Series lectures of phase-field model

05. Interfacial Energy from diffused interfafce profile

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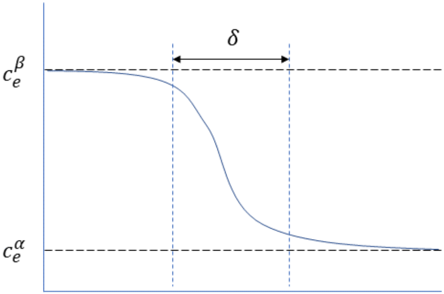
Interfacial Energy of diffused interface

- Compute the interfacial profile through a planar interface.
- Free energy of the interface is the excess energy associated with the interface, subtract from F the energy associate uniform composition up to the interface.

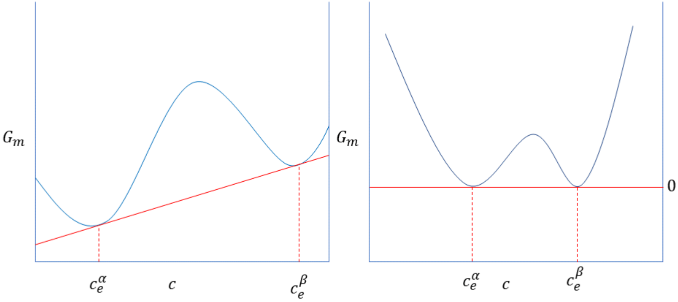
$$F = A \int \left[f(c) + \kappa \left(\frac{dc}{dx} \right)^2 \right] dx$$



- Interface energy is given by

$$\sigma = \frac{F^{\text{nonuniform}} - F^{\text{uniform}}}{A} = \int_{-\infty}^{\infty} \left[f(c) + \kappa \left(\frac{dc}{dx} \right)^2 \right] dx$$

- To minimize F, σ have to be minimized.



Interfacial Energy of diffused interface

- To obtain $c(x)$ within the interface region, we get Euler-Lagrange equation

$$\frac{\delta\sigma}{\delta c} = \frac{\partial f(c)}{\partial c} - 2\kappa\frac{d^2 c}{dx^2} = 0$$

enforce conservation of mass by saying the composition go to the equilibrium compositions at $\pm\infty$.

- Integrate the Euler-Lagrange equation

$$\int \frac{\partial f(c)}{\partial c} dc - 2\kappa \int \frac{d^2 c}{dx^2} dc = A$$

$$f(c) - 2\kappa \int \frac{d^2 c}{dx^2}\frac{dc}{dx} dx = A$$

we have

$$\frac{d}{dx}\left(\frac{dc}{dx}\right)^2 = 2\frac{dc}{dx}\frac{d^2 c}{dx^2}$$

- Finally,

$$f(c) - \kappa \left(\frac{dc}{dx} \right)^2 = A$$

- In the limit $x \to \pm\infty$

$$\frac{dc}{dx} \to 0 \qquad\qquad f(c) \to 0$$

$$f(c) - \kappa \left(\frac{dc}{dx} \right)^2 = 0 \to f(c) = \kappa \left(\frac{dc}{dx} \right)^2$$

$$\sigma = \int_{-\infty}^{\infty} \left[f(c) + \kappa \left(\frac{dc}{dx} \right)^2 \right] dx = \int_{-\infty}^{\infty} \left[2\kappa \left(\frac{dc}{dx} \right)^2 \right] dx$$