Series lectures of phase-field model

13. Phase-field method with elasticity

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Phase-field method with elasticity

- The eigenstrain is given by

$$\varepsilon^{\circ}_{ij} = \varepsilon\delta_{ij}$$

- For spinodal decomposition, we generally assumes that

$$\varepsilon^{\circ}_{ij} = \eta(c - c_0)\delta_{ij}$$

where

$$\eta = \frac{1}{a}\frac{da}{dc}$$

a is the lattice parameter.

- The stress is

$$\sigma_{ij} = C_{ijkl}\big(\varepsilon_{kl} - \eta(c - c_0)\delta_{kl}\big)$$

Incorporate elasticity in free energy

- The free energy for Cahn-Hilliard equation with consideration of elasticity is

$$F = \int_V \left[f(c) + \underbrace{W_e(\varepsilon_{ij}, c)}_{\text{elastic effect}} + \kappa |\nabla c|^2 \right] dV$$

- To make total amount of c conserved,

$$\int (c - c_0) dV = 0$$

- Finally, we reach

$$F = \int_V \left[f(c) + W_e(\varepsilon_{ij}, c) + \kappa |\nabla c|^2 - \lambda (c - c_0) \right] dV$$

- At equilibrium

$$\delta \int W_e(\varepsilon_{ij}, c)dV = 0$$
$$= \int \left[\frac{\partial W_e}{\partial \varepsilon_{ij}}\delta\varepsilon_{ij} + \frac{\partial W_e}{\partial c}\delta c\right]dV \quad (1)$$
$$= \int \left[\sigma_{ij}\delta\varepsilon_{ij} + \frac{\partial W_e}{\partial c}\delta c\right]dV$$

- First term of RHS of (1) is

$$\int \sigma_{ij}\delta\varepsilon_{ij}dV = \int \sigma_{ij}\frac{1}{2}\delta(u_{i,j} + u_{j,i})dV$$
$$= \int \sigma_{ij}\delta u_{i,j}dV = \int \sigma_{ij}(\delta u_i)_{,j}dV \quad (2)$$

For further development,

$$(\sigma_{ij}\delta u_i)_{,j} = \sigma_{ij,j}\delta u_i + \sigma_{ij}(\delta u_i)_{,j} \quad (3)$$

- By divergence theorem,

$$\int (\sigma_{ij}\delta u_i)_{,j} dV = \int \sigma_{ij} n_j \delta u_i dS \tag{4}$$

- Combine (2) to (4),

$$\begin{aligned}\int \sigma_{ij}\delta\varepsilon_{ij} dV &= \int \sigma_{ij}(\delta u_i)_{,j} dV = \int (\sigma_{ij}\delta u_i)_{,j} dV - \int \sigma_{ij,j}\delta u_i dV \\ &= \int \sigma_{ij} n_j \delta u_i dS - \int \sigma_{ij,j}\delta u_i dV\end{aligned} \tag{5}$$

- The elastic energy

$$
\begin{aligned}
W_e &= \frac{1}{2}\sigma_{kl}\varepsilon^e_{kl} = \frac{1}{2}C_{ijkl}\varepsilon^e_{ij}\varepsilon^e_{kl} \\
&= \frac{1}{2}C_{ijkl}(\varepsilon_{ij} - \eta(c - c_0)\delta_{ij})(\varepsilon_{kl} - \eta(c - c_0)\delta_{kl})
\end{aligned}
$$

- The derivative

$$
\begin{aligned}
\left.\frac{W_e}{\partial c}\right|_{\varepsilon_{ij}} &= \frac{1}{2}C_{ijkl}\Big[-\eta\delta_{ij}(\varepsilon_{kl} - \eta(c - c_0)\delta_{kl}) \\
&\quad - \eta\delta_{kl}(\varepsilon_{ij} - \eta(c - c_0)\delta_{ij})\Big] \\
&= -C_{ijkl}\eta\delta_{ij}(\varepsilon_{kl} - \eta(c - c_0)\delta_{kl}) \\
&= -C_{jjkl}\eta(\varepsilon_{kl} - \eta(c - c_0)\delta_{kl}) \\
&= -\eta\sigma_{jj}
\end{aligned}
$$

- Derivative of the free energy becomes

$$\delta F = \int \left[\left[\frac{\partial f}{\partial c} - \kappa \nabla^2 c - \eta \sigma_{jj} - \lambda \right] \delta c - \sigma_{ij,j} \delta u_j \right] dV + \int \sigma_{ij} n_j \delta u_i dS = 0$$

