

PRISMS-PF: Precipitate Evolution

1 Variational formulation

The total free energy of the system (neglecting boundary terms) is of the form,

$$\Pi(c, \eta_1, \eta_2, \eta_3, \epsilon) = \int_{\Omega} f(c, \eta_1, \eta_2, \eta_3, \epsilon) dV \quad (1)$$

where c is the concentration of the β phase, η_p are the structural order parameters and ϵ is the small strain tensor. f , the free energy density is given by

$$f(c, \eta_1, \eta_2, \eta_3, \epsilon) = f_{chem}(c, \eta_1, \eta_2, \eta_3) + f_{grad}(\eta_1, \eta_2, \eta_3) + f_{elastic}(c, \eta_1, \eta_2, \eta_3, \epsilon) \quad (2)$$

where

$$f_{chem}(c, \eta_1, \eta_2, \eta_3) = f_{\alpha}(c) (1 - H(\eta_1) - H(\eta_2) - H(\eta_3)) + f_{\beta}(c) (H(\eta_1) + H(\eta_2) + H(\eta_3)) + W f_{Landau}(\eta_1, \eta_2, \eta_3) \quad (3)$$

$$f_{grad}(\eta_1, \eta_2, \eta_3) = \frac{1}{2} \sum_{p=1}^3 \kappa_{ij}^{\eta_p} \eta_{p,i} \eta_{p,j} \quad (4)$$

$$f_{elastic}(c, \eta_1, \eta_2, \eta_3, \epsilon) = \frac{1}{2} \mathbf{C}_{ijkl}(\eta_1, \eta_2, \eta_3) (\epsilon_{ij} - \epsilon_{ij}^0(c, \eta_1, \eta_2, \eta_3)) (\epsilon_{kl} - \epsilon_{kl}^0(c, \eta_1, \eta_2, \eta_3)) \quad (5)$$

$$\epsilon^0(c, \eta_1, \eta_2, \eta_3) = H(\eta_1) \epsilon_{\eta_1}^0(c) + H(\eta_2) \epsilon_{\eta_2}^0(c) + H(\eta_3) \epsilon_{\eta_3}^0(c) \quad (6)$$

$$\mathbf{C}(\eta_1, \eta_2, \eta_3) = H(\eta_1) \mathbf{C}_{\eta_1} + H(\eta_2) \mathbf{C}_{\eta_2} + H(\eta_3) \mathbf{C}_{\eta_3} + (1 - H(\eta_1) - H(\eta_2) - H(\eta_3)) \mathbf{C}_{\alpha} \quad (7)$$

Here $\epsilon_{\eta_p}^0$ are the composition dependent stress free strain transformation tensor corresponding to each structural order parameter.

2 Required inputs

- $f_{\alpha}(c), f_{\beta}(c)$ - Homogeneous chemical free energy of the components of the binary system, example form given in Appendix I
- $f_{Landau}(\eta_1, \eta_2, \eta_3)$ - Landau free energy term that controls the interfacial energy and prevents precipitates with different orientation variants from overlapping, example form given in Appendix I
- W - Barrier height for the Landau free energy term, used to control the thickness of the interface
- $H(\eta_p)$ - Interpolation function for connecting the α phase and the p^{th} orientation variant of the β phase, example form given in Appendix I
- κ^{η_p} - gradient penalty tensor for the p^{th} orientation variant of the β phase
- \mathbf{C}_{η_p} - fourth order elasticity tensor (or its equivalent second order Voigt representation) for the p^{th} orientation variant of the β phase
- \mathbf{C}_{α} - fourth order elasticity tensor (or its equivalent second order Voigt representation) for the α phase
- $\epsilon_{\eta_p}^0$ - stress free strain transformation tensor for the p^{th} orientation variant of the β phase

In addition, to drive the kinetics, we need:

- M - mobility value for the concentration field
- L - mobility value for the structural order parameter field

3 Variational treatment

From the variational derivatives given in Appendix II, we obtain the chemical potentials for the concentration and the structural order parameters:

$$\mu_c = f_{\alpha,c} (1 - H(\eta_1) - H(\eta_2) - H(\eta_3)) + f_{\beta,c} (H(\eta_1) + H(\eta_2) + H(\eta_3)) + \mathbf{C}_{ijkl}(-\varepsilon_{ij,c}^0) (\varepsilon_{kl} - \varepsilon_{kl}^0) \quad (8)$$

$$\mu_{\eta_p} = (f_{\beta} - f_{\alpha})H(\eta_p)_{,\eta_p} + W f_{Landau,\eta_p} - \kappa_{ij}^{\eta_p} \eta_{p,ij} + \mathbf{C}_{ijkl}(-\varepsilon_{ij,\eta_p}^0) (\varepsilon_{kl} - \varepsilon_{kl}^0) + \frac{1}{2} \mathbf{C}_{ijkl,\eta_p} (\varepsilon_{ij} - \varepsilon_{ij}^0) (\varepsilon_{kl} - \varepsilon_{kl}^0) \quad (9)$$

