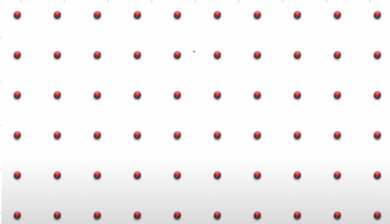
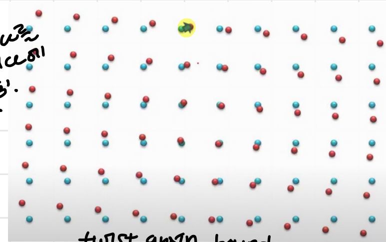
HW#2 20212568 강승연

1) CSL (Coincidence site lattice) boundary

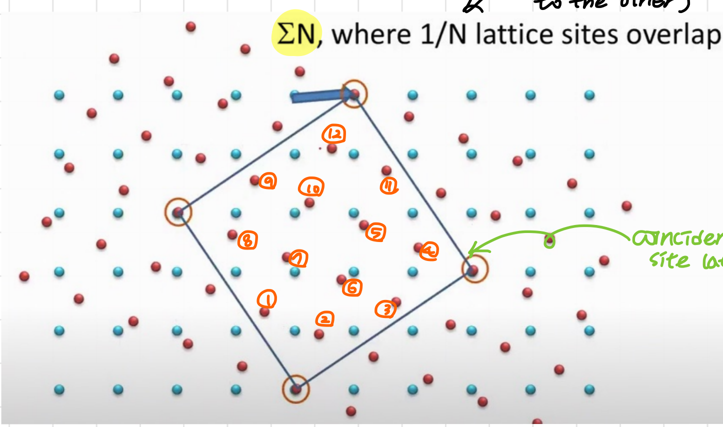
- special orientation rotation angles that can happen
- sitting directly on top of each other



빨간 lattice를 파랑 lattice에 대해 돌려줌.



twist grain boundary
(start rotate one of those with respect to the other)



coincidence site lattice

⇒ Some of these atoms are coincident with the position of the atoms on the lattice

⇒ how many red lattice sites there are in this square = total 13 lattice sites.
(∵ red on the corner only counts as one ; 4 corner = 1개)

⇒ that is, in this picture
↳ we can call it Σ13 (Sigma 13) CSL relationship.
↳ one out of 13 of those lattice sites are overlapping b/w the red & blue lattices

※ 이때 Σ는 홀수값만 가짐.

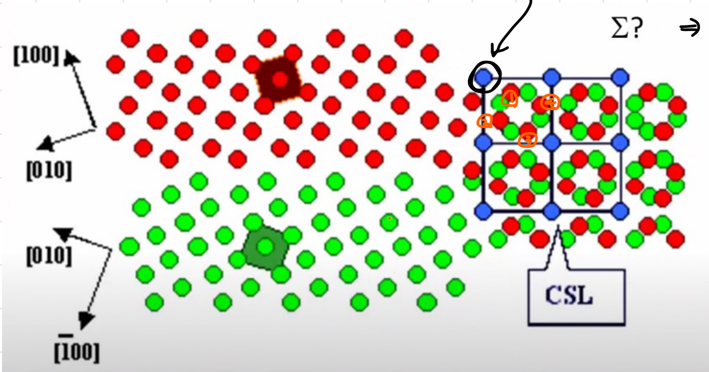
* Σ1 = 완전히 같은 orientation의 grain들간의 관계 ; perfect crystal

Σ3 = twin boundary

Σ가 낮을 수록 일치하는 격자점↑

blue dot = both red + green dot

Σ? ⇒ Count one of the lattices, so let's pick red



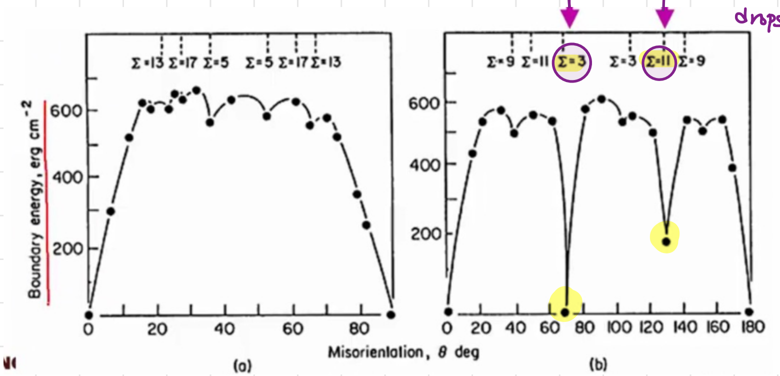
(tilted one with respect to the other)

⇒ how many red sites in the square? = total $\underline{\underline{5}}$

↳ Σ5 CSL boundary.

