Series lectures of phase-field model

06. Interface energy of an alloy

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November 21, 2024

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Interface energy of an alloy

- The free energy of $\alpha - \beta$ two phases system per volume is

$$G_\mathsf{a} = \Omega_\alpha f^\alpha\left(c_\alpha^\mathsf{e}\right) + \Omega_\beta f^\beta\left(c_\beta^\mathsf{e}\right) + G^\mathsf{xs}$$

- There are excess solute atoms near the interface, and G^xs exists by these atoms.

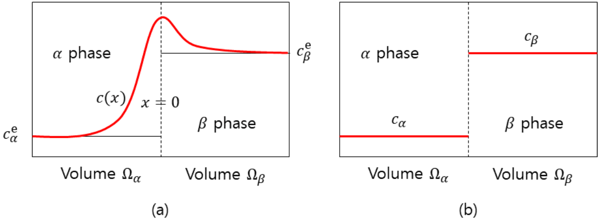

Figure: Profiles of concentration within two phase system (a) With interface (b) Without interface

- Total moles of solute at interface is given by

$$\Gamma^{\mathsf{xs}} = \frac{\Omega_\alpha}{v_m}\int_{-\infty}^{0}\left(c(x) - c_\alpha^{\mathsf{e}}\right)dx + \frac{\Omega_\beta}{v_m}\int_{0}^{\infty}\left(c(x) - c_\beta^{\mathsf{e}}\right)dx$$

- The interface energy when the area of interface A is given by

$$\sigma = \frac{\Omega_\alpha}{A}\left[f^\alpha(c_\alpha^{\mathsf{e}}) - f^\alpha(c_\alpha)\right] + \frac{\Omega_\beta}{A}\left[f^\beta(c_\beta^{\mathsf{e}}) - f^\beta(c_\beta)\right] + \frac{G^{\mathsf{xs}}}{A}$$

- To conserve number of solute atoms,

$$\frac{1}{v_m}\left(c_\alpha^{\mathsf{e}}\Omega_\alpha + c_\beta^{\mathsf{e}}\Omega_\beta\right) + \Gamma^{\mathsf{xs}} = \frac{1}{v_m}\left(c_\alpha\Omega_\alpha + c_\beta\Omega_\beta\right)$$

or

$$\left(c_\alpha^{\mathsf{e}} - c_\alpha\right)\Omega_\alpha + \left(c_\beta^{\mathsf{e}} - c_\beta\right)\Omega_\beta = -v_m\Gamma^{\mathsf{xs}} \tag{1}$$

- By Taylor's series, we take the first term

$$f^{\alpha}(c_{\alpha}) = f^{\alpha}(c_{\alpha}^{\mathsf{e}}) + (c_{\alpha} - c_{\alpha}^{\mathsf{e}})\frac{df^{\alpha}(c_{\alpha})}{dc}$$

$$f^{\beta}(c_{\beta}) = f^{\beta}(c_{\beta}^{\mathsf{e}}) + (c_{\beta} - c_{\beta}^{\mathsf{e}})\frac{df^{\beta}(c_{\beta})}{dc}$$

then the interface energy is

$$\sigma = \frac{\Omega_{\alpha}}{A}(c_{\alpha}^{\mathsf{e}} - c_{\alpha})\frac{df^{\alpha}(c_{\alpha})}{dc} + \frac{\Omega_{\beta}}{A}(c_{\beta}^{\mathsf{e}} - c_{\beta})\frac{df^{\beta}(c_{\beta})}{dc} + \frac{G^{\mathsf{xs}}}{A}$$

- With common tangent condition, we have

$$\sigma = \frac{1}{A}\Big(\Omega_{\alpha}(c_{\alpha}^{\mathsf{e}} - c_{\alpha}) + \Omega_{\beta}(c_{\beta}^{\mathsf{e}} - c_{\beta})\Big)\tilde{\mu}^{\mathsf{e}} + \frac{G^{\mathsf{xs}}}{A}$$

- With Eq. 1,

$$\sigma = \frac{G^{\mathsf{xs}}}{A} - v_m\frac{\Gamma^{\mathsf{xs}}}{A}\tilde{\mu}^{\mathsf{e}} \tag{2}$$