Department of Materials Science and Engineering Pohang University of Science and Technology

AMSE502 Phase Transformations

due Date: Mar. 23, 2021Prof. Byeong-Joo LeeProblem Set #2calphad@postech.ac.kr

Room 1-311

- 1. Study and summarize CSL(coincidence site lattice) boundary.
- 2. 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)

$$\frac{X_i^{\phi}}{X_n^{\phi}} = \frac{X_i^B}{X_n^B} e^{-\Delta G^{seg}/RT} \quad \text{where} \quad \Delta G^{seg} = \left[{}^o G_i^{\phi} - {}^o G_i^B\right] - \left[{}^o G_n^{\phi} - {}^o G_n^B\right] + RT \ln \frac{\gamma_i^{\phi} \gamma_n^B}{\gamma_n^{\phi} \gamma_i^B}$$

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

$$X_{i}^{\phi} = \frac{X_{i}^{B} e^{-\Delta G_{i}^{seg}/RT}}{1 + \sum_{j=1}^{n-1} X_{j}^{B} (e^{-\Delta G_{j}^{seg}/RT} - 1)}$$
 Hint: use $\sum_{i=1}^{n-1} x_{i}^{\phi} x_{n}^{B} = \sum_{j=1}^{n-1} x_{j}^{B} x_{n}^{\phi} e^{-\Delta G_{j}^{seg}/RT}$