To satisfy it,

$$\lambda = \frac{\partial f}{\partial c} - \kappa \nabla^2 c - \eta \sigma_{jj} \qquad \sigma_{ij,j} = 0 \qquad \sigma_{ij} n_j |_{\Omega} = 0$$

- Since

$$\mathbf{J} = -M \nabla \lambda \qquad \frac{\partial c}{\partial t} = \nabla \cdot \mathbf{J}$$

$$\frac{\partial c}{\partial t} = M \left[\frac{\partial^2 f}{\partial c^2} \nabla^2 c - \eta \nabla^2 \sigma_{jj} - \kappa \nabla^4 c \right]$$

Mechanical equilibrium condition

- How do we determine σ_{ij}?

$$\sigma_{ij,j} = 0 \tag{6}$$

$$\sigma_{ij} = C_{ijkl}\big(\varepsilon_{kl} - \eta\delta_{kl}(c - c_0)\big) = C_{ijkl}\big(u_{k,l} - \eta\delta_{kl}(c - c_0)\big)$$

$$\sigma_{ij,j} = C_{ijkl}\big(u_{k,lj} - \eta c_{,j}\delta_{kl}\big) \tag{7}$$

$$c_{,j} = \frac{\partial c}{\partial x_j}$$

- Combining (6) and (7), we reach

$$C_{ijkl}u_{k,lj} = C_{ijkl}\eta c_{,j}\delta_{kl} \tag{8}$$

Linear equation for $u_{k,lj}$, however it is coupled.

- Coupled linear problem can be relatively easily approached by the Fourier transform.

- Fourier transforms, not worry about boundaries at ∞.

$$u_{k,lj} = \frac{\partial^2 u_k}{\partial x_l \partial x_j}$$

- Take Fourier transforms of $u_{k,lj}$

$$\int \frac{\partial^2 u_k}{\partial x_l \partial x_j} e^{-i\mathbf{k}\cdot\mathbf{x}} d\mathbf{x} = -k_l k_j \tilde{u}_k$$

- (8) can be rewritten after taking Fourier transform,

$$C_{ijkl} k_l k_j \tilde{u}_k(\mathbf{k}) = i\eta C_{ijkl} k_j \tilde{c}(\mathbf{k}) \delta_{kl}$$

- Three equations ($k = 1, 2, 3$) for three unknowns.

Cramer's rule

- For the linear problem

$$\mathbf{A}\tilde{\mathbf{U}} = \mathbf{b}$$

where

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \quad \tilde{\mathbf{U}} = \begin{bmatrix} \tilde{u}_1 \\ \tilde{u}_2 \\ \tilde{u}_3 \end{bmatrix} \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

$\mathbf{A}^i$ is a matrix with column i replaced by $\mathbf{b}$.

$$\tilde{u}_i = \frac{|\mathbf{A}^i|}{|\mathbf{A}|}$$

$$A_{ik} = C_{ijkl} k_l k_j$$

$$|\mathbf{A}^i| = b_i N_{ij}$$

where N_{ij} is the cofactor matrix.

- Proceed to

$$|\mathbf{A}^1| = \begin{bmatrix} b_1 & a_{12} & a_{13} \\ b_2 & a_{22} & a_{23} \\ b_3 & a_{32} & a_{33} \end{bmatrix} = b_1 \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} + b_2 \begin{vmatrix} a_{12} & a_{13} \\ a_{32} & a_{33} \end{vmatrix} + b_3 \begin{vmatrix} a_{12} & a_{13} \\ a_{22} & a_{23} \end{vmatrix}$$

$$|\mathbf{A}^i| = iC_{jlmk}\delta_{mk}\eta\tilde{c}(\mathbf{k})k_l N_{ij}$$

$$\tilde{u}_i(\mathbf{k}) = iC_{jlmm}\eta k_l \tilde{c}(\mathbf{k}) \frac{N_{ij}}{|\mathbf{A}|}$$

Introduce $\Omega_{ij} = \frac{N_{ij}}{|\mathbf{A}|}$

$$\tilde{u}_i(\mathbf{k}) = iC_{jlmm}\eta k_l \tilde{c}(\mathbf{k})\Omega_{ij}$$

Finally we have

$$\sigma_{rs} = C_{rskl}\big(u_{k,l}(\mathbf{x}) - \eta(c(\mathbf{x}) - c_0)\delta_{kl}\big)$$

with

$$u_k(\mathbf{x}) = \int \tilde{u}_k(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{k} \qquad c(\mathbf{x}) - c_0 = \int \tilde{c}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{k}$$