4 Kinetics

Now the PDE for Cahn-Hilliard dynamics is given by:

$$\frac{\partial c}{\partial t} = -\nabla \cdot (M \nabla \mu_c) \quad (10)$$

and the PDE for Allen-Cahn dynamics is given by:

$$\frac{\partial \eta_p}{\partial t} = -L \mu_{\eta_p} \quad (11)$$

where M and L are the constant mobilities.

5 Mechanics

Considering variations on the displacement u of the form $u + \epsilon w$, we have

$$\delta_u \Pi = \int_{\Omega} \nabla w : \mathbf{C}(\eta_1, \eta_2, \eta_3) : (\varepsilon - \varepsilon^0(c, \eta_1, \eta_2, \eta_3)) \, dV = 0 \quad (12)$$

$$(13)$$

where $\boldsymbol{\sigma} = \mathbf{C}(\eta_1, \eta_2, \eta_3) : (\varepsilon - \varepsilon^0(c, \eta_1, \eta_2, \eta_3))$ is the stress tensor.

Now consider

$$R = \int_{\Omega} \nabla w : \mathbf{C}(\eta_1, \eta_2, \eta_3) : (\varepsilon - \varepsilon^0(c, \eta_1, \eta_2, \eta_3)) \, dV = 0 \quad (14)$$

We solve for $R = 0$ using a gradient scheme which involves the following linearization:

$$R|_u + \frac{\delta R}{\delta u} \Delta u = 0 \quad (15)$$

$$\Rightarrow \frac{\delta R}{\delta u} \Delta u = -R|_u \quad (16)$$

This is the linear system $Ax = b$ which we solve implicitly using the Conjugate Gradient scheme. For clarity, here in the left hand side (LHS) $A = \frac{\delta R}{\delta u}$, $x = \Delta u$ and the right hand side (RHS) is $b = -R|_u$.

6 Time discretization

Using forward Euler explicit time stepping, equations 10 and 11 become:

$$c^{n+1} = c^n + \Delta t [\nabla \cdot (M \nabla \mu_c)] \quad (17)$$

$$\eta_p^{n+1} = \eta_p^n - \Delta t L \mu_{\eta_p} \quad (18)$$

7 Weak formulation

Writing equations 10 and 11 in the weak form, with the arbitrary variation given by w yields:

$$\int_{\Omega} w c^{n+1} dV = \int_{\Omega} w c^n + w \Delta t [\nabla \cdot (M \nabla \mu_c)] dV \quad (19)$$

$$\int_{\Omega} w \eta_p^{n+1} dV = \int_{\Omega} w \eta_p^n - w \Delta t L \mu_{\eta_p} dV \quad (20)$$

The gradient of μ_c is:

$$\begin{aligned} \nabla \mu_c = & \nabla c \left[f_{\alpha, cc} + \sum_{p=1}^3 H(\eta_p) (f_{\beta, cc} - f_{\alpha, cc}) \right] + \sum_{p=1}^3 \nabla \eta_p H(\eta_p)_{,\eta_p} (f_{\beta, c} - f_{\alpha, c}) \\ & + \left[\sum_{p=1}^3 (C_{ijkl}^{\eta_p} - C_{ijkl}^{\alpha}) \nabla \eta_p H(\eta_p)_{,\eta_p} \right] (-\epsilon_{ij, c}^0) (\epsilon_{ij} - \epsilon_{ij}^0) \\ & - C_{ijkl} \left[\sum_{p=1}^3 H(\eta_p)_{,\eta_p} \epsilon_{ij, c}^{0\eta_p} \nabla \eta_p + H(\eta_p) \epsilon_{ij, cc}^{0\eta_p} \nabla c \right] (\epsilon_{kl} - \epsilon_{kl}^0) \\ & + C_{ijkl} (-\epsilon_{ij, c}^0) \left[\nabla \epsilon_{ij} - \left(\sum_{p=1}^3 H(\eta_p)_{,\eta_p} \epsilon_{kl}^{0\eta_p} \nabla \eta_p + H(\eta_p) \epsilon_{kl, c}^{0\eta_p} \nabla c \right) \right] \end{aligned} \quad (21)$$