Something special relationship

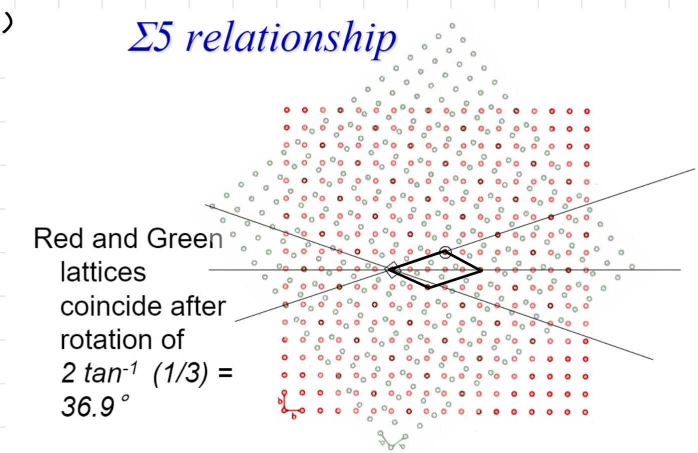
⇒ boundary energy drops dramatically



(sigma grain boundary)

→ tilt grain boundary

e.g.)



2) $\frac{X_{\bar n}^{\phi}}{X_n^{\phi}} = \frac{X_{\bar n}^{B}}{X_n^{B}} e^{-\Delta G^{seg}/RT} \Rightarrow \frac{1}{X_n^{\phi}} = \frac{X_{\bar n}^{B}}{X_{\bar n}^{\phi} X_n^{B}} e^{-\Delta G_{\bar n}^{seg}/RT}$

$\left(\because 1 = X_n + \sum_{\bar n=1}^{n-1} X_{\bar n}^{\phi}\right)$

$$\Rightarrow \frac{X_n + \sum_{\bar n=1}^{n-1} X_{\bar n}^{\phi}}{X_n^{\phi}} = \frac{X_{\bar n}^{B}}{X_{\bar n}^{\phi} X_n^{B}} e^{-\Delta G_{\bar n}^{seg}/RT}$$

$$\Rightarrow X_{\bar n}^{\phi} X_n^{B} \left(1 + \frac{\sum_{\bar n=1}^{n-1} X_{\bar n}^{\phi}}{X_n^{\phi}}\right) = X_{\bar n}^{B} e^{-\Delta G_{\bar n}^{seg}/RT}$$

$$\Rightarrow X_{\bar n}^{\phi} X_n^{B} + \frac{X_{\bar n}^{\phi}}{X_n^{\phi}} \sum_{\bar n=1}^{n-1} X_{\bar n}^{\phi} X_n^{B} = X_{\bar n}^{B} e^{-\Delta G_{\bar n}^{seg}/RT}$$

(Hint: $\sum_{\bar n=1}^{n-1} X_{\bar n}^{\phi} X_n^{B} = \sum_{j=1}^{n-1} X_j^{B} X_n^{\phi} e^{-\Delta G_j^{seg}/RT}$)

$$\Rightarrow X_{\bar n}^{\phi} X_n^{B} + \frac{X_{\bar n}^{\phi}}{X_n^{\phi}} \sum_{j=1}^{n-1} X_j^{B} X_n^{\phi} e^{-\Delta G_j^{seg}/RT} = X_{\bar n}^{B} e^{-\Delta G_{\bar n}^{seg}/RT}$$

$$\Rightarrow \boxed{X_{\bar n}^{\phi}} \left(X_n^{B} + \sum_{j=1}^{n-1} X_j^{B} e^{-\Delta G_j^{seg}/RT}\right) = X_{\bar n}^{B} e^{-\Delta G_{\bar n}^{seg}/RT}$$

$$\Rightarrow X_{\bar n}^{\phi} = \frac{X_{\bar n}^{B} e^{-\Delta G_{\bar n}^{seg}/RT}}{1 + \sum_{j=1}^{n-1} X_j^{B} \left(e^{-\Delta G_j^{seg}/RT} - 1\right)}$$

$X_n^{B} = 1 - \sum_{j=1}^{n-1} X_j^{B}$

∎