Series lectures of phase-field model

04. Cahn-Hilliard Equation II

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Solution for small fluctuation case

- Assume the small fluctuation,

$$c(x,t) = c_0 + \varepsilon\tilde{c}(x,t) \qquad \varepsilon \ll 1$$

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial t}\left(c_0 + \varepsilon\tilde{c}(x,t)\right) = \varepsilon\frac{\partial \tilde{c}}{\partial t}$$

$$\frac{\partial^4 c}{\partial x^4} = \frac{\partial^4}{\partial x^4}\left(c_0 + \varepsilon\tilde{c}(x,t)\right) = \varepsilon\frac{\partial^4 \tilde{c}}{\partial x^4}$$

- By Taylor series

$$\frac{\partial^2 f(c)}{\partial c^2} = \left.\frac{\partial^2 f}{\partial c^2}\right|_{c_0} + \left.\frac{\partial^3 f}{\partial c^3}\right|_{c_0}\varepsilon\tilde{c}(x,t)$$

$$\frac{\partial}{\partial x}\left(\frac{\partial^2 f}{\partial c^2}\frac{\partial c}{\partial x}\right) = \frac{\partial}{\partial x}\left[\left(\left.\frac{\partial^2 f}{\partial c^2}\right|_{c_0} + \left.\frac{\partial^3 f}{\partial c^3}\right|_{c_0}\varepsilon\tilde{c}(x,t)\right)\varepsilon\frac{\partial \tilde{c}}{\partial x}\right]$$

$$= \frac{\partial}{\partial x}\left(\left.\frac{\partial^2 f}{\partial c^2}\right|_{c_0}\varepsilon\frac{\partial \tilde{c}}{\partial x}\right) + \frac{\partial}{\partial x}\left(\left.\frac{\partial^3 f}{\partial c^3}\right|_{c_0}\cancel{\varepsilon^2}\tilde{c}(x,t)\frac{\partial \tilde{c}}{\partial x}\right)$$

- Therefore,

$$\varepsilon\frac{\partial \tilde{c}}{\partial t} = M\left[\varepsilon\left(\left.\frac{\partial^2 f}{\partial c^2}\right|_{c_0}\frac{\partial^2 \tilde{c}}{\partial x^2}\right) - 2\varepsilon\kappa\frac{\partial^4 \tilde{c}}{\partial x^4}\right]$$

- Let

$$f''(c_0) = \left.\frac{\partial^2 f}{\partial c^2}\right|_{c_0}$$

then we have

$$\frac{\partial \tilde{c}}{\partial t} = M\left[\left(f''(c_0)\frac{\partial^2 \tilde{c}}{\partial x^2}\right) - 2\kappa\frac{\partial^4 \tilde{c}}{\partial x^4}\right]$$

- Recall Fourier transform,

$$\tilde{c}(x,t) = \int_{-\infty}^{\infty}\Phi(k,t)e^{-ikx}dk$$

$$\Phi(k,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\tilde{c}(x,t)e^{ikx}dx$$

- Take forward Fourier transform

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\partial\tilde{c}}{\partial t}e^{ikx}dx = \frac{1}{2\pi}\frac{d}{dt}\int_{-\infty}^{\infty}\tilde{c}(x,t)e^{ikx}dx = \frac{1}{2\pi}\frac{d\Phi(k,t)}{dt}$$

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\partial^2\tilde{c}e^{ikx}}{\partial x^2}dx = -\frac{k^2}{2\pi}\Phi(k,t)$$

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\partial^4\tilde{c}e^{ikx}}{\partial x^4}dx = \frac{k^4}{2\pi}\Phi(k,t)$$

- Then Cahn-Hilliard equation becomes

$$\frac{d\Phi(k,t)}{dt} = -M\left[k^2 f''(c_0) + 2\kappa k^4\right]\Phi(k,t)$$

- Initial condition is

$$\Phi(k,0) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\tilde{c}(x,0)e^{ikx}dx$$

