Theoretical and Computational Mechanics of Materials Group

- Fundamental coupling of mathematics, materials science, and theoretical/computational mechanics of materials.
- The design, use, and computational representation of materials for applications involving extreme loading conditions remains a key research area.
- We seek to develop physically-based theory and computational tools to describe real material behaviors at a mechanistic level demonstrated through experiments.
- Our vision is to offer new approaches to the study and prediction of multi-physics events taking place within materials exposed to extreme loading.
Ductile damage models

- Statistical Distribution of Nucleated Pores
- Statistical Distribution of Thick-walled Spheres

- Pressure $P$
- Cavitation Pressure $p_c = [p_c = \infty]$

- Porosity $\rho(r) = \frac{\pi (r)^3}{2} [\rho(r)]$
- Ensemble Porosity $\bar{\rho} = \frac{\int \rho(r) \, dr}{\int 1 \, dr}$

- Statistical Model for Pore Nucleation
- Distribution of Thick-walled Spheres
- No Sphere Coupling
- Application to high triaxiality

Damage region
- Tantalum sample
- Plate impact simulation
- von Mises stress
- Tantalum flyer
- Aluminum flyer
- Axis of symmetry
Non-Schmid Crystal Plasticity

Resolved Shear Stress
\[ \tau^\alpha = (C^T S)^\alpha \approx T \sum \alpha \omega \beta S \beta \]

Schmid Tensor
\[ S^\alpha_0 = m^\alpha_0 \otimes n^\alpha_0 \]
\[ \tilde{\tau}^\alpha = T^T (S^\alpha_0 + \tilde{S}^\alpha_0) \]

Non-Schmid Effect Tensor
\[ \tilde{S}^\alpha_0 = \sum_{i=1}^3 \omega_i \tilde{S}^{i,\alpha}_0 \]
\[ \tilde{S}^{i,\alpha}_0 = m^\alpha_0 \otimes n^\alpha_0, \quad \tilde{S}^{2,\alpha}_0 = (n^\alpha_0 \times m^\alpha_0) \otimes m^\alpha_0, \quad \tilde{S}^{3,\alpha}_0 = (n^\alpha_0 \times m^\alpha_0) \otimes n^\alpha_0 \]
\[ \omega_{0,0} = 0.483, \quad \omega_{2,0} = 0.659, \quad \omega_{0,0,k} = 0.967 \]

Plastic Flow Rule
\[ \dot{\gamma}^\alpha = \dot{\gamma}_0 \exp \left[ \frac{F}{kT} \left( 1 - \frac{|\tau^\alpha|}{s^\alpha - \frac{\mu_0}{\mu_0}} \right)^p \right] \operatorname{sgn}(\tau^\alpha) \]
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Micro-mechanics of Additively Manufactured Materials

\[ s_\rho^\alpha = s_\alpha + \frac{k_{gr}}{\sqrt{d_{gr}}} + \mu b \sum_{\beta} a_{\alpha\beta} \rho^\beta \]

Slip resistance

\[ \dot{\rho}^\alpha = \frac{1}{b} \left( \sqrt{\sum_{\beta} d_{\alpha\beta}^\rho \rho^\beta - 2r_c \rho^\alpha} \right) \]

Dislocation density

\[ d_{\alpha\beta}^\rho = \frac{a_{\alpha\beta}^\rho}{k_e} \]

Intersecting slip systems

\[ d_{\alpha\beta}^{\alpha\beta} = \frac{a_{\alpha\beta}^{\alpha\beta}}{k_{nc}} \]

Self and coplanar systems

\[ r_c = r_{c0} \left( \frac{\gamma_c}{\gamma_0} \right)^{\frac{1}{n}} \]

Annihilation capture radius

316L Stainless Steel

\begin{itemize}
  \item **Wrought**
    \begin{itemize}
      \item Grain size = 15.9 µm
      \item \( \rho_0 = 9.0 \times 10^7 \text{ mm}^2 \)
    \end{itemize}
  \item **Additively Manufactured**
    \begin{itemize}
      \item Grain size = 4.4 µm
      \item \( \rho_0 = 2.3 \times 10^8 \text{ mm}^2 \)
    \end{itemize}
  \item **Additively Manufactured + heat treated**
    \begin{itemize}
      \item Grain size = 18.8 µm
      \item \( \rho_0 = 9.0 \times 10^7 \text{ mm}^2 \)
    \end{itemize}
\end{itemize}

In Collaboration with MST-8
Los Alamos National Laboratory
Explicit Deformation Twin Representation

Deformation Gradient Outside Twin

Deformation Gradient Within Twin

Probabilistic Twin Nucleation

\[
P(\tau > \tau_a) = P\left(N(t) \geq 1\right) = 1 - \exp\left(-\Lambda(\tau)\right)
\]

\[
\Lambda(\tau) = \frac{\tau}{\tau_c}
\]

\[
P(\tau > \tau_a) = 1 - e^{-\Lambda(\tau)} > P_0
\]

Thermal Activated Propagation & Growth

\[
i_{\tau} = v_e \exp\left[-\frac{G_s c}{k\theta} \left(1 - \frac{\tau}{s_i}\right)^\mu \right]
\]

\[
i_{\tau} = v_s \exp\left[-\frac{G_s c}{k\theta} \left(1 - \frac{\tau}{s_i}\right)^\mu \right]
\]
Shock Loaded Ti Bi-crystal

