Prof. Curt Bronkhorst

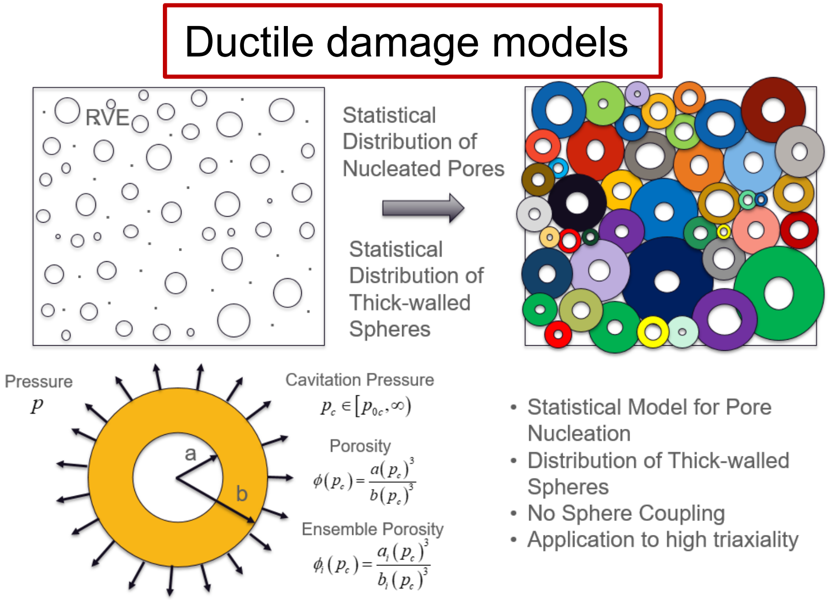
Engineering Physics Department

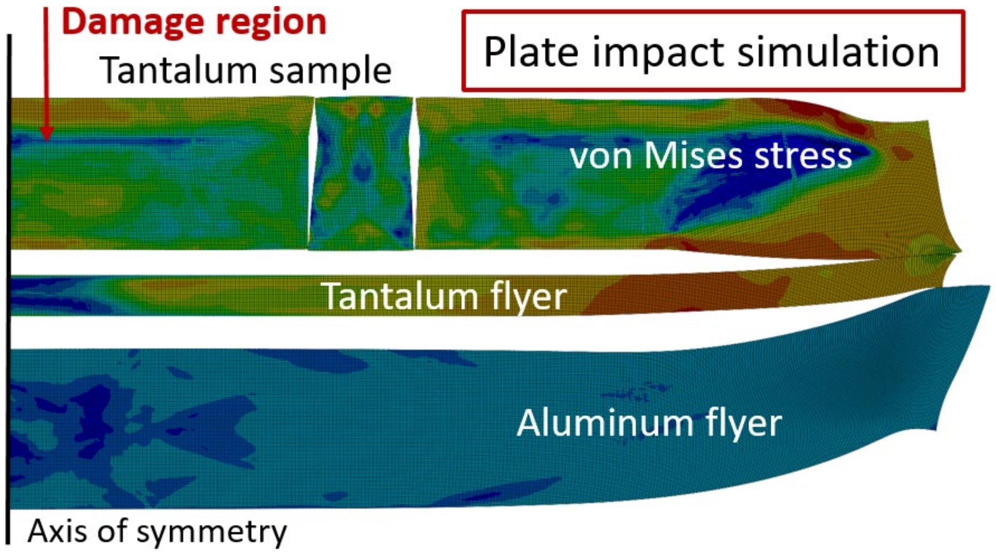
Theoretical and Computational Mechanics of Materials Group

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.