- The solution is

$$\Phi(k,t) = \Phi(k,0)\exp\Big[-M(f''k^2 + 2\kappa k^4)t\Big]$$

- Finally, we can calculate fluctuation

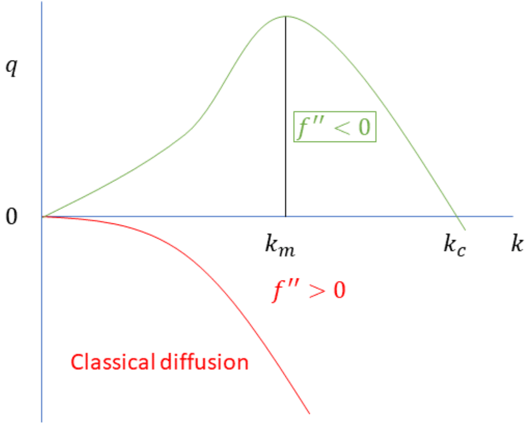
$$\tilde{c}(x,t) = \int_{-\infty}^{\infty} \Phi(k,0)\exp\big[-M(f''k^2 + 2\kappa k^4)t\big]\exp\left(-ikx\right)dk$$

- Whether a fluctuation grow or shrink depends on sign of $-M(f''k^2 + 2\kappa k^4)$.
- Introduce the amplification factor

$$q = -M(f''k^2 + 2\kappa k^4) = -D\left(k^2 + \frac{2\kappa}{f''}k^4\right) \qquad D = Mf''$$

- κ regularizes the diffusion equation.

$$q(k_c) = 0 \qquad \left.\frac{dq}{dk}\right|_{k=k_m} = 0$$



- k_m is the wave number with maximum growth rate.
- When $k > k_c$, then $q < 0$ means all fluctuation will shrink.
- When $k < k_c$, all fluctuation will grow.

$$f''k_c^2 + 2\kappa k_c^4 = 0 \rightarrow k_c^2(f'' + 2\kappa k_c^2) = 0$$

$$k_c = \sqrt{-\frac{f''}{2\kappa}}$$

$$\left.\frac{dq}{dk}\right|_{k=k_m} = 0 \rightarrow 2k_m f'' + 8\kappa k_m^3 = 0$$

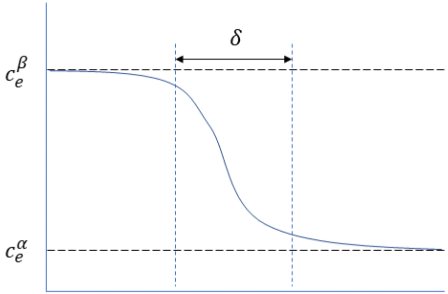
$$2k_m(f'' + 4\kappa k_m^2) = 0$$

$$k_m = \sqrt{-\frac{f''}{4\kappa}} = \frac{k_c}{\sqrt{2}}$$

Diffused interface approach

- 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.

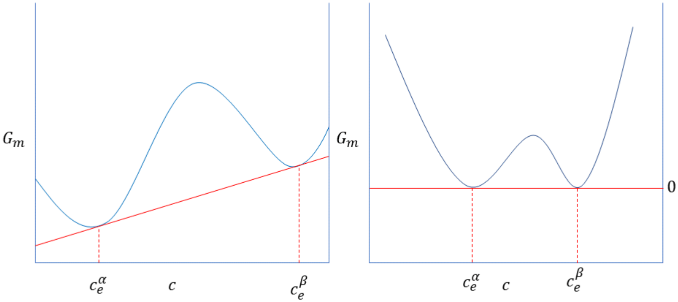
$$F = A \int \left[f(c) + \kappa \left(\frac{dc}{dx} \right)^2 \right] dx$$



- 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.