Finite Deformation

\[ \mathbf{F} = \mathbf{F}_{st} \mathbf{F}_{pt} \mathbf{F}_{tw} \]

Finite Elasticity

\[ \mathbf{\sigma} = \frac{1}{\text{det} \mathbf{F}_{st}} \mathbf{F}_{st} \cdot (\mathbf{C} \cdot \mathbf{E}_{st}) \cdot \mathbf{F}_{st}^{-1} \]

Dislocation Slip

\[ \dot{\mathbf{F}}_{sl} \cdot \mathbf{F}_{sl}^{-1} = \sum_i \sum_p c_i \mathbf{y}_{pi} \left( \mathbf{s}_{pi} \otimes \mathbf{m}_{pi} \right) \]

Deformation Twinning

\[ \dot{\mathbf{F}}_{tw} \cdot \mathbf{F}_{tw}^{-1} = \sum_i \dot{c}_i \mathbf{y}_{ni} \otimes \mathbf{m}_i \]

Phase Transformation

\[ \dot{\mathbf{F}}_{pt} = \sum_{i=1}^{13} \dot{c}_i \mathbf{e}_{i, pt} \]

\[ \dot{c}_{i, pt} = \left[ 1 - \left( \frac{X_{i, pt}}{\beta_{pt}} \right) \right] w \frac{X_{i, pt}}{\beta_{pt}} \exp \left( \frac{X_{i, pt}}{\beta_{pt}} \right) \]
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**Computational Framework for Adiabatic Shear Banding**

\[
\int_{\Omega} f(\mathbf{x}) d\Omega \approx \sum_{q=1}^{N_q} J(\mathbf{x}_q) w_q \left[ \frac{V^B q(\mathbf{d}_g)}{V^e} f(\mathbf{x}_q)^B + \left( 1 - \frac{V^B q(\mathbf{d}_g)}{V^e} \right) f(\mathbf{x}_q)^M \right]
\]

**Rate-dependent Nucleation Condition**

Level set function \( \mathcal{G}(\mathbf{x}) \) \:

\[
\nabla \cdot \mathbf{q} = 0 \\
\mathbf{q} = -\kappa_\mathcal{G} \nabla \mathcal{G} \\
\mathcal{G} = \mathcal{G}_0 \\
\mathbf{q} \cdot \mathbf{v} = 0
\]

**Global Level Set via Displacement Field**

**Quadrature Rule with band size and position**

Temperature Evolution:

\[
\dot{\theta} = \frac{\beta k_B}{c_v} \mathbf{\sigma} : \dot{\varepsilon}^{pl} \\
\dot{\chi} = \frac{\kappa_s}{\mu_T} \mathbf{\sigma} : \dot{\varepsilon}^{pl} \left( 1 - \frac{\chi}{\chi_0} \right)
\]

**Effective Temperature Evolution**

\[
\beta = \frac{\chi - \theta}{\chi_0 - \theta}
\]

**Dislocation Density Evolution**

\[
\dot{\rho} = \kappa_1 \frac{\mathbf{\sigma} : \dot{\varepsilon}^{pl}}{v^2 \mu_T} \left( 1 - \frac{\rho}{\rho_{ss}} \right)
\]

**Grain Boundary Density Evolution**

\[
\dot{\xi} = \kappa_d \frac{\mathbf{\sigma} : \dot{\varepsilon}^{pl}}{\mu_T} \left( 1 - \frac{\xi}{\xi_{ss}} \right)
\]

**Plastic Flow Rule**

\[
\dot{\varepsilon}^{pl} = \sqrt{\frac{\rho}{2r}} \frac{S}{s} \exp \left( -\frac{c_p}{\theta} \varepsilon^{-\gamma/s} \right)
\]
Single Crystal Stored Energy of Cold Work

\[ \chi = \frac{\partial U_C}{\partial S_C} \]

**Effective Temperature (Stored Energy)**

\[ S_D = -\sum_a \left( -\rho a \ln (\alpha a \rho a) + \rho a \right) \]

**Dislocation Entropy and Energy Densities**

\[ U_D = \frac{1}{2} \left( \sum_a \sum_{\beta} f^{ab\beta} \rho a \rho \beta \right) \]

**Dislocation Density Evolution**

\[ \dot{\rho a} = \frac{\rho a}{\mu} \left( 1 - \frac{\rho a}{\rho a} \right) \]

**Effective Temperature (Stored Energy) Evolution**

\[ \dot{\chi} = \frac{K_{\chi}}{e_{D}} \left( \sum_{\beta} \epsilon^\beta \dot{\gamma}^\beta \right) \]

**Thermal Temperature Evolution**

\[ \dot{T} = \frac{1}{\rho B c_p} \left( \beta_T \sum_{\beta} \epsilon^\beta \dot{\gamma}^\beta + K \nabla^2 T \right) \]

**Slip System Flow Rule**

\[ \dot{\gamma}^\alpha = \frac{\rho a}{\alpha a} \frac{b}{b_0} \exp \left( -\frac{T_D}{T} e^{-v/a} \right) \]
To Learn More

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