Applying the divergence theorem to equation 19, one can derive the residual terms r_c and r_{cx} :

$$\int_{\Omega} w c^{n+1} dV = \int_{\Omega} w \underbrace{c^n}_{r_c} + \nabla w \cdot \underbrace{(-\Delta t M \nabla \mu_c)}_{r_{cx}} dV \quad (22)$$

Expanding μ_{η_p} in equation 20 and applying the divergence theorem yields the residual terms r_{η_p} and $r_{\eta_p x}$:

$$\begin{aligned} \int_{\Omega} w \eta_p^{n+1} dV = & \int_{\Omega} w \left\{ \underbrace{\eta_p^n - \Delta t L \left[(f_{\beta} - f_{\alpha}) H(\eta_p^n)_{,\eta_p} + W f_{Landau, \eta_p} - C_{ijkl} \left(H(\eta_p)_{,\eta_p} \epsilon_{ij}^{0\eta_p} \right) (\epsilon_{kl} - \epsilon_{kl}^0) \right]}_{r_{\eta_p}} \right. \\ & \left. + \frac{1}{2} \left[(C_{ijkl}^{\eta_p} - C_{ijkl}^{\alpha}) H(\eta_p)_{,\eta_p} \right] (\epsilon_{ij} - \epsilon_{ij}^0) (\epsilon_{kl} - \epsilon_{kl}^0) \right\} \\ & \underbrace{\left. \right]}_{r_{\eta_p} \text{ cont.}} \\ & + \nabla w \cdot \underbrace{(-\Delta t L \kappa_{ij}^{\eta_p} \eta_{p,i}^n)}_{r_{\eta_p x}} dV \end{aligned} \quad (23)$$

8 Appendix I: Example functions for f_{α} , f_{β} , f_{Landau} , $H(\eta_p)$

$$f_{\alpha}(c) = A_{2,\alpha} c^2 + A_{1,\alpha} c + A_{0,\alpha} \quad (24)$$

$$f_{\beta}(c) = A_{2,\beta} c^2 + A_{1,\beta} c + A_{0,\beta} \quad (25)$$

$$f_{Landau}(\eta_1, \eta_2, \eta_3) = (\eta_1^2 + \eta_2^2 + \eta_3^2) - 2(\eta_1^3 + \eta_2^3 + \eta_3^3) + (\eta_1^4 + \eta_2^4 + \eta_3^4) + 5(\eta_1^2 \eta_2^2 + \eta_2^2 \eta_3^2 + \eta_1^2 \eta_3^2) + 5(\eta_1^2 \eta_2^2 \eta_3^2) \quad (26)$$

$$H(\eta_p) = 3\eta_p^2 - 2\eta_p^3 \quad (27)$$

9 Appendix II: Variational Derivatives

Variational derivative of Π with respect to η_p (where η_q and η_r correspond to the structural order parameters for the other two orientational variants):

$$\delta_{\eta_p} \Pi = \frac{d}{d\alpha} \left[\int_{\Omega} f_{chem}(c, \eta_p + \alpha w, \eta_q, \eta_r) + f_{grad}(\eta_p + \alpha w, \eta_q, \eta_r) + f_{el}(c, \eta_p + \alpha w, \eta_q, \eta_r, \epsilon) dV \right]_{\alpha=0} \quad (28)$$

Breaking up each of these terms yields:

$$\begin{aligned} \frac{d}{d\alpha} [f_{chem}(c, \eta_p + \alpha w, \eta_q, \eta_r)]_{\alpha=0} &= f_{\alpha}(c) \left[-\frac{\partial H(\eta_p + \alpha w)}{\partial(\eta_p + \alpha w)} \frac{\partial(\eta_p + \alpha w)}{\partial\alpha} \right]_{\alpha=0} \\ &+ f_{\beta}(c) \left[\frac{\partial H(\eta_p + \alpha w)}{\partial(\eta_p + \alpha w)} \frac{\partial(\eta_p + \alpha w)}{\partial\alpha} \right]_{\alpha=0} \\ &+ W \left[\frac{\partial f_{Landau}(\eta_p + \alpha w, \eta_q, \eta_r)}{\partial(\eta_p + \alpha w)} \frac{\partial(\eta_p + \alpha w)}{\partial\alpha} \right]_{\alpha=0} \\ &= f_{\alpha}(c) \left[-\frac{\partial H(\eta_p)}{\partial\eta_p} w \right] + f_{\beta}(c) \left[\frac{\partial H(\eta_p)}{\partial\eta_p} w \right] + W \left[\frac{\partial f_{Landau}(\eta_p, \eta_q, \eta_r)}{\partial\eta_p} w \right] \end{aligned} \quad (29)$$