- Proceed to

$$\sigma_{rs}(\mathbf{x}) = C_{rskl}\left[i\int k_l \tilde{u}_k(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{k} - \eta\int \tilde{c}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}\delta_{kl}d\mathbf{k}\right]$$

$$= C_{rskl}\left[\eta\int C_{jnmm}k_l k_n \Omega_{kj}\tilde{c}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{k} - \eta\int \tilde{c}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}\delta_{kl}d\mathbf{k}\right]$$

$$= C_{rskl}\eta\int\left[C_{jnmm}k_l k_n \Omega_{kj} - \delta_{kl}\right]\tilde{c}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{k}$$

- Then Cahn-Hilliard equation becomes

$$\frac{\partial c}{\partial t} = M\left[f''(c)c_{,ii} - \eta\sigma_{kk,ii} - \kappa c_{,iiii}\right]$$

- Take Fourier transform

$$\sigma_{rs}(\mathbf{x}) = \int \tilde{\sigma}_{rs}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} d\mathbf{k}$$

$$\sigma_{rs,ii}(\mathbf{x}) = -\int k^2 \tilde{\sigma}_{rs}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} d\mathbf{k}$$
$$= -\int k^2 \eta C_{rsoi} \Big[C_{jlmn} k_l k_i \Omega_{oj} - \delta_{oj} \Big] \tilde{c}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} d\mathbf{k}$$

$$\sigma_{kk,ii}(\mathbf{x}) = -\int k^2 \eta B(\mathbf{k}) \tilde{c}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} d\mathbf{k}$$

where

$$B(\mathbf{k}) = -C_{kkoi} \Big[C_{jlmm} k_l k_j \Omega_{oj} - \delta_{oj} \Big]$$

- We have the relation

$$c(\mathbf{x}, t) = \hat{c}(\mathbf{x}) e^{q(\mathbf{k})t}$$

- Cahn-Hillard equation becomes

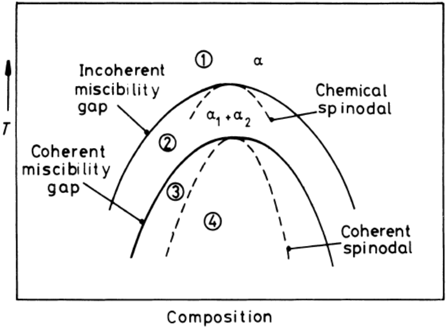
$$\frac{\partial \hat{c}(\mathbf{x})}{\partial t} = -M\left[(f'' + B(\mathbf{k})\eta^2)k^2 + \kappa k^4\right]\hat{c}(\mathbf{x})$$

where

$$q(\mathbf{k}) = -M\left[(f'' + B(\mathbf{k})\eta^2)k^2 + \kappa k^4\right]$$

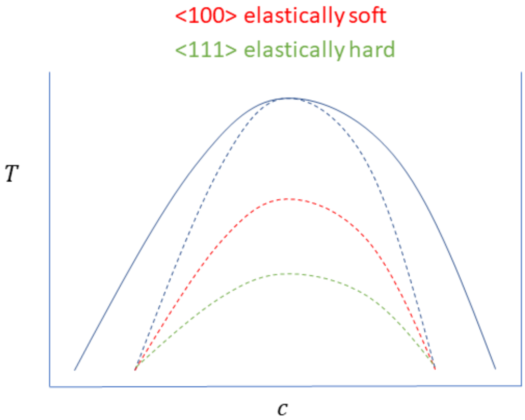
$q(\mathbf{k})$ now depends on the crystallography.

- If
$$f'' + \eta^2 B(\mathbf{k}) + \kappa k^2 < 0$$
hold for all k,
$$f'' + \eta^2 B(\mathbf{k}) < 0$$
if $f'' < 0$, $B(\mathbf{k}) > 0$ then it is possible for the system to be stable even though $f'' < 0$



- $B(\mathbf{k})$ can be anisotropic.
- For cubic crystal the anisotropy factor is

$$2C_{44} - C_{11} + C_{12}$$



- For cubic crystal, we can generally say

$$B(\mathbf{k}) = \frac{1}{2}(C_{11} + 2C_{12})\eta^2 \left[3 - \frac{C_{11} + 2C_{12}}{C_{11} + 2(2C_{44} - C_{11} + C_{12})(k_1^2 k_2^2 + k_3^2 k_2^2 + k_1^2 k_3^2)} \right]$$