Theoretical and Computational Mechanics of Materials Group





Theoretical and Computational Mechanics of Materials Group

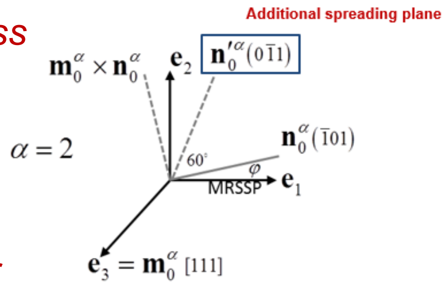
Non-Schmid Crystal Plasticity

$\tau^\alpha = \left(\mathbf{C}^*\mathbf{T}^*\right)\mathbf{S}_0^\alpha \approx \mathbf{T}^*\mathbf{S}_0^\alpha$ *Resolved Shear Stress*

$\mathbf{S}_0^\alpha = \mathbf{m}_0^\alpha \otimes \mathbf{n}_0^\alpha$ *Schmid Tensor*

$\tilde{\tau}^\alpha = \mathbf{T}^*\left(\mathbf{S}_0^\alpha + \tilde{\mathbf{S}}_0^\alpha\right)$

$\tilde{\mathbf{S}}_0^\alpha = \sum_{i=1}^{3} \omega_i \tilde{\mathbf{S}}_0^{i,\alpha}$ *Non-Schmid Effect Tensor*



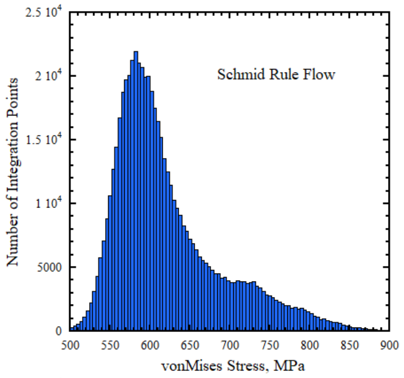
$\tilde{\mathbf{S}}_0^{1,\alpha} = \mathbf{m}_0^\alpha \otimes \mathbf{n}'^\alpha_0,\ \tilde{\mathbf{S}}_0^{2,\alpha} = \left(\mathbf{n}_0^\alpha \times \mathbf{m}_0^\alpha\right) \otimes \mathbf{n}_0^\alpha,\ \tilde{\mathbf{S}}_0^{3,\alpha} = \left(\mathbf{n}'^\alpha_0 \times \mathbf{m}_0^\alpha\right) \otimes \mathbf{n}'^\alpha_0$

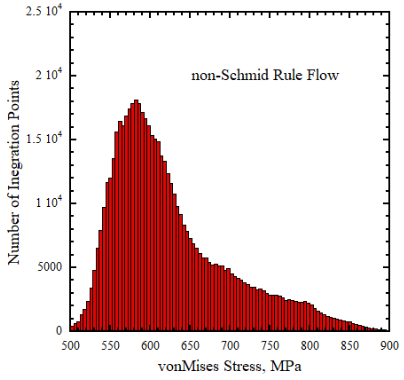
$\omega_{1,0K} = 0.483$

$\omega_{2,0K} = 0.659$

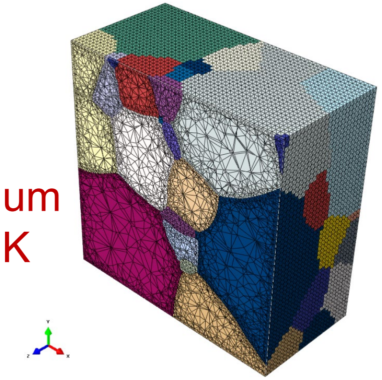
$\omega_{3,0K} = 0.967$

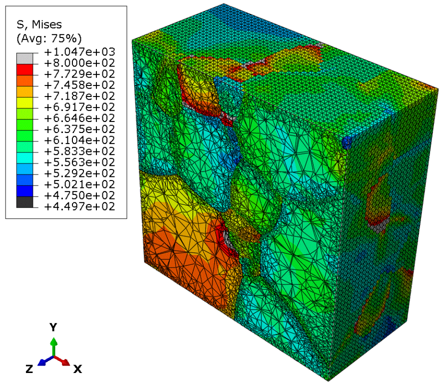
$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \exp\left[-\frac{F_0}{k\theta}\left\langle 1 - \left\langle \frac{\left|\tilde{\tau}^\alpha\right| - s^\alpha \frac{\mu}{\mu_0}}{s_l^\alpha \frac{\mu}{\mu_0}} \right\rangle^p \right\rangle^q\right] \operatorname{sgn}\left(\tau^\alpha\right)$$ *Plastic Flow Rule*





