~~$(1 - X_1^\phi) X_n^B / X_n^\phi$~~

Homework #2

20222980 정대훈

Date No.

1.

$$\Delta W = {}^\circ G_1^\phi - {}^\circ G_1^B + RT\ln\frac{\gamma_1^\phi}{\gamma_1^B} + RT\ln\frac{X_1^\phi}{X_1^B}$$

$$\Delta W = {}^\circ G_2^\phi - {}^\circ G_2^B + RT\ln\frac{\gamma_2^\phi}{\gamma_2^B} + RT\ln\frac{X_2^\phi}{X_2^B}$$

$$\vdots$$

$$\Delta W = {}^\circ G_n^\phi - {}^\circ G_n^B + RT\ln\frac{\gamma_n^\phi}{\gamma_n^B} + RT\ln\frac{X_n^\phi}{X_n^B}$$

$$\rightarrow \begin{cases} X_1^\phi X_n^B = X_1^B X_n^\phi e^{-\Delta G_1^{seg}/RT} \\ X_2^\phi X_n^B = X_2^B X_n^\phi e^{-\Delta G_2^{seg}/RT} \\ \vdots \\ X_{n-1}^\phi X_n^B = X_{n-1}^B X_n^\phi e^{-\Delta G_{n-1}^{seg}/RT} \quad \cdots (1) \\ X_n^\phi X_n^B = X_n^B X_n^\phi \end{cases}$$

$$\rightarrow X_i^\phi = \frac{X_n^\phi}{X_n^B} X_i^B e^{-\Delta G_i^{seg}/RT} \quad \cdots (2)$$

from (1),

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

$$\rightarrow (X_1^\phi + X_2^\phi + \cdots + X_{n-1}^\phi + X_n^\phi) X_n^B = \sout{(X_1^B + X_2^B + \cdots + X_{n-1}^B) X_n^\phi e^{-\Delta G}}$$

$$\left(X_1^B e^{-\Delta G_1^{seg}/RT} + X_2^B e^{-\Delta G_2^{seg}/RT} + \cdots X_{n-1}^B e^{-\Delta G^{seg}/RT}\right) X_n^\phi + X_n^B$$

$$\rightarrow \frac{X_n^\phi}{X_n^B} = \frac{\sum_1^n X_j^\phi}{\sum_{j=1}^{n-1} X_j^B e^{-\Delta G_j^{seg}/RT} + X_n^B}$$

$$= \frac{1}{1 + \sum_{j=1}^{n-1} X_j^B (e^{-\Delta G_j^{seg}/RT} - 1)} \quad \cdots (3) \qquad (\because X_1^B + X_2^B + \cdots X_n^B = 1)$$

from (2) & (3),

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

MooKEUK

Date No.

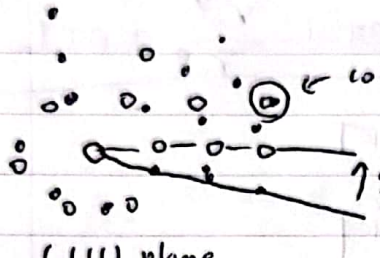
2.

Coincidence site lattice

: 두 격자를 회전시켰을 때 특정 각도에서 일치하는 부분이 생기는 격자 쌍.

- fraction of atoms in coincidence : density of ~~coincidence~~ coincidence sites

ex)



(twist boundary)

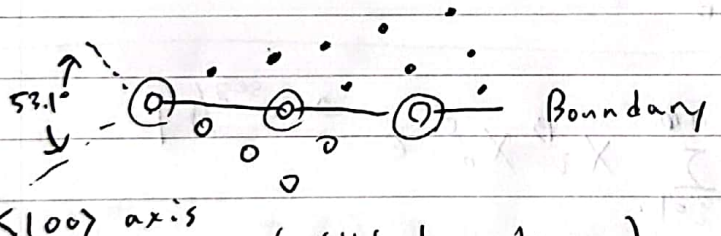
$N = 1^2+1^2+1^2 = 3$

$\Sigma = 2^2+1\times3 = 7$

coordinates of coincidence : (x, y) in (hkl) plane

→ $\Sigma = x^2+y^2N$ $(N = h^2+k^2+l^2)$

ex 2)



(tilt boundary)

$\Sigma = x^2+y^2 = 5$

Σ must have an odd number (ex) $\Sigma = 5$ $(x=3, y=1)$

→ $\frac{x^2+y^2}{2} = 5$

Boundary energy 가 다르다.

ex)