

KKS Phase Field Model of Precipitate Evolution

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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

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

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

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

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

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

Here $\epsilon_{\eta_p}^0$ are the composition dependent stress free strain transformation tensor corresponding to each structural order parameter, which is a function of the β phase concentration, c_{β} , defined below.

In the KKS model (Kim 1999), the interfacial region is modeled as a mixture of the α and β phases with concentrations c_{α} and c_{β} , respectively. The homogenous free energies for each phase, f_{α} and f_{β} in this case, are typically given as functions of c_{α} and c_{β} , rather than directly as functions of c and η_p . Thus, $f_{chem}(c, \eta_1, \eta_2, \eta_3)$ can be rewritten as

$$f_{chem}(c, \eta_1, \eta_2, \eta_3) = f_{\alpha}(c_{\alpha}) \left(1 - \sum_{p=1}^3 H(\eta_p) \right) + f_{\beta}(c_{\beta}) \sum_{p=1}^3 H(\eta_p) + W f_{Landau}(\eta_1, \eta_2, \eta_3) \quad (8)$$

The concentration in each phase is determined by the following system of equations:

$$c = c_{\alpha} \left(1 - \sum_{p=1}^3 H(\eta_p) \right) + c_{\beta} \sum_{p=1}^3 H(\eta_p) \quad (9)$$

$$\frac{\partial f_{\alpha}(c_{\alpha})}{\partial c_{\alpha}} = \frac{\partial f_{\beta}(c_{\beta})}{\partial c_{\beta}} \quad (10)$$

Given the following parabolic functions for the single-phase homogenous free energies:

$$f_{\alpha}(c_{\alpha}) = A_2 c_{\alpha}^2 + A_1 c_{\alpha} + A_0 \quad (11)$$

$$f_{\beta}(c_{\beta}) = B_2 c_{\beta}^2 + B_1 c_{\beta} + B_0 \quad (12)$$

the single-phase concentrations are:

$$c_\alpha = \frac{B_2 c + \frac{1}{2}(B_1 - A_1) \sum_{p=1}^3 H(\eta_p)}{A_2 \sum_{p=1}^3 H(\eta_p) + B_2 \left(1 - \sum_{p=1}^3 H(\eta_p)\right)} \quad (13)$$

$$c_\beta = \frac{A_2 c + \frac{1}{2}(A_1 - B_1) \left[1 - \sum_{p=1}^3 H(\eta_p)\right]}{A_2 \sum_{p=1}^3 H(\eta_p) + B_2 \left[1 - \sum_{p=1}^3 H(\eta_p)\right]} \quad (14)$$

2 Required inputs

- $f_\alpha(c_\alpha), f_\beta(c_\beta)$ - Homogeneous chemical free energy of the components of the binary system, example form given above
- $f_{Landau}(\eta_1, \eta_2, \eta_3)$ - 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
- C_{η_p} - fourth order elasticity tensor (or its equivalent second order Voigt representation) for the p^{th} orientation variant of the β phase
- 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

We obtain chemical potentials for the chemical potentials for the concentration and the structural order parameters by taking variational derivatives of Π :

$$\mu_c = f_{\alpha,c}(1 - H(\eta_1) - H(\eta_2) - H(\eta_3)) + f_{\beta,c}(H(\eta_1) + H(\eta_2) + H(\eta_3)) + C_{ijkl}(-\epsilon_{ij,c}^0)(\epsilon_{kl} - \epsilon_{kl}^0) \quad (15)$$

$$\mu_{\eta_p} = [f_\beta - f_\alpha - (c_\beta - c_\alpha)f_{\beta,c_\beta}]H(\eta_p)_{,\eta_p} + W f_{Landau,\eta_p} - \kappa_{ij}^{\eta_p} \eta_{p,ij} + C_{ijkl}(-\epsilon_{ij,\eta_p}^0)(\epsilon_{kl} - \epsilon_{kl}^0) + \frac{1}{2} C_{ijkl,\eta_p}(\epsilon_{ij} - \epsilon_{ij}^0) \quad (16)$$

4 Kinetics

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

$$\frac{\partial c}{\partial t} = -\nabla \cdot \left(\frac{1}{f_{,cc}} M \nabla \mu_c \right) \quad (17)$$

where M is a constant mobility and the factor of $\frac{1}{f_{,cc}}$ is added to guarantee constant diffusivity in the two phases. The PDE for Allen-Cahn dynamics is given by:

$$\frac{\partial \eta_p}{\partial t} = -L\mu_{\eta_p} \quad (18)$$

where L is a constant mobility.

