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Micromechanical Model for the Delta Ferrite-to-Austenite Transition

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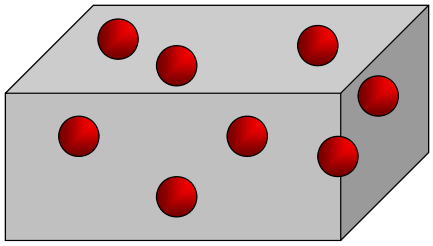
Objectives

- 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

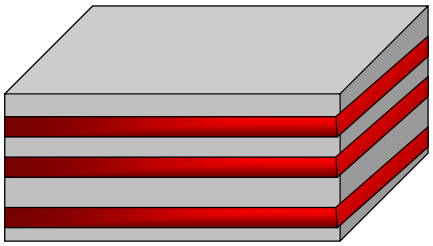
Mixture Rules

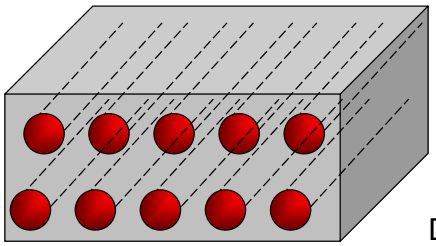
- Some properties depend on microstructure



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

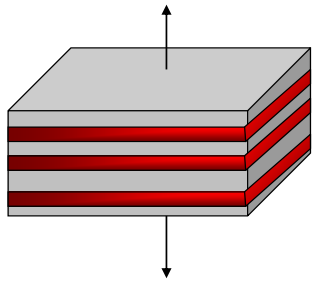
$$\bar{\rho} = \rho_1 f_1 + \rho_2 f_2 + \cdots$$

f_i is **volume** fraction

  - This holds no matter what the microstructure

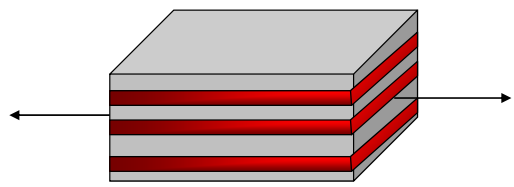
Mechanical Mixture Rules

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



(same stress)
"Reuss average"

$$\frac{1}{\bar{E}_{\perp}} = \frac{f_1}{E_1} + \frac{f_2}{E_2} + \cdots$$



(same strain)
"Voigt average"

$$\bar{E}_{||} = E_1 f_1 + E_2 f_2 + \cdots$$

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 ansiotropic

- 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

$$\bar{\sigma}_{ij}^{2} = \sigma_{ij}^{\circ} + \bar{\sigma}_{ij}^{1}$$

σ_{ij}° 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:
T. Mura, *Micromechanics of Defects in Solids*, 2e. Kluwer Academic Publishers, 1987.

Nominal Phase 2 Stress

- Eshelby's method provides the stress in an "inclusion" with a given "eigenstrain"

$$\sigma_{ij}^{\circ} = C_{ijkl}\left(S_{klmn} - \delta_{mk}\delta_{nl}\right)\varepsilon_{mn}^{*}$$

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

$$\varepsilon_{mn}^{*} = \left(\varepsilon_{mn}^{th,2} - \varepsilon_{mn}^{th,1}\right) + \left(\varepsilon_{mn}^{pl,2} - \varepsilon_{mn}^{pl,1}\right) + \varepsilon_{mn}^{tr}$$

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

$$\dot{\sigma}_{ij} = (1-2f)\dot{\sigma}_{ij}^{\bigcirc} + 2\dot{f}\sigma_{ij}^{\bigcirc}$$

$$\dot{\sigma}_{ij}^{\bigcirc} = C_{ijkl}\left(S_{klmn} - \delta_{mk}\delta_{nl}\right)\dot{\varepsilon}_{mn}^{*}$$

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

Strains

$$\dot{\varepsilon}^{\gamma}\left(s^{-1}\right) = f(C)\left[\sigma - f_1(T)\varepsilon\left|\varepsilon\right|^{f_2(T)-1}\right]^{f_3(T)} \exp\left(-\frac{4.465\times10^4(K)}{T}\right)$$

$$f_1(T) = 130.5 - 5.128\times10^{-3}T$$
$$f_2(T) = -0.6289 + 1.114\times10^{-3}T$$
$$f_3(T) = 8.132 - 1.54\times10^{-3}T$$
$$f(C) = 4.655\times10^4 + 7.14\times10^4 C + 1.2\times10^5 C^2$$

