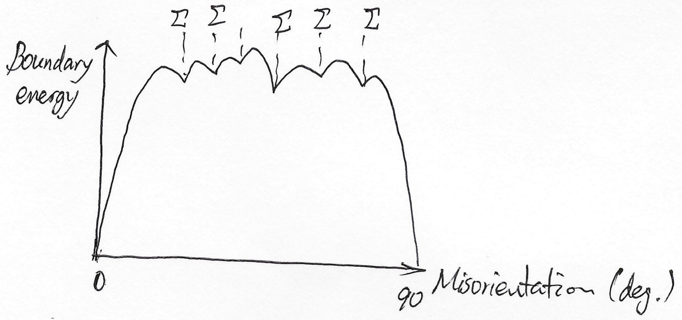
[AMSE 502] Phase Transformations

Problem Set #2 20202966 이정완

1. CSL boundaries, Coincidence site lattice boundaries are characterized by specific values of misorientation which allow atoms from neighboring lattices to notionally coincide, and the reciprocal density of coinciding sites is designated Σ. [1] which has low boundary energy. Generally, the improvement in properties was attributed to an increase in the proportion of low Σ CSL boundaries, which were referred to as 'special' boundaries.

This term Σ is defined as the relation between the number of lattice points in the unit cell of a CSL and the number of lattice points in a unit cell of the generating lattice. This is the unit cell volume of the CSL in units of the unit cell volume of the elementary cells of the crystals.



Reference

[1] V. Randle, Twinning-related grain boundary engineering, Acta Mater. 52 (2004) 4067-4081.

2. According to the interfacial phenomena,

from $\mu_i^\phi = \mu_i^B$ where μ is partial molar G.

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

We're going to use the hint given as $\sum_{i=1}^{n-1} X_i^\phi X_n^B = \sum_{j=1}^{n-1} X_j^B X_i^\phi e^{-\frac{\Delta G_j^{seg}}{RT}}$

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

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

$$(1-X_n^\phi) X_n^B = X_n^\phi \sum_{i=1}^{n-1} X_i^B e^{-\frac{\Delta G^{seg}}{RT}}$$

$$\therefore \frac{X_n^\phi}{X_n^B} = \frac{1-X_n^\phi}{\sum_{i=1}^{n-1} X_i^B e^{-\frac{\Delta G^{seg}}{RT}}}$$

From the given equation,

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

$$= \frac{X_i^B (1 - X_n^{\phi}) e^{-\frac{\Delta G^{seg}}{RT}}}{\sum_{i=1}^{n-1} X_i^B e^{-\frac{\Delta G^{seg}}{RT}}}$$

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

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

In here, we can say $X_n^B = 1 - \sum_{i=1}^{n-1} X_i^B$

$$X_i^{\phi}\left(\sum_{i=1}^{n-1} X_i^B e^{-\frac{\Delta G^{seg}}{RT}} + 1 - \sum_{i=1}^{n-1} X_i^B \right) = X_i^B e^{-\frac{\Delta G^{seg}}{RT}}$$

$$X_i^{\phi}\left\{ 1 + \sum_{i=1}^{n-1} X_i^B \left(e^{-\frac{\Delta G^{seg}}{RT}} - 1 \right) \right\} = X_i^B e^{-\frac{\Delta G^{seg}}{RT}}$$

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