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

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

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

- Integrate the Euler-Lagrange equation

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

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

we have

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

finally,

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

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

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

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

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

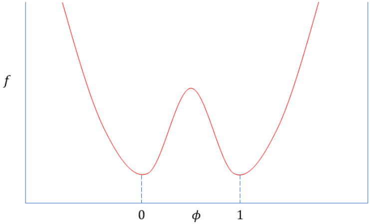
Analytic solution for double well potential

- Start from

$$\sigma = 2\kappa \int_{-\infty}^{\infty} \left(\frac{dc}{dx}\right)^2 \qquad\qquad f(c) - \kappa\left(\frac{dc}{dx}\right)^2 = 0$$

- To obtain analytic solution, we do not use regular solution model. We will use polynomial approximation, so called Landau expansions.

$$\phi = \frac{c - c_e^\alpha}{c_e^\beta - c_e^\alpha} \qquad f = A\phi^2(1-\phi)^2$$



- To obtain the equilibrium value,

$$\frac{\partial f}{\partial \phi} = 0 \rightarrow \phi = 1, 0, \frac{1}{2}$$

- E-L equation becomes

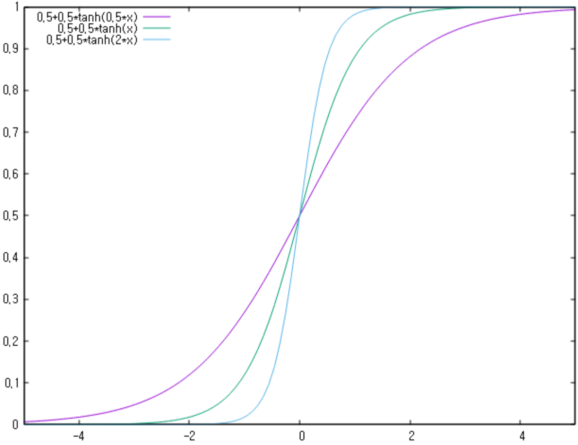
$$f(\phi) - \kappa\left(\frac{d\phi}{dx}\right)^2 = A\phi^2(1-\phi)^2 - \kappa\left(\frac{d\phi}{dx}\right)^2 = 0$$

$$\left(\frac{d\phi}{dx}\right)^2 = \left[\frac{A\phi^2(1-\phi)^2}{\kappa}\right] \rightarrow \frac{d\phi}{dx} = \sqrt{\frac{A}{\kappa}}\phi(1-\phi)$$

$$\int \frac{d\phi}{\phi(1-\phi)} = \int \sqrt{\frac{A}{\kappa}}dx \rightarrow -2\tanh^{-1}(1-2\phi) = \sqrt{\frac{A}{\kappa}}x$$

$$2\phi - 1 = \tanh\left[\sqrt{\frac{A}{\kappa}}\frac{x}{2}\right]$$

$$\phi = \frac{1}{2} + \frac{1}{2}\tanh\left[\frac{x}{2\delta}\right] \quad \text{where} \quad \delta = \sqrt{\frac{\kappa}{A}}$$



0.5+0.5*tanh(0.5*x)
0.5+0.5*tanh(x)
0.5+0.5*tanh(2*x)
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-4
-2
0
2
4

- To evaluate interfacial energy

$$\sigma = 2\kappa \int_{-\infty}^{\infty} \left(\frac{d\phi}{dx}\right)^2$$

$$\frac{d\phi}{dx} = \frac{1}{2}\left[1 - \tanh^2\left(\frac{x}{2\delta}\right)\right]\frac{1}{2\delta} = \frac{1}{4\delta}\left[1 - \tanh^2\left(\frac{x}{2\delta}\right)\right]$$

- Therefore,

$$\begin{aligned}
\sigma &= 2\int_{-\infty}^{\infty} \frac{\kappa}{16\delta^2}\left[1 - \tanh^2\left(\frac{2}{2\delta}\right)\right]^2 dx \\
&= \frac{\kappa}{8\delta^2}\int_{-\infty}^{\infty} \mathrm{sech}^4\left(\frac{x}{2\delta}\right) dx \\
&= \frac{\kappa}{3\delta} = \frac{\sqrt{A\kappa}}{3}
\end{aligned}$$