REPORT

POSTECH

POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY

제목 : Homework #2

수강과목 :	상변태론
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1. Assuming a one atomic layer surface phase and considering equilibrium between bulk and surface phases, one can derive the following relation between surface composition and bulk composition. (B means "bulk" and ϕ means "surface". i means arbitrary solute elements while n means solvent element)

$$\frac{X_i^\phi}{X_n^\phi}=\frac{X_i^B}{X_n^B}\,e^{-\Delta G^{seg}/RT} \qquad \text{where} \quad \Delta G^{seg}=[{}^oG_i^\phi-{}^oG_i^B]-[{}^oG_n^\phi-{}^oG_n^B]+RT\ln\frac{\gamma_i^\phi\gamma_n^B}{\gamma_n^\phi\gamma_i^B}$$

Change the above equation into the following, more general multicomponent form:

$$X_i^\phi=\frac{X_i^B e^{-\Delta G_i^{seg}/RT}}{1+\sum_{j=1}^{n-1}X_j^B(e^{-\Delta G_j^{seg}/RT}-1)} \qquad \text{Hint: use} \quad \sum_{i=1}^{n-1}x_i^\phi x_n^B=\sum_{j=1}^{n-1}x_j^B x_n^\phi\, e^{-\Delta G_j^{seg}/RT}$$

sol)

$$\frac{X_i^\phi}{X_n^\phi}=\frac{X_i^B}{X_n^B}\exp\left(-\frac{\Delta G_i^{seg}}{RT}\right), \quad X_i^\phi=\frac{X_i^B\exp(-\frac{\Delta G_i^{seg}}{RT})}{\frac{X_n^B}{X_n^\phi}}$$

$$\frac{X_n^B}{X_n^\phi}=X_n^B\left(1+\frac{1-X_n^\phi}{X_n^\phi}\right)=X_n^B\left(1+\frac{\sum_{i=1}^{n-1}X_i^\phi}{X_n^\phi}\right) \quad (\textstyle\sum_{i=1}^{n}X_i=1)$$

$$\rightarrow X_n^B\left(1+\frac{\sum_{i=1}^{n-1}X_i}{X_n^\phi}\right)=X_n^B+\frac{\sum_{i=1}^{n-1}X_i^B X_n^\phi}{X_n^\phi}\exp\left(-\frac{\Delta G_i^{seg}}{RT}\right)$$

$$\rightarrow X_n^B+\frac{\sum_{i=1}^{n-1}X_j^B X_n^\phi\exp(-\frac{\Delta G_i^{seg}}{RT})}{X_n^\phi}=X_n^B+\sum_{i=1}^{n-1}X_j^B\exp\left(-\frac{\Delta G_i^{seg}}{RT}\right)$$

$$=1-\sum_{i=1}^{n-1}X_j^B+\sum_{i=1}^{n-1}X_j^B\exp\left(-\frac{\Delta G_i^{seg}}{RT}\right)$$

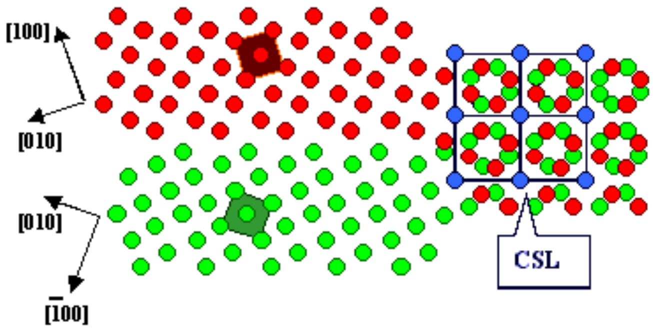
$$=1+\sum_{i=1}^{n-1}X_j^B\left(\exp\left(-\frac{\Delta G_i^{seg}}{RT}\right)-1\right)$$

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

$$X_i^\phi=\frac{X_i^B\exp(-\frac{\Delta G_i^{seg}}{RT})}{\frac{X_n^B}{X_n^\phi}}=\frac{X_i^B\exp(-\frac{\Delta G_i^{seg}}{RT})}{1+\sum_{i=1}^{n-1}X_j^B\left(\exp(-\frac{\Delta G_i^{seg}}{RT})-1\right)}$$

#2

Coincidence Site Lattice (CSL) is a special grain boundary that occurs in polycrystalline materials and has matching lattice points between two adjacent particles.



The degree of fit(Σ) : draw the lattice for the 2 grains and count the number of atoms that are shared (coincidence sites), and the total number of atoms on the boundary (total number of site)

Σ=(volume of CSL unit cell)/(volume of standard crystal unit cell)

Characteristics of CSL Boundaries

Unlike other grain boundaries, CSL has high symmetry and a well-defined structure. In addition, CSL can act as a potential barrier and affect the grain growth of materials, changing mechanical properties.

Low-sigma CSLs' coordinates are low index directions (<110>, <111) where many atoms are arranged.

In conclusion, CSL boundaries are special types of particle boundaries with high symmetry. Occurs when the lattice points match between two adjacent particles. CSL boundaries have unique properties that make them different from other grain boundaries and have several applications in materials science and engineering. Understanding CSL boundaries is essential for designing materials with desired properties.