CSL boundary

- CSL (coincidence site lattice) boundary

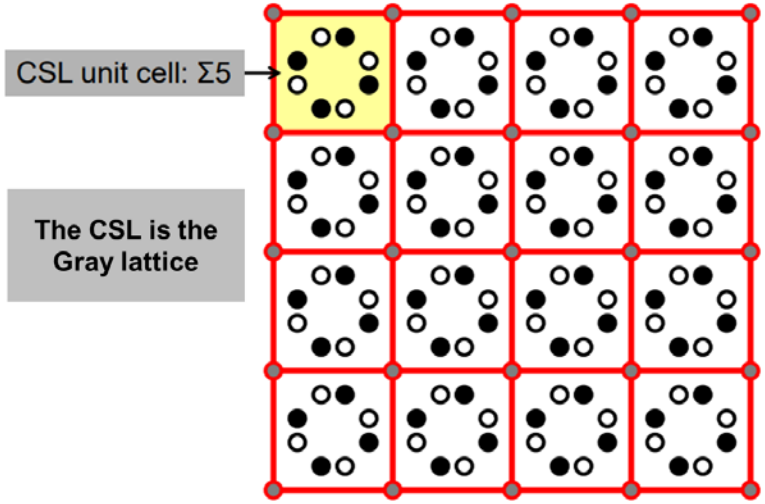
  특정 angle에서 두 grain의 lattice point가 정확히 일치하는 경우 두 grain 사이의 boundary를 CSL boundary 라고 한다.

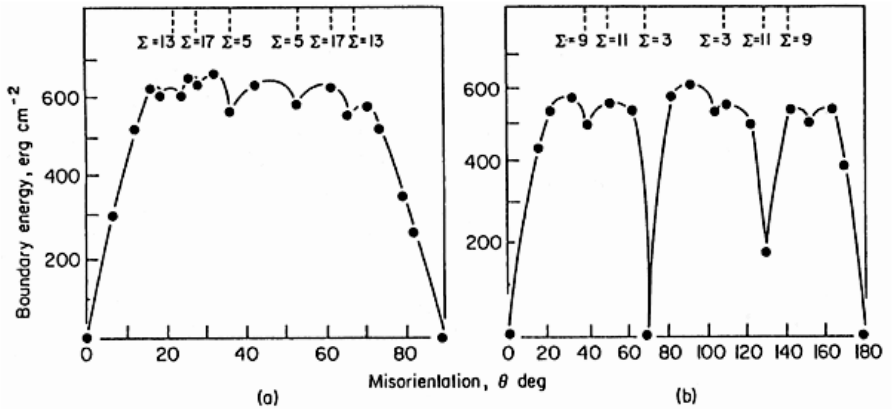
- Σ (sigma)

  unit cell 내에서 CSL의 lattice point 수와 전체 lattice point 수 사이의 관계를 나타낸다.

$$\Sigma = \frac{The\ number\ of\ lattice\ points\ in\ a\ unit\ cell}{The\ number\ of\ lattice\ points\ in\ the\ unit\ cell\ of\ a\ CSL}$$

  Σ가 낮을 수록 일치하는 lattice point가 많음을 의미함으로 일반적으로 낮은 grain boundary energy를 가진다.





$$\frac{X_i^{\phi}}{X_n^{\phi}} = \frac{X_i^{B}}{X_n^{B}} e^{-\Delta G_i^{seg}/RT}$$

$$\Rightarrow X_i^{\phi} = \left(\frac{X_n^{\phi}}{X_n^{B}}\right) X_i^{B} e^{-\Delta G_i^{seg}/RT}$$

$$\sum_{i=1}^{n-1} X_i^{\phi} X_n^{B} = \sum_{j=1}^{n-1} X_j^{B} X_n^{\phi} e^{-\Delta G_j^{seg}/RT}$$

$$\Rightarrow \sum_{i=1}^{n-1} X_i^{\phi} X_n^{B} + X_n^{\phi} X_n^{B} = \sum_{j=1}^{n-1} X_j^{B} X_n^{\phi} e^{-\Delta G_j^{seg}/RT} + X_n^{\phi} X_n^{B}$$

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

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

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

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