γ constitutive model

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

$$f(C) = 1.3678\times10^4 (C)^{-5.56\times10^{-2}}$$
$$m = -9.4156\times10^{-5}T + 0.3495$$
$$n = 1/1.617\times10^{-4}T - 0.06166$$

δ constitutive model

$$\dot{\varepsilon}_{ij}^{pl} = \frac{3}{2}\frac{\dot{\varepsilon}}{\sigma}\sigma'_{ij} \qquad \sigma'_{ij} = \sigma_{ij} - \sigma_{kk}/3$$

Prandtl-Reuss equations

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

Thermal strain

δ-γ Transition

- Take eigenstrain as:

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

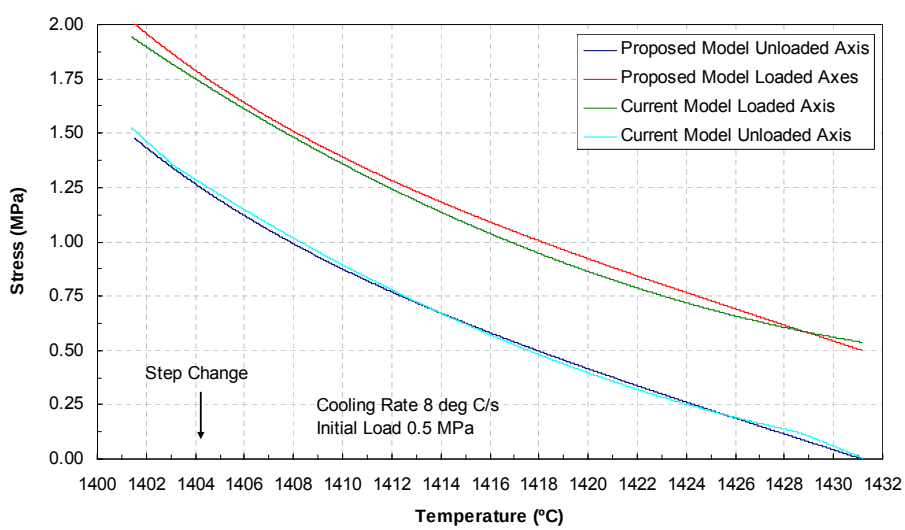
- Take Eshelby tensor for spherical particles:

$$S_{1111} = \frac{7-5\nu}{15(1-\nu)} \qquad S_{1122} = \frac{5\nu-1}{15(1-\nu)} \qquad S_{1212} = \frac{4-5\nu}{15(1-\nu)}$$

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

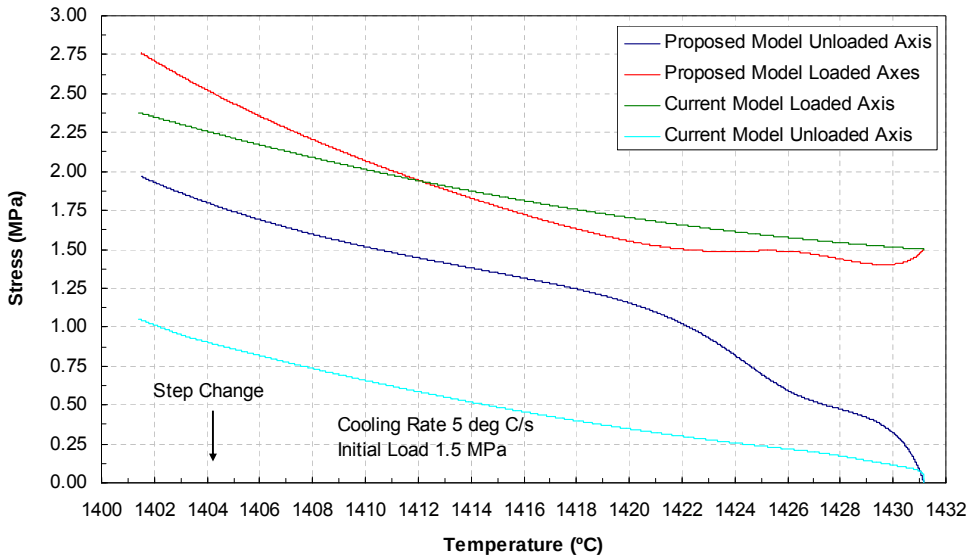
δ-γ Transition

- 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



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

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

Acknowledgements

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