$$\begin{aligned} \frac{d}{d\alpha} [f_{grad}(\eta_p + \alpha w, \eta_q, \eta_r)]_{\alpha=0} &= \frac{1}{2} \left[\kappa_{ij}^{\eta_p}(\eta_p + \alpha w)_{,i}(\eta_p + \alpha w)_{,j} + \kappa_{ij}^{\eta_q}(\eta_q)_{,i}(\eta_q)_{,j} + \kappa_{ij}^{\eta_r}(\eta_r)_{,i}(\eta_r)_{,j} \right]_{\alpha=0} \\ &= \kappa_{ij} w_{,i} \eta_{p,j} \end{aligned} \quad (30)$$

$$\begin{aligned} \frac{d}{d\alpha} [f_{el}(c, \eta_p + \alpha w, \eta_q, \eta_r, \epsilon)]_{\alpha=0} &= \frac{1}{2} \left[\frac{\partial C_{ijkl}(\eta_p + \alpha w, \eta_q, \eta_r)}{\partial(\eta_p + \alpha w)} \frac{\partial(\eta_p + \alpha w)}{\partial\alpha} \right. \\ &\cdot (\epsilon_{ij} - \epsilon_{ij}^0(c, \eta_p + \alpha w, \eta_q, \eta_r)) (\epsilon_{kl} - \epsilon_{kl}^0(c, \eta_p + \alpha w, \eta_q, \eta_r)) \\ &+ C_{ijkl}(\eta_p + \alpha w, \eta_q, \eta_r) \left(-\frac{\partial \epsilon_{ij}^0(c, \eta_p + \alpha w, \eta_q, \eta_r)}{\partial(\eta_p + \alpha w)} \frac{\partial(\eta_p + \alpha w)}{\partial\alpha} \right) \\ &\cdot (\epsilon_{kl} - \epsilon_{kl}^0(c, \eta_p + \alpha w, \eta_q, \eta_r)) \\ &+ C_{ijkl}(\eta_p + \alpha w, \eta_q, \eta_r) (\epsilon_{ij} - \epsilon_{ij}^0(c, \eta_p + \alpha w, \eta_q, \eta_r)) \\ &\cdot \left(-\frac{\partial \epsilon_{kl}^0(c, \eta_p + \alpha w, \eta_q, \eta_r)}{\partial(\eta_p + \alpha w)} \frac{\partial(\eta_p + \alpha w)}{\partial\alpha} \right) \left. \right]_{\alpha=0} \\ &= \frac{1}{2} \left[\frac{\partial C_{ijkl}(\eta_p, \eta_q, \eta_r)}{\partial\eta_p} w (\epsilon_{ij} - \epsilon_{ij}^0(c, \eta_p, \eta_q, \eta_r)) (\epsilon_{kl} - \epsilon_{kl}^0(c, \eta_p, \eta_q, \eta_r)) \right] \\ &+ C_{ijkl}(\eta_p, \eta_q, \eta_r) \left(-\frac{\partial \epsilon_{ij}^0(c, \eta_p, \eta_q, \eta_r)}{\partial\eta_p} w \right) (\epsilon_{kl} - \epsilon_{kl}^0(c, \eta_p, \eta_q, \eta_r)) \end{aligned} \quad (31)$$

Putting the terms back together yields:

$$\begin{aligned}
\delta_{\eta_p} \Pi = & \int_{\Omega} f_{\alpha}(c) \left[-\frac{\partial H(\eta_p)}{\partial \eta_p} w \right] + f_{\beta}(c) \left[\frac{\partial H(\eta_p)}{\partial \eta_p} w \right] + W \left[\frac{\partial f_{Landau}(\eta_p, \eta_q, \eta_r)}{\partial \eta_p} w \right] \\
& + \kappa_{ij} w_{,i} \eta_{p,j} \\
& + \frac{1}{2} \left[\frac{\partial C_{ijkl}(\eta_p, \eta_q, \eta_r)}{\partial (\eta_p)} w (\epsilon_{ij} - \epsilon_{ij}^0(c, \eta_p, \eta_q, \eta_r)) (\epsilon_{kl} - \epsilon_{kl}^0(c, \eta_p, \eta_q, \eta_r)) \right] \\
& + C_{ijkl}(\eta_p, \eta_q, \eta_r) \left(-\frac{\partial \epsilon_{ij}^0(c, \eta_p, \eta_q, \eta_r)}{\partial \eta_p} w \right) (\epsilon_{kl} - \epsilon_{kl}^0(c, \eta_p, \eta_q, \eta_r)) dV
\end{aligned} \tag{32}$$

