Series lectures of phase-field model

11. Eshelby's inclusion theory

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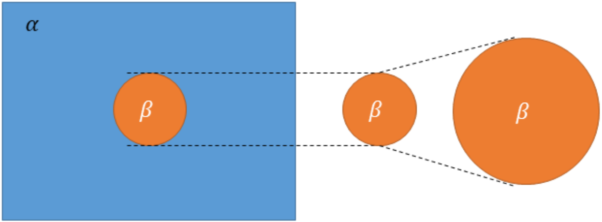
Effects of elasticity on Phase transformations

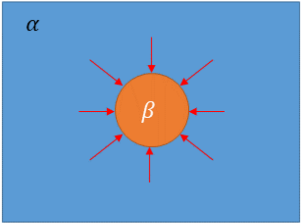
- Source of stress 1: Lattice parameter can be a function of composition: Lattice planes are continuous, no dislocation.
- Source of stress 2: Difference in lattice parameters between two phases: Eigenstrain, misfit strain



- Make β phase lattice parameter match α - coherent.
- Eigenstrain

$$\varepsilon_{ij} = \frac{a^\beta - a^\alpha}{a^\alpha}\delta_{ij}$$

where a^β is lattice parameter of β phase and a^α is lattice parameter of α phase.



Elastic stress surrounding a coherent spherical precipitate

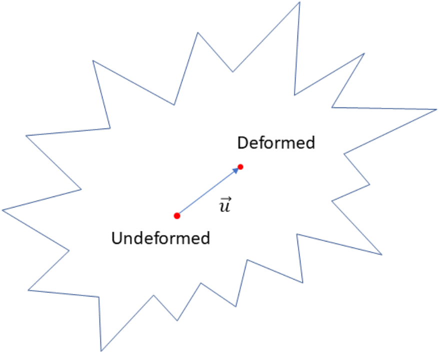
- Coherent lattice
- Dilatational misfit
- Linear isotropic inhomogeneous elasticity
- Inhomogeneous elastic constant of α and β can be different.
- Spherical particle

Strain

- Strain is related to the gradients in the displacement

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right) \qquad 3 \times 3 \text{ tensor}$$

$$u_{i,j} = \frac{\partial u_i}{\partial x_j}$$



- With 4th-order rank elastic constant

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$$

implicitly means (Einstein notation)

$$\sigma_{ij} = \sum_{k=1}^{3}\sum_{l=1}^{3} C_{ijkl}\varepsilon_{kl}$$

- For isotropic materials

$$\sigma_{ij} = \lambda\varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij}$$

where λ is Lame's constant and μ is the shear modulus.

Mechanical equilibrium

- Condition for equilibrium

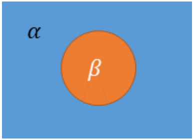
$$\nabla \cdot [\sigma] = 0 \rightarrow \sigma_{ij,j} = 0$$

- For an isotropic material

$$(\lambda + \mu)\nabla(\nabla \cdot \mathbf{u}) + \mu\nabla^2\mathbf{u} = 0$$

- In spherical coordinates, for spherical particle at $\alpha - \beta$ interface coherent

$$\mathbf{u}^{\alpha}(R) = \mathbf{u}^{\beta}(R)$$



- Force balance at interface

$$\sigma_{rr}^{\beta}(R) - \sigma_{rr}^{\alpha}(R) = -\frac{2f}{R}$$

- For spherical particle and assume the spherical symmetry

$$\mathbf{u} = u\hat{r}$$

then the force balance equation becomes

$$\frac{d^2u}{dr^2} + \frac{2}{r}\frac{du}{dr} - \frac{2u}{r^2} = 0$$

$$\frac{d}{dr}\left[\frac{1}{r^2}\frac{d(r^2u)}{dr}\right] = 0 \rightarrow \frac{d(r^2u)}{dr} = A'r^2$$

$$u = Ar + \frac{B}{r^2}$$

- When $r \to 0$, u have to be finite. Therefore, $B = 0$.
- When $r \to \infty$, $u \to 0$. Therefore, $A = 0$
- Therefore,

$$u^{\beta} = Ar \qquad u^{\alpha} = \frac{B}{r^2}$$

- According to continuum mechanics,

$$\varepsilon_{rr} = \frac{du}{dr} \qquad \varepsilon_{\theta\theta} = \varepsilon_{\phi\phi} = \frac{u}{r}$$

- Eigenstrains, misfit strains

$$\underbrace{\varepsilon_{ij}}_{\text{Total strain compatible}} = \underbrace{\varepsilon_{ij}^{e}}_{\text{elastic strain}} + \underbrace{\varepsilon_{ij}^{\circ}}_{\text{eigenstrain}}$$

- By Hooke's law

$$\sigma_{ij}^{\beta} = C_{ijkl}^{\beta}\varepsilon_{ij}^{\beta,e} = C_{ijkl}^{\beta}(\varepsilon_{ij}^{\beta} - \varepsilon_{ij}^{\circ})$$

- Assuming no holes or overlap of material

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$$

- For isotropic materials and assume $\varepsilon^{\circ}_{ij} = \varepsilon\delta_{ij}$

$$\sigma^{\beta}_{ij} = \lambda^{\beta}\varepsilon^{\beta}_{kk}\delta_{ij} + 2\mu^{\beta}\varepsilon^{\beta}_{ij} - 3K^{\beta}\varepsilon\delta_{ij}$$

where K^{β} is bulk modulus of β phase.

$$\sigma^{\alpha}_{ij} = \lambda^{\alpha}\varepsilon^{\alpha}_{kk}\delta_{ij} + 2\mu^{\alpha}\varepsilon^{\alpha}_{ij}$$

