

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

$$\downarrow$$

$$\sum_{i=1}^{n-1} \frac{X_i^\phi}{X_n^\phi} = \sum_{j=1}^{n-1} \frac{X_j^\beta}{X_n^\beta} \exp\left(-\frac{\Delta G_j^{\text{seg}}}{RT}\right) \quad \text{I}$$

Since $\sum_{i=1}^{n-1} X_i^\phi = X_1^\phi + \dots + X_{n-1}^\phi$ and $X_1^\phi + \dots + X_n^\phi = 1$

then $\sum_{i=1}^{n-1} X_i^\phi = 1 - X_n^\phi \quad \text{II}$

by plugging II in I $\rightarrow \frac{1 - X_n^\phi}{X_n^\phi} = \sum_{j=1}^{n-1} \frac{X_j^\beta}{X_n^\beta} \exp\left(-\frac{\Delta G_j^{\text{seg}}}{RT}\right)$

then $\frac{1}{X_n^\phi} = \sum_{j=1}^n \frac{X_j^\beta}{X_n^\beta} \exp\left(-\frac{\Delta G_j^{\text{seg}}}{RT}\right) + \frac{1}{X_n^\phi} \quad \text{III}$ (IV) $1 = \frac{X_n^\beta}{X_n^\beta}$

by plugging IV in III we have

$$X_n^\phi = \frac{X_n^\beta}{\sum_{j=1}^{n-1} \frac{X_j^\beta}{X_n^\beta} \exp\left(-\frac{\Delta G_j^{\text{seg}}}{RT}\right) + X_n^\beta} = \frac{X_n^\beta}{\sum_{j=1}^{n-1} X_j^\beta \exp\left(-\frac{\Delta G_j^{\text{seg}}}{RT}\right) + 1 - \sum_{j=1}^{n-1} X_j^\beta}$$

then $X_n^\phi = \frac{X_n^\beta}{\sum_{j=1}^{n-1} X_j^\beta \left(\exp\left(-\frac{\Delta G_j^{\text{seg}}}{RT}\right) - 1\right) + 1} \quad \text{(V)}$

we know

$$X_n^\beta = X_i^\beta \exp\left(-\frac{\Delta G_i^{\text{seg}}}{RT}\right) \cdot X_n^\phi / X_i^\phi \quad \text{(VI)}$$

by plugging vI in v we have

$$\cancel{X_n^\phi} X_i^\phi = \frac{\cancel{X_n^\phi} X_i^\beta \exp(-\Delta G_i^{\text{seg}}/RT)}{\sum_j^{n-1} X_j^\beta (\exp(-\frac{\Delta G_j^{\text{seg}}}{RT}) - 1) + 1}$$

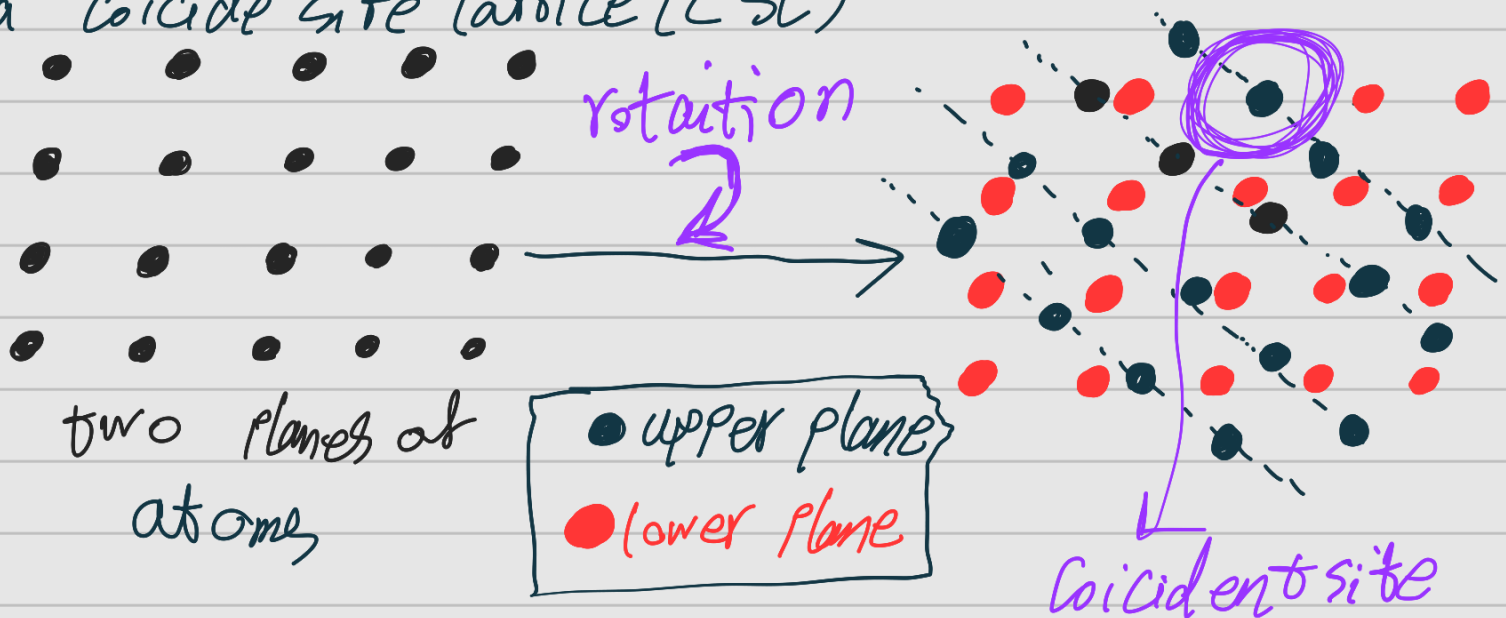
then we have

$$X_i^\phi = \frac{X_i^\beta \exp(-\Delta G_i^{\text{seg}}/RT)}{\sum_{j=1}^{n-1} X_j^\beta (\exp(-\frac{\Delta G_j^{\text{seg}}}{RT}) - 1) + 1}$$

equation successfully proved ✓

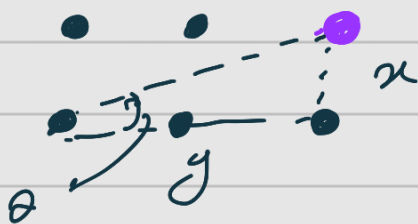
The CSL is a geometrical construction based on the geometry of the lattice

If two grains of same crystal are placed on top of each other each atom has its own position. Now if the upper plane starts to rotate at different angles and some atoms sit on top of each other that means a finite number of lattice sites coincide between two lattices. Then one can define a coincident site lattice (CSL)



The reason that CSL is important is that when a boundary that contains a high number of lattice points in a CSL is expected to have good atomic fit and thus low energy.

The angle of rotation can be determined from the lattice geometry because of discrete nature of lattice based on coordinates of coincident site.



$$\theta = 2 \tan^{-1} \left(\frac{y}{x} \right) \star$$

y should be on same primary position of atom in coincident site before rotation.