twist>

(c) Σ5[001]/(001)

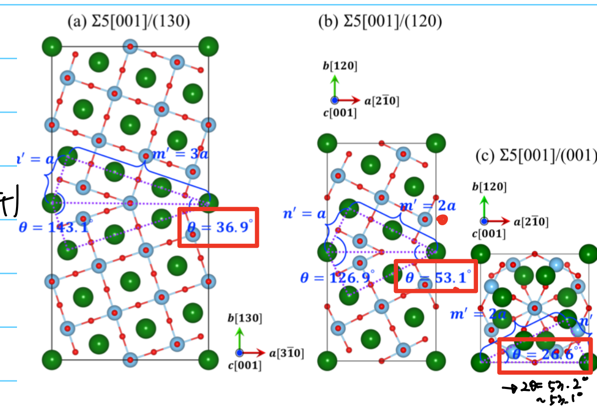


격자내 site # = 5 → $\Sigma 5$

or

unit cell volume $= \sqrt{5}a \times \sqrt{5}a \times \sqrt{5}a = 5\sqrt{5}a^3$
coincidence cell volume $= \frac{1}{2} \times 2a \times a \times \sqrt{5}a = \sqrt{5}a^3$

$\rightarrow \frac{5\sqrt{5}a^3}{\sqrt{5}a^3} = 5 \rightarrow \Sigma 5$



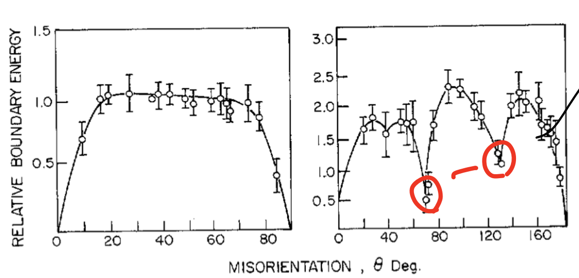
$A = \alpha\Sigma = m^2 + (u^2+v^2+w^2)n^2$ / $\tan\frac{\theta}{2} = \frac{n}{m}(u^2+v^2+w^2)^{1/2}$

ex) $\Sigma 5(001) \Rightarrow 5\alpha = m^2+n^2$ (α, m, n must be Integer, 약수)

i) $\alpha=1$. $5=m^2+n^2$, $(m,n)=(2,1), (1,2) \rightarrow \theta = 53.1°, 126.9°$ same

ii) $\alpha=2$. $10=m^2+n^2$, $(m,n)=(3,1) \rightarrow \theta = 36.9°$

iii) $\alpha=4$. $20=m^2+n^2$, $(m,n)=(4,2) \rightarrow (2,1)$ ∴ $\alpha=1$과 동일



special grain boundary가 생기도함.

[100] and [110] tilt Boundary energy of Al