Tantalum
298 K





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Micro-mechanics of Additively Manufactured Materials

$$s_{\rho}^{\alpha} = s_{\infty} + \frac{k_{gr}}{\sqrt{d_{gr}}} + \mu b \sqrt{\sum_{\beta} a^{\alpha\beta} \rho^{\beta}}$$ *Slip resistance*

$$\dot{\rho}^{\alpha} = \frac{1}{b} \left(\sqrt{\sum_{\beta} d^{\alpha\beta} \rho^{\beta}} - 2 r_c \rho^{\alpha} \right) \left| \dot{\gamma}^{\alpha} \right|$$ *Dislocation density*

$$d^{\alpha\beta} = \frac{a^{\alpha\beta}}{k_c^2}$$ *Intersecting slip systems*

$$d^{\alpha\beta} = \frac{a^{\alpha\beta}}{k_{nc}^2}$$ *Self and coplanar systems*

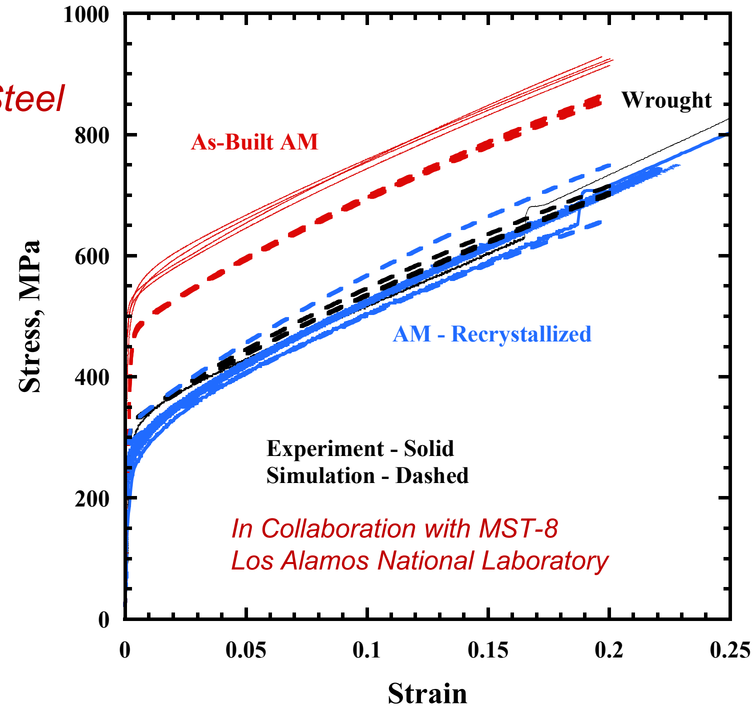
$$r_c = r_{c0} \left(\frac{\left| \dot{\gamma}^{\alpha} \right|}{\dot{\gamma}_0} \right)^{\frac{k\theta}{A}}$$ *Annihilation capture radius*

316L Stainless Steel

Wrought
Grain size = 15.9 μm
ρ_0 *= 9.0 × 10*^{7} *mm*^{2}

Additively Manufactured
Grain size = 4.4 μm
ρ_0 *= 2.3 × 10*^{8} *mm*^{2}

Additively Manufactured + heat treated
Grain size = 18.8 μm
ρ_0 *= 9.0 × 10*^{7} *mm*^{2}



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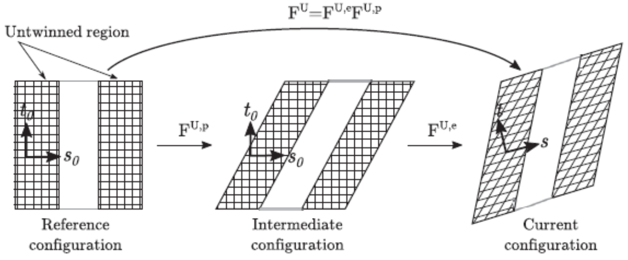
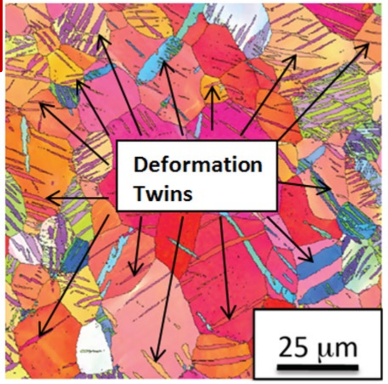
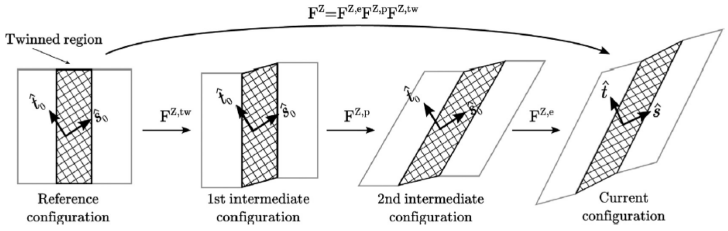
Explicit Deformation Twin Representation

