Micromechanical Model for the Delta Ferrite-to-Austenite Transition

Lance C. Hibbeler
(Ph.D. Student)

Department of Mechanical Science and Engineering
University of Illinois at Urbana-Champaign

Objectives

• Propose better mixture rule for mechanical behavior of delta-to-gamma transition
• Compare with mixture rule in current UMAT/CON2D model
• Implement into UMAT/CON2D
Mixture Rules

• Some properties depend on microstructure

- Random particles

Directed laminates

Directed fibers

Mixture Rules

• How do we describe on a macroscopic scale the behavior of a system composed of different materials?

• For some properties, a volume-weighted average of constituent parts makes sense
  – Mass density: total mass is the sum of the parts

\[
\bar{\rho} = \rho_1 f_1 + \rho_2 f_2 + \cdots
\]

  \( f_i \) is volume fraction

  – This holds no matter what the microstructure
Mechanical Mixture Rules

- Consider the effective Young’s modulus of a laminate microstructure

\[
\frac{1}{E_{\perp}} = f_1 \frac{E_1}{E_1} + f_2 \frac{E_2}{E_2} + \ldots
\]

- “Reuss average”

\[
\bar{E}_{\parallel} = E_1 f_1 + E_2 f_2 + \ldots
\]

- “Voigt average”

Mixture Rules

- These rules bound the effective properties
  - Iso-(stress, heat flux, etc) are lower bounds
  - Iso-(strain, temperature, etc) are upper bounds

- Macroscopic properties become anisotropic

- What about other microstructure shapes?
- What about inelastic behavior?
Mori-Tanaka Theory*

- Without external loads, the average stress in each phase of a mixture must balance
  \[ (1 - f) \bar{\sigma}_{ij}^{1} + f \bar{\sigma}_{ij}^{2} = 0 \]
  \( \bar{\sigma}_{ij}^{1} \) Average stress in phase 1
  \( \bar{\sigma}_{ij}^{2} \) Average stress in phase 2
  \( f \) Volume fraction of phase 2

- Change \( f \) by tiny amount; new phase 2 average stress is
  \[ \bar{\sigma}_{ij}^{2} = \sigma_{ij}^{\circ} + \bar{\sigma}_{ij}^{1} \]
  \( \sigma_{ij}^{\circ} \) Nominal stress inside phase 2

- Can solve for individual phase and macroscopic stresses
  \[ \bar{\sigma}_{ij}^{1} = -f \sigma_{ij}^{\circ} \]
  \[ \bar{\sigma}_{ij}^{2} = (1 - f) \sigma_{ij}^{\circ} \]
  \[ \sigma_{ij} = \bar{\sigma}_{ij}^{1} + \bar{\sigma}_{ij}^{2} = (1 - 2f) \sigma_{ij}^{\circ} \]
  Macroscopic stress

*As a general reference, see:

Nominal Phase 2 Stress

- Eshelby’s method provides the stress in an “inclusion” with a given “eigenstrain”
  \[ \sigma_{ij}^{\circ} = C_{ijkl} (S_{klnn} - \delta_{mk} \delta_{nl}) \varepsilon_{mn}^{\ast} \]
  \( S_{ijkl} \) Eshelby’s tensor, accounts for shape of phase 2

- Isotropic elastic moduli:
  \[ C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu \delta_{ik} \delta_{jl} + \mu \delta_{il} \delta_{jk} \]

- Eigenstrain accounts for any difference in strain between phases
  - Thermal, inelastic, transformation, etc
    \[ \varepsilon_{mn}^{\ast} = (\varepsilon_{mn}^{\text{th},2} - \varepsilon_{mn}^{\text{th},1}) + (\varepsilon_{mn}^{\text{pl},2} - \varepsilon_{mn}^{\text{pl},1}) + \varepsilon_{mn}^{tr} \]
**Δ-γ Transition**

