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

AMSE502   Phase Transformations

due Date: Oct. 04, 2012 _____ Prof. Byeong-Joo Lee

Problem Set #2   calphad@postech.ac.kr

Room 1- 311

1. Study and summarize CSL 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)

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

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

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