Deformation Gradient Outside Twin



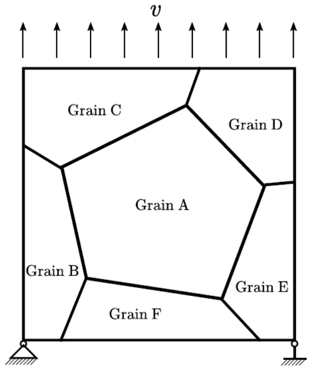


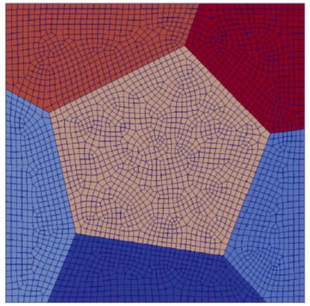
Deformation Gradient Within Twin



Thermal Activated Dislocation Glide

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \exp\left[-\frac{F_0}{k\theta}\left\langle 1 - \left\langle \frac{|\tau^\alpha|}{\frac{\mu}{\mu_0}\left(s_\rho^\alpha + s_l^\alpha\right)} \right\rangle^p \right\rangle^q\right] \mathrm{sgn}\left(\tau^\alpha\right)$$



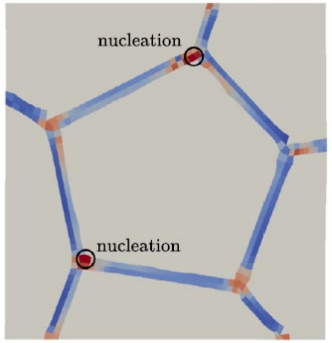


Probabilistic Twin Nucleation

$$P(\tau > \tau_n) = P\left(N(\tau) \geq 1\right) = 1 - \exp\left(-\Lambda(\tau)\right)$$

$$\Lambda(\tau) = \left(\frac{\tau}{\tau_c}\right)^\beta$$

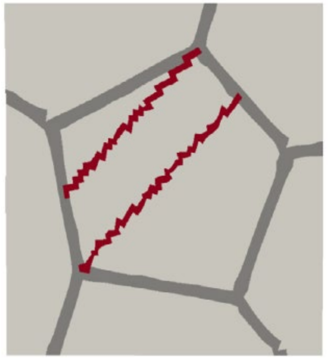
$$P\left(\tau > \tau_n\right) = 1 - e^{-\Lambda(\tau)} > P_0$$



Thermal Activated Propagation & Growth

$$\dot{l}_{tw} = v_l \exp\left[\frac{-G_{tw}}{k\theta}\left\langle 1 - \left(\frac{\tau}{s_l}\right)^p \right\rangle^q\right]$$

$$\dot{b}_{tw} = v_b \exp\left[\frac{-G_{tw}}{k\theta}\left\langle 1 - \left(\frac{\tau}{s_l}\right)^p \right\rangle^q\right]$$



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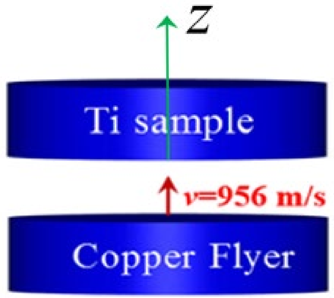


Thermo-mechanics of Single Crystal Phase Transformation

Finite Deformation $\mathbf{F} = \mathbf{F}_e \mathbf{F}_{sl} \mathbf{F}_{pt} \mathbf{F}_{tw}$