- Current model: if \( f_δ > 10\% \), use \( δ \), else use \( γ \)
- Proposed model: \( δ \) matrix with growing \( γ \) particles
- Rate forms of above equations more useful given the high temperatures involved

\[
\dot{\sigma}_{ij} = (1 - 2f) \dot{\sigma}^0_{ij} + 2 f \dot{\sigma}^0_{ij}
\]

\[
\dot{\sigma}^0_{ij} = C_{ijkl} (S_{klmn} - \delta_{mk} \delta_{nl}) \dot{\varepsilon}_{mn}^*
\]

\[
\dot{\varepsilon}_{mn}^* = \left( \dot{\varepsilon}_{mn}^{th,2} - \dot{\varepsilon}_{mn}^{th,1} \right) + \left( \dot{\varepsilon}_{mn}^{pl,2} - \dot{\varepsilon}_{mn}^{pl,1} \right)
\]

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**Strains**

\[
\dot{\varepsilon}^\gamma (s^{-1}) = f(C) \left[ \sigma - f_1(T) \varepsilon \right] \exp\left( \frac{-4.465 \times 10^4 (K)}{T} \right)
\]

\( f_1(T) = 130.5 - 5.128 \times 10^{-3} T \)  
\( f_2(T) = -0.6289 + 1.114 \times 10^{-3} T \)  
\( f_3(T) = 8.132 - 1.54 \times 10^{-3} T \)  
\( f(C) = 4.655 \times 10^4 + 7.14 \times 10^4 C + 1.2 \times 10^4 C^2 \)

\[
\dot{\varepsilon}^\delta (s^{-1}) = 0.1 \left[ \frac{\sigma}{f(C)(T/300)^{5.52} (1 + 1000 \varepsilon)^m} \right]^{n}
\]

\( f(C) = 1.3678 \times 10^4 \left( C^{-5.56 \times 10^{-2}} \right) \)  
\( m = -9.4156 \times 10^{-5} T + 0.3495 \)  
\( n = 1/1.617 \times 10^{-4} T - 0.06166 \)

\[
\dot{\varepsilon}_{ij}^{pl} = \frac{3}{2} \frac{\dot{\varepsilon}}{\sigma} \sigma'_{ij} \quad \sigma'_{ij} = \sigma_{ij} - \sigma_{kk}/3
\]

\[
\dot{\varepsilon}_{ij}^{th} = \alpha \dot{T} \delta_{ij}
\]

Prandtl-Reuss equations

Thermal strain
δ-γ Transition

• Take eigenstrain as:

\[ \dot{\varepsilon}_{ij}^* = (\alpha^\gamma - \alpha^\delta) \dot{T} \delta_{ij} + (\dot{\varepsilon}_{ij}^{pl,\gamma} - \dot{\varepsilon}_{ij}^{pl,\delta}) \]

• Take Eshelby tensor for spherical particles:

\[ S_{111} = \frac{7 - 5\nu}{15(1 - \nu)} \quad S_{112} = \frac{5\nu - 1}{15(1 - \nu)} \quad S_{121} = \frac{4 - 5\nu}{15(1 - \nu)} \]

– Need to have isotropic macroscopic response for current integration scheme in UMAT

\[
\begin{array}{c}
\text{Proposed Model Unloaded Axis} \\
\text{Proposed Model Loaded Axes}
\end{array}
\]

\[
\begin{array}{c}
\text{Current Model Loaded Axis} \\
\text{Current Model Unloaded Axis}
\end{array}
\]

δ-γ Transition

• Consider a cube of material with an initial biaxial load (i.e., found in CC shells)
**δ-γ Transition**

- Slower cooling rate, larger initial load

![Graph showing stress-strain relationship](image)

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**δ-γ Transition**

- Inelastic behavior misfit important when there is existing inelastic behavior
- Thermal expansion mismatch eventually dominates macroscopic response
  - “Low initial load” case, immediately
  - “High initial load” case, at about 36% austenite

![Graph showing temperature vs. stress](image)
Discussion / Conclusion

• Two different models for δ-γ transition provide comparable results (for spherical particles)
• Previous model is quite reasonable
• Proposed model
  – Can extend to columnar grains with different S_{ijkl}
  – Can incorporate growth of austenite with d/dt(S_{ijkl}) term
  – Difficult integrals
  – Anisotropic response
• Any incorporation of anisotropic plasticity requires complete rewriting of UMAT

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