Variational derivative of Π with respect to c :

$$\delta_c \Pi = \frac{d}{d\alpha} \left[\int_{\Omega} f_{chem}(c + \alpha w, \eta_p, \eta_q, \eta_r) + f_{grad}(\eta_p, \eta_q, \eta_r) + f_{el}(c + \alpha w, \eta_p, \eta_q, \eta_r, \epsilon) dV \right]_{\alpha=0} \tag{33}$$

Breaking up each of these terms yields:

$$\begin{aligned}
\frac{d}{d\alpha} [f_{chem}(c + \alpha w, \eta_p, \eta_q, \eta_r)]_{\alpha=0} &= \left[\frac{\partial f_{\alpha}(c + \alpha w)}{\partial (c + \alpha w)} \frac{\partial (c + \alpha w)}{\partial \alpha} \left(1 - \sum_{p=1}^3 H(\eta_p) \right) \right. \\
&+ \frac{\partial f_{\beta}(c + \alpha w)}{\partial (c + \alpha w)} \frac{\partial (c + \alpha w)}{\partial \alpha} \left(\sum_{p=1}^3 H(\eta_p) \right) + W \frac{\partial f_{Landau}(\eta_p, \eta_q, \eta_r)}{\partial (c + \alpha w)} \frac{\partial (c + \alpha w)}{\partial \alpha} \left. \right]_{\alpha=0} \\
&= \frac{\partial f_{\alpha}(c)}{\partial c} w \left(1 - \sum_{p=1}^3 H(\eta_p) \right) + \frac{\partial f_{\beta}(c)}{\partial c} w \left(\sum_{p=1}^3 H(\eta_p) \right)
\end{aligned} \tag{34}$$

$$\frac{d}{d\alpha} [f_{grad}(\eta_p, \eta_q, \eta_r)]_{\alpha=0} = 0 \tag{35}$$

$$\begin{aligned}
\frac{d}{d\alpha} [f_{el}(c + \alpha w, \eta_p, \eta_q, \eta_r, \epsilon)]_{\alpha=0} &= \frac{1}{2} C_{ijkl}(\eta_p, \eta_q, \eta_r) \left[-\frac{\partial \epsilon_{ij}^0(c + \alpha w, \eta_p, \eta_q, \eta_r)}{\partial (c + \alpha w)} \frac{\partial (c + \alpha w)}{\partial \alpha} (\epsilon_{kl} - \epsilon_{kl}^0(c + \alpha w, \eta_p, \eta_q, \eta_r)) \right. \\
&- (\epsilon_{ij} - \epsilon_{ij}^0(c + \alpha w, \eta_p, \eta_q, \eta_r)) \frac{\partial \epsilon_{ij}^0(c + \alpha w, \eta_p, \eta_q, \eta_r)}{\partial (c + \alpha w)} \frac{\partial (c + \alpha w)}{\partial \alpha} \left. \right]_{\alpha=0} \\
&= -C_{ijkl}(\eta_p, \eta_q, \eta_r) \frac{\partial \epsilon_{ij}^0(c, \eta_p, \eta_q, \eta_r)}{\partial c} w (\epsilon_{kl} - \epsilon_{kl}^0(c + \alpha w, \eta_p, \eta_q, \eta_r))
\end{aligned} \tag{36}$$

Putting the terms back together yields:

$$\begin{aligned}
\delta_c \Pi = & \int_{\Omega} \frac{\partial f_{\alpha}(c)}{\partial c} w \left(1 - \sum_{p=1}^3 H(\eta_p) \right) + \frac{\partial f_{\beta}(c)}{\partial c} w \left(\sum_{p=1}^3 H(\eta_p) \right) \\
& - C_{ijkl}(\eta_p, \eta_q, \eta_r) \frac{\partial \epsilon_{ij}^0(c, \eta_p, \eta_q, \eta_r)}{\partial c} w (\epsilon_{kl} - \epsilon_{kl}^0(c + \alpha w, \eta_p, \eta_q, \eta_r)) dV
\end{aligned} \tag{37}$$