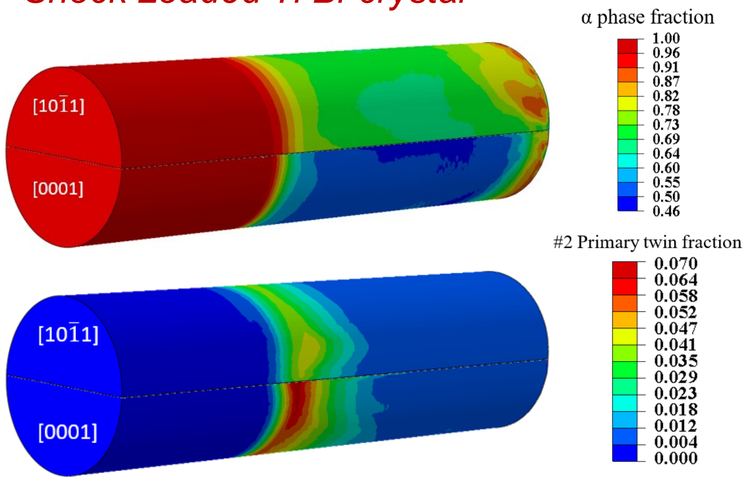
Finite Elasticity $\boldsymbol{\sigma} = \left(\frac{1}{\det \mathbf{F}_e} \cdot \mathbf{F}_e \cdot (\mathbf{C} : \mathbf{E}_e) \cdot \mathbf{F}_e^t \right)_{dev} - p_{eos}\mathbf{I} \qquad p_{eos} = -\frac{\partial \psi_{eos}}{\partial v}$

Dislocation Slip $\dot{\mathbf{F}}_{sl} \cdot \mathbf{F}_{sl}^{-1} = \sum_i \sum_\beta c_i \dot{\gamma}_{\beta i} \left(\mathbf{s}_{\alpha i} \otimes \mathbf{m}_{\alpha i} \right) \qquad \dot{\gamma}_{\beta i} = b_{\beta i} \rho_{M \beta i} v_{\beta i}$

Deformation Twinning $\dot{\mathbf{F}}_{tw} \cdot \mathbf{F}_{tw}^{-1} = \sum_i \dot{c}_{i-tw} \gamma_{tw} \mathbf{b}_i \otimes \mathbf{n}_i \qquad \dot{c}_{i-tw}\big|_{i=1,2,\ldots,6} = \left(1 - \sum_{j=7}^{13} c_j \right) \left(1 - c_i^{b_0} \right) \frac{\dot{\gamma}_0}{\gamma_{tw}} \left(\frac{\tau_{tw-i}}{S_{tw}} \right)^{d_0}$

Phase Transformation $\dot{\mathbf{F}}_{pt} = \sum_{i=7}^{13} \dot{c}_i \boldsymbol{\varepsilon}_{i-pt} \qquad \dot{c}_{i-pt} = \left[1 - \left(c_{i-pt} \right)^{p_1} \right] w \frac{X_{i-pt}}{\beta_{tr}} \exp\left\{ \left(\frac{X_{i-pt}}{\beta_{tr}} \right)^{q_1} \right\}$

Shock Loaded Ti Bi-crystal



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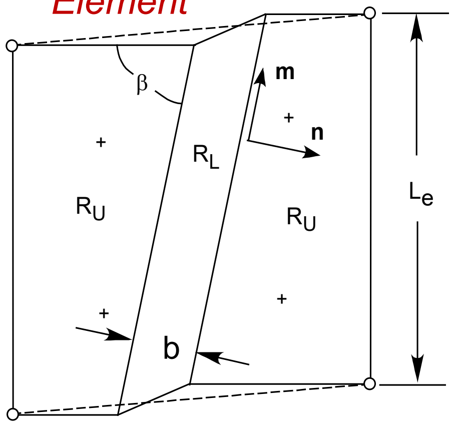
Computational Framework for Adiabatic Shear Banding

Embedded Weak Discontinuity Element



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

Quadrature Rule with band size and position

$$\text{Level set function } \vartheta(\mathbf{x}) \Rightarrow \begin{cases} \nabla\cdot\mathbf{q}=0 \\ \mathbf{q}=-\kappa_\vartheta\cdot\nabla\vartheta \\ \vartheta=\vartheta_0 \\ \mathbf{q}\cdot\mathbf{v}=0 \end{cases}$$

$$\kappa_\vartheta = (1+\varepsilon)\mathbf{1}-\mathbf{n}\otimes\mathbf{n}$$

Global Level Set via Displacement Field

$$\dot{\theta} = \frac{\beta k_B}{c_v}\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}^{pl}$$