In other notations, we have

$$\sigma^{\alpha} = \sigma^{\alpha}_{11} = \sigma^{\alpha}_{22} = \sigma^{\alpha}_{33} = \left(C^{\alpha}_{11} + 2C^{\alpha}_{12}\right)\varepsilon^{\alpha} \tag{1}$$

where

$$\varepsilon^{\alpha} = \varepsilon^{\alpha}_{11} = \varepsilon^{\alpha}_{22} = \varepsilon^{\alpha}_{33}$$

- Note that

$$C_{11} = \lambda + 2\mu \qquad C_{12} = \lambda$$

- Inside precipitate,

$$\begin{aligned}\sigma_{rr}^{\beta} &= \lambda^{\beta}\left[\varepsilon_{rr}^{\beta} + \varepsilon_{\theta\theta}^{\beta} + \varepsilon_{\phi\phi}^{\beta}\right] + 2\mu^{\beta}\varepsilon_{rr}^{\beta} - 3K^{\beta}\varepsilon \\ &= \lambda^{\beta}\left[\frac{du^{\beta}}{dr} + \frac{2u^{\beta}}{r}\right] + 2\mu^{\beta}\frac{du^{\beta}}{dr} - 3K^{\beta}\varepsilon \\ &= \lambda^{\beta}[A + 2A] + 2\mu^{\beta} \times A - 3K^{\beta}\varepsilon \\ &= 3K^{\beta}(A - \varepsilon)\end{aligned}$$

where

$$K^{\beta} = \frac{3\lambda^{\beta} + 2\mu^{\beta}}{3}$$

- For matrix

$$\begin{aligned}\sigma_{rr}^{\alpha} &= \lambda^{\alpha}\left[\frac{du^{\alpha}}{dr} + \frac{2u^{\alpha}}{r}\right] + 2\mu^{\alpha}\frac{du^{\alpha}}{dr} \\ &= \lambda^{\alpha}\left[-\frac{2B}{r^3} + \frac{2B}{r^3}\right] - \frac{4\mu^{\alpha}B}{r^3} = -\frac{4\mu^{\alpha}B}{r^3}\end{aligned}$$

- At interface

$$\sigma_{rr}^{\alpha}(R) = -\frac{4\mu^{\alpha}B}{R^3}$$

- Apply force balance at interface

$$\sigma_{rr}^{\beta}(R) - \sigma_{rr}^{\alpha}(R) = \frac{4\mu^{\alpha}B}{R^3} + 3K^{\beta}(A - \varepsilon) = -\frac{2f}{R}$$

- Displacement condition

$$u^{\alpha}(R) = u^{\beta}(R) \rightarrow AR = \frac{B}{R^2} \rightarrow B = AR^3$$

- We have

$$A = \frac{3K^{\beta}\varepsilon - 2f/R}{3K^{\beta} + 4\mu^{\alpha}}$$

Evaluating stress and strain

- Inside the particle

$$\varepsilon^{\beta}_{rr} = \varepsilon^{\beta}_{\theta\theta} = \varepsilon^{\beta}_{\phi\phi} = A$$

$$\sigma^{\beta}_{rr} = \sigma^{\beta}_{\theta\theta} = \sigma^{\beta}_{\phi\phi} = 3K^{\beta}(A - \varepsilon)$$

where

$$\varepsilon = \frac{1}{3}\frac{V^{\beta}_{m} - V^{\alpha}_{m}}{V^{\alpha}_{m}}$$

- For matrix,

$$\varepsilon^{\alpha}_{rr} = \frac{du}{dr} = -\frac{2B}{r^3} \qquad \varepsilon^{\alpha}_{\theta\theta} = \varepsilon^{\alpha}_{\phi\phi} = \frac{B}{r^3}$$

$$\sigma^{\alpha}_{rr} = -\frac{4B\mu^{\alpha}}{r^3} \qquad \sigma^{\alpha}_{\theta\theta} = \sigma^{\alpha}_{\phi\phi} = 2\mu^{\alpha}\left(\frac{B}{r^3}\right)$$

- Note that

$$\sigma^{\alpha}_{rr} + \sigma^{\alpha}_{\theta\theta} + \sigma^{\alpha}_{\phi\phi} = 0$$

Stress in precipitate

- Stress field and strain field are constants.
- Pure hydrostatic pressure.
- Assume no surface stress $f = 0$,

$$A = \frac{3K^\beta \varepsilon}{3K^\beta + 4\mu^\alpha} \qquad \sigma_{rr}^\beta = \frac{-4\mu^\alpha \varepsilon}{3K^\beta + 4\mu^\alpha}$$

- For case $\varepsilon > 0 \rightarrow \sigma_{rr} < 0$, it means particle is under compression. $(V_m^\beta > V_m^\alpha)$
- For the case of $f \neq 0$ and $\varepsilon = 0$

$$A = \frac{1}{3K^\beta}\left(-\frac{2f}{R}\right) \qquad \sigma_{rr}^\beta = \sigma_{\theta\theta}^\beta = \sigma_{\phi\phi}^\beta = -\frac{2f}{R}$$

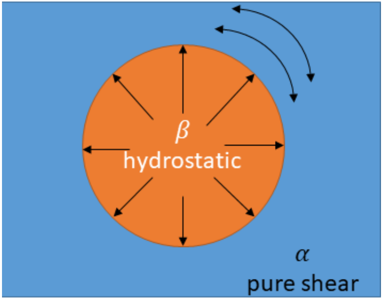
The pressure inside the particle

$$P^\beta = -\frac{1}{3}\sigma_{kk} = \frac{2f}{R}$$

Stress in matrix phase

- Pure shear stress

$$\sigma_{kk} = 0$$



Stress at interface