5 Mechanics

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

$$\delta_u \Pi = \int_{\Omega} \nabla w : \mathbf{C}(\eta_1, \eta_2, \eta_3) : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^0(c, \eta_1, \eta_2, \eta_3)) \, dV = 0 \quad (19)$$

$$(20)$$

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

6 Time discretization

Using forward Euler explicit time stepping, equations 17 and 18 become:

$$c^{n+1} = c^n + \Delta t \left[\nabla \cdot \left(\frac{1}{f_{,cc}} M \nabla \mu_c \right) \right] \quad (21)$$

$$\eta_p^{n+1} = \eta_p^n - \Delta t L \mu_{\eta_p} \quad (22)$$

7 Weak formulation

Writing equations 17 and 18 in the weak form, with the arbitrary variation given by w yields:

$$\int_{\Omega} w c^{n+1} dV = \int_{\Omega} w c^n + w \Delta t \left[\nabla \cdot \left(\frac{1}{f_{,cc}} M \nabla \mu_c \right) \right] dV \quad (23)$$

$$\int_{\Omega} w \eta_p^{n+1} dV = \int_{\Omega} w \eta_p^n - w \Delta t L \mu_{\eta_p} dV \quad (24)$$

The expression of $\frac{1}{f_{,cc}} \mu_c$ can be written as:

$$\begin{aligned} \frac{1}{f_{,cc}} \nabla \mu_c = & \nabla c + (c_{\alpha} - c_{\beta}) \sum_{p=1}^3 H(\eta_p)_{,\eta_p} \nabla \eta_p \\ & + \frac{1}{f_{,cc}} \left[\sum_{p=1}^3 (C_{ijkl}^{\eta_p} - C_{ijkl}^{\alpha}) \nabla \eta_p H(\eta_p)_{,\eta_p} \right] (-\epsilon_{ij,c}^0)(\epsilon_{ij} - \epsilon_{ij}^0) \\ & - \frac{1}{f_{,cc}} C_{ijkl} \left[\sum_{p=1}^3 \left(H(\eta_p)_{,\eta_p} \epsilon_{ij,c}^{0\eta_p} + \sum_{q=1}^3 \left(H(\eta_p) \epsilon_{ij,c\eta_q}^{0\eta_p} \right) \right) \nabla \eta_p + H(\eta_p) \epsilon_{ij,cc}^{0\eta_p} \nabla c \right] (\epsilon_{kl} - \epsilon_{kl}^0) \\ & + \frac{1}{f_{,cc}} C_{ijkl} (-\epsilon_{ij,c}^0) \left[\nabla \epsilon_{kl} - \left(\sum_{p=1}^3 \left(H(\eta_p)_{,\eta_p} \epsilon_{kl}^{0\eta_p} - \sum_{q=1}^3 \epsilon_{kl,\eta_q}^{\eta_q} H(\eta_q) \right) \nabla \eta_p + H(\eta_p) \epsilon_{kl,c}^{0\eta_p} \nabla c \right) \right] \end{aligned} \quad (25)$$

Applying the divergence theorem to equation 23, one can derive the residual terms r_c and r_{cx} :

$$\int_{\Omega} w c^{n+1} dV = \int_{\Omega} w \underbrace{c^n}_{r_c} + \underbrace{\nabla w \cdot \left(-\Delta t M \frac{1}{f_{,cc}} \nabla \mu_c \right)}_{r_{cx}} dV \quad (26)$$

Expanding μ_{η_p} in equation 24 and applying the divergence theorem yields the residual terms r_{η_p} and $r_{\eta_p x}$:

$$\begin{aligned} \int_{\Omega} w \eta_p^{n+1} dV = & \int_{\Omega} w \left\{ \underbrace{\eta_p^n - \Delta t L \left[(f_{\beta} - f_{\alpha}) H(\eta_p^n)_{,\eta_p} - (c_{\beta} - c_{\alpha}) f_{\beta, c_{\beta}} H(\eta_p^n)_{,\eta_p} + W f_{Landau, \eta_p} \right]}_{r_{\eta_p}} \right. \\ & \left. - C_{ijkl} \left(H(\eta_p)_{,\eta_p} \epsilon_{ij}^{0\eta_p} \right) (\epsilon_{kl} - \epsilon_{kl}^0) + \frac{1}{2} \left[(C_{ijkl}^{\eta_p} - C_{ijkl}^{\alpha}) H(\eta_p)_{,\eta_p} \right] (\epsilon_{ij} - \epsilon_{ij}^0) (\epsilon_{kl} - \epsilon_{kl}^0) \right\} \\ & \underbrace{\left. \right)}_{r_{\eta_p} \text{ cont.}} \\ & + \nabla w \cdot \underbrace{\left(-\Delta t L \kappa_{ij}^{\eta_p} \eta_{p,i}^n \right)}_{r_{\eta_p x}} dV \end{aligned} \quad (27)$$

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

$$f_{\alpha}(c_{\alpha}) = A_2 c_{\alpha}^2 + A_1 c_{\alpha} + A_0 \quad (28)$$

$$f_{\beta}(c_{\beta}) = B_2 c_{\beta}^2 + B_1 c_{\beta} + B_0 \quad (29)$$

$$f_{Landau}(\eta_1, \eta_2, \eta_3) = (\eta_1^2 + \eta_2^2 + \eta_3^2) - 2(\eta_1^3 + \eta_2^3 + \eta_3^3) + (\eta_1^4 + \eta_2^4 + \eta_3^4) + 5(\eta_1^2 \eta_2^2 + \eta_2^2 \eta_3^2 + \eta_1^2 \eta_3^2) + 5(\eta_1^2 \eta_2^2 \eta_3^2) \quad (30)$$

$$H(\eta_p) = 3\eta_p^2 - 2\eta_p^3 \quad (31)$$