Temperature Evolution

$$-\frac{\beta}{\rho c_v}\frac{\partial\hat{\sigma}_f}{\partial\theta} > \frac{1}{\hat{\sigma}_f}\frac{\partial\hat{\sigma}_f}{\partial\bar{\varepsilon}^{vp}}$$

Rate-dependent Nucleation Condition

$$\dot{\chi} = \frac{\kappa_2}{\mu_T}\boldsymbol{\sigma}:\boldsymbol{\varepsilon}^{pl}\left(1-\frac{\chi}{\chi_0}\right)$$

Effective Temperature Evolution

$$\dot{\boldsymbol{\varepsilon}}^{pl} = \frac{\sqrt{\rho}}{2\tau}\frac{\mathbf{S}}{\bar{s}}\exp\left(-\frac{e_p}{\theta}e^{-s/s_T}\right)$$

Plastic Flow Rule

$$\dot{\rho} = \kappa_1\frac{\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}^{pl}}{\nu^2\mu_T}\left(1-\frac{\rho}{\rho_{ss}}\right)$$

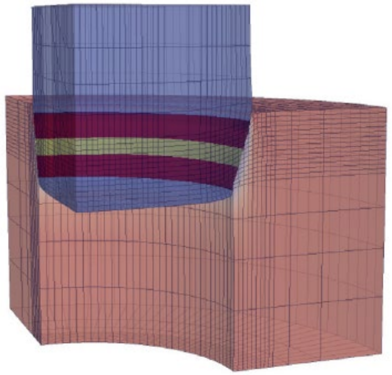
Dislocation Density Evolution

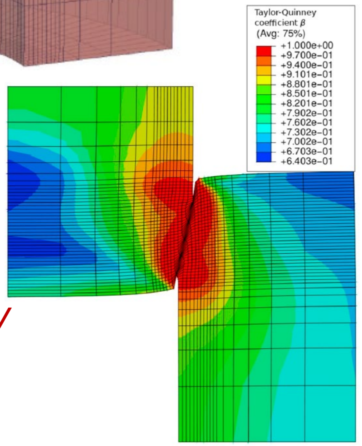
$$\beta = \frac{\chi-\theta}{\chi_0-\theta}$$

Taylor-Quinney Coefficient

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

Grain Boundary Density Evolution





Theoretical and Computational Mechanics of Materials Group

Single Crystal Stored Energy of Cold Work

$$U_{tot} = U_K + U_C$$
$$S_{tot} = S_K + S_C$$

Kinetic, Configuration Energy and Entropy

$$\chi \equiv \frac{\partial U_C}{\partial S_C}$$

Effective Temperature (Stored Energy)

$$\beta_T \approx \frac{\chi}{\chi_{ss}}$$

Taylor-Quinney Coefficient

$$S_D = \frac{1}{a}\sum_{\alpha}\left[-\rho^{\alpha}\ln\left(a^2\rho^{\alpha}\right)+\rho^{\alpha}\right]$$

$$U_D = \frac{1}{a}\left(\sum_{\alpha} e_D\rho^{\alpha} + \frac{b^2 e_N}{2}\sum_{\alpha}\sum_{\beta} f^{\alpha\beta}\rho^{\alpha}\rho^{\beta}\right)$$

Dislocation Entropy and Energy Densities

$$\dot{\rho}^{\alpha} = \frac{\kappa_{\rho}^{\alpha}}{a^2}\frac{\tau^{\alpha}\dot{\gamma}^{\alpha}}{\mu}\left(1-\frac{\rho^{\alpha}}{\rho_{ss}^{\alpha}}\right)$$

Dislocation Density Evolution

$$\frac{\dot{\chi}}{e_D} = \frac{\kappa_{\chi}}{\mu}\left[\sum_{\beta}\tau^{\beta}\dot{\gamma}^{\beta}\left(1-\frac{\chi}{\chi_{ss}}\right)+K_C\nabla^2\chi\right]$$

