Series lectures of phase-field model

07. Curvature effect on equilibrium

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Curvature effect on equilibrium

- With adopting sharp interface assumption, the interface energy is

$$\sigma = \left(\frac{\delta G}{\delta A} \right)_{N_1, N_2, \cdots, T, p}$$

- The driving force for $\alpha \to \beta$ phase transformation, Δf_p is

$$\Delta f_p = f^\beta(c_\beta) - f^\alpha(c_\alpha) - (c_\beta - c_\alpha) \frac{df^\alpha(c_\alpha)}{dc} + \sigma \frac{\delta A}{\delta \Omega}$$

- Under the equilibrium, when curvature σ, we have

$$f^\beta(c_\beta) - f^\alpha(c_\alpha) - (c_\beta - c_\alpha) \frac{df^\alpha(c_\alpha)}{dc} + \sigma\kappa = 0 \qquad (1)$$

$$\frac{df^\alpha(c_\alpha)}{dc} = \frac{df^\beta(c_\beta)}{dc} = \text{const}$$

- Assume that curvature and interface energy does not depend on the concentration,

$$\frac{d\big(f^{\beta}(c_{\beta})+\sigma\kappa\big)}{dc}=\frac{d\big(f^{\alpha}(c_{\alpha})\big)}{dc}=\frac{\big(f^{\beta}(c_{\beta})+\sigma\kappa\big)-f^{\alpha}(c_{\alpha})}{c_{\beta}-c_{\alpha}}$$

or

$$\frac{d\big(f^{\beta}(c_{\beta})\big)}{dc}=\frac{d\big(f^{\alpha}(c_{\alpha})-\sigma\kappa\big)}{dc}=\frac{f^{\beta}(c_{\beta})-\big(f^{\alpha}(c_{\alpha})-\sigma\kappa\big)}{c_{\beta}-c_{\alpha}}$$

- Without curvature, $\sigma=0$, $R=\infty$, under the equilibrium,

$$f^{\beta}\left(c_{\beta}^{\mathsf{e}}\right)-f^{\alpha}\left(c_{\alpha}^{\mathsf{e}}\right)-\left(c_{\beta}^{\mathsf{e}}-c_{\alpha}^{\mathsf{e}}\right)\frac{df^{\alpha}\left(c_{\alpha}^{\mathsf{e}}\right)}{dc}=0$$

$$\frac{df^{\alpha}\left(c_{\alpha}^{\mathsf{e}}\right)}{dc}=\frac{df^{\beta}\left(c_{\beta}^{\mathsf{e}}\right)}{dc}$$

- The spherical β phase with curvature κ, we express the concentration at this situation as c_α^κ and c_β^κ.

$$f^\beta\left(c_\beta^\kappa\right) - f^\alpha\left(c_\alpha^\kappa\right) - \left(c_\beta^\kappa - c_\alpha^\kappa\right)\frac{df^\alpha\left(c_\alpha^\kappa\right)}{dc} + \sigma\kappa = 0 \qquad (2)$$

$$\frac{df^\alpha\left(c_\alpha^\kappa\right)}{dc} = \frac{df^\beta\left(c_\beta^\kappa\right)}{dc}$$

- By Taylor series, we have

$$f^p\left(c_p^\kappa\right) \simeq f^p\left(c_p^{\mathsf{e}}\right) + \frac{df^p\left(c_p^{\mathsf{e}}\right)}{dc}\left(c_p^\kappa - c_p^{\mathsf{e}}\right)$$

then Eq. 2 becomes

$$\left[f^\beta\left(c_\beta^{\mathsf{e}}\right) + \frac{df^\beta\left(c_\beta^{\mathsf{e}}\right)}{dc}\left(c_\beta^\kappa - c_\beta^{\mathsf{e}}\right)\right] - \left[f^\alpha\left(c_\alpha^{\mathsf{e}}\right) + \frac{df^\alpha\left(c_\alpha^{\mathsf{e}}\right)}{dc}\left(c_\alpha^\kappa - c_\alpha^{\mathsf{e}}\right)\right]$$
$$- \left(c_\beta^\kappa - c_\alpha^\kappa\right)\frac{df^\alpha\left(c_\alpha^\kappa\right)}{dc} + \sigma\kappa = 0$$

- With assumption

$$c_\beta^\kappa - c_\alpha^\kappa \simeq c_\beta^{\mathsf{e}} - c_\alpha^{\mathsf{e}}$$

we have

$$\frac{df^\beta\left(c_\beta^\kappa\right)}{dc} - \frac{df^\beta\left(c_\beta^{\mathsf{e}}\right)}{dc} = \frac{\sigma\kappa}{c_\beta^{\mathsf{e}} - c_\alpha^{\mathsf{e}}}$$

$$\frac{df^\alpha\left(c_\alpha^\kappa\right)}{dc} - \frac{df^\alpha\left(c_\alpha^{\mathsf{e}}\right)}{dc} = \frac{\sigma\kappa}{c_\beta^{\mathsf{e}} - c_\alpha^{\mathsf{e}}}$$

- With assumptions

$$\frac{df^p\left(c_p^\kappa\right)}{dc} \simeq \frac{df^p\left(c_p^{\mathsf{e}}\right)}{dc} + \frac{d^2 f^p\left(c_p^{\mathsf{e}}\right)}{dc^2}\left(c_p^\kappa - c_p^{\mathsf{e}}\right)$$

Finally, we have

$$c_\beta^\kappa - c_\beta^{\mathsf{e}} = \frac{\sigma\kappa}{\left(c_\beta^{\mathsf{e}} - c_\alpha^{\mathsf{e}}\right)\left(d^2 f^\beta\left(c_\beta^{\mathsf{e}}\right)/dc^2\right)}$$

$$c_\alpha^\kappa - c_\alpha^{\mathsf{e}} = \frac{\sigma\kappa}{\left(c_\beta^{\mathsf{e}} - c_\alpha^{\mathsf{e}}\right)\left(d^2 f^\alpha\left(c_\alpha^{\mathsf{e}}\right)/dc^2\right)}$$