Effective Temperature (Stored Energy) Evolution

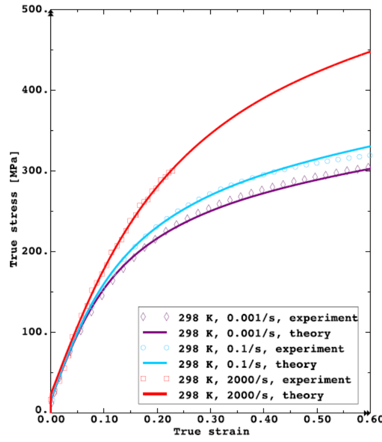
$$\dot{T} = \frac{1}{\bar{\rho}_M c_p}\left[\beta_T\sum_{\beta}\tau^{\beta}\dot{\gamma}^{\beta}+K\nabla^2 T\right]$$

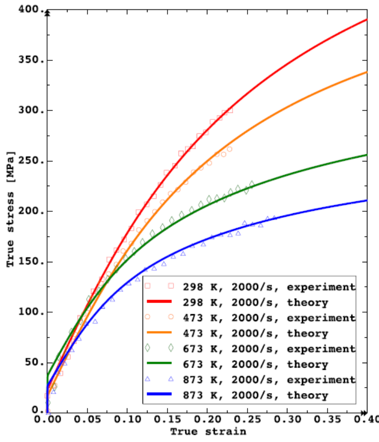
Thermal Temperature Evolution

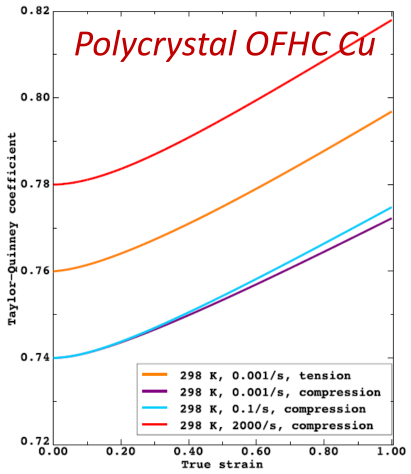
$$\dot{\gamma}^{\alpha} = \frac{\rho^{\alpha}l^{\alpha}b}{t_0}\exp\left(-\frac{T_P}{T}e^{-\tau^{\alpha}/s_T^{\alpha}}\right)$$

Slip System Flow Rule

Parameter	Definition or meaning	Value
$\bar{\rho}_M$	Mass density	8960 kg m^{-3}
c_p	Specific heat capacity	380 J kg^{-1} K^{-1}
C_{11}^0	Elastic moduli parameter	179.5 GPa
m_{11}	Elastic moduli parameter	–36.3 MPa K^{-1}
C_{12}^0	Elastic moduli parameter	126.4 GPa
m_{12}	Elastic moduli parameter	–16.4 MPa K^{-1}
C_{44}^0	Elastic moduli parameter	82.5 GPa
m_{44}	Elastic moduli parameter	25.7 MPa K^{-1}
μ_1	Shear modulus adjustment	6 GPa
α_T	Stress scale parameter	2
b	Burgers vector	0.257 nm
a^{self}	Dislocation interaction coefficient	0.122
a^{copl}	Dislocation interaction coefficient	0.122
a^{hirth}	Dislocation interaction coefficient	0.070
a^{colli}	Dislocation interaction coefficient	0.625
a^{gliss}	Dislocation interaction coefficient	0.137
a^{lomer}	Dislocation interaction coefficient	0.122
k_c	Mean free path parameter	12.0
k_{nc}	Mean free path parameter	180.0
a	Atomic length scale	5.14 nm
$(a/b)t_0$	Atomic time scale	1 ps
T_P	Depinning barrier	40800 K
χ_{ss}	Steady-state effective temperature (in units of e_D)	0.25
κ_1^{α}	Hardening parameter	100.0
κ_{χ}	Effective temperature increase rate	6.0







Large Deformation

Evolving Taylor-Quinney Coefficient

To Learn More

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UW Web Site: https:/directory.engr.wisc.edu/ep/Faculty/Bronkhorst_Curt/

Group Web Site: https://uwtcmmg.wiscweb.wisc.edu/group-overview/