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A multi-scale model of dislocation plasticity in α-Fe: Incorporating temperature, strain rate and non-Schmid effects

Hojun Lim[1], Lucas Hale[2], Jonathan Zimmerman[3], Corbett Battaile[1] and Christopher Weinberger[4]

[1]Computational Materials & Data Science, [3]Materials Physics,
Sandia National Laboratories

[2]Thermodynamics and Kinetics Group,
National Institute of Standards and Technology

[4]Department of Mechanical Engineering & Mechanics,
Drexel University

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Outline

- **Introduction**
- **BCC plasticity model**
- **Atomistic calculations**
- **CP-FEM calculations**
- **Summary**

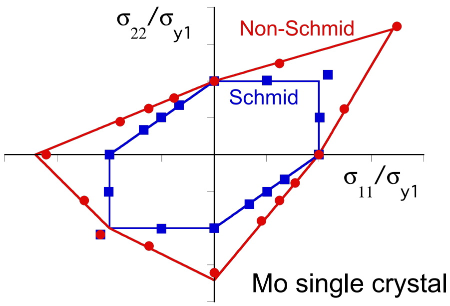
Lim, H., Hale, L. M., Zimmerman, J. A., Battaile, C. C., Weinberger, C. R., "A Multi-scale Model of Dislocation Plasticity in α-Iron: Incorporating Temperature, Strain Rate and Non-Schmid Effects", *Int. J. Plasticity*, 2015, In press.

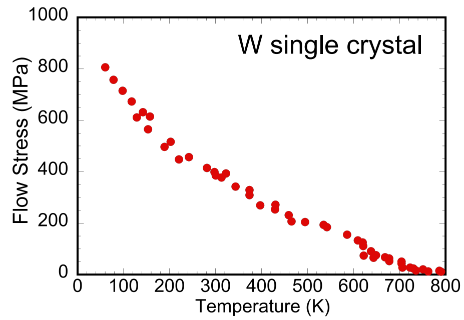
Hale, L. M., Lim, H., Weinberger, C. R., Zimmerman, J. A., Battaile, C. C., "Insights on Activation Enthalpy for Non-Schmid Slip in BCC Metals" *Scripta Mat.*, 2015, 99. 89-92.

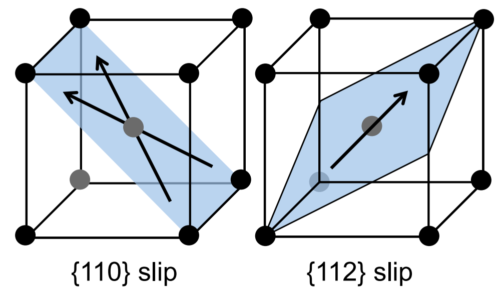
Introduction

❖ Need *physically-based* model for BCC metals

- **Complex response compared to FCC**
  - *Non-Schmid effects*, *large temp. & rate dep. flow behavior,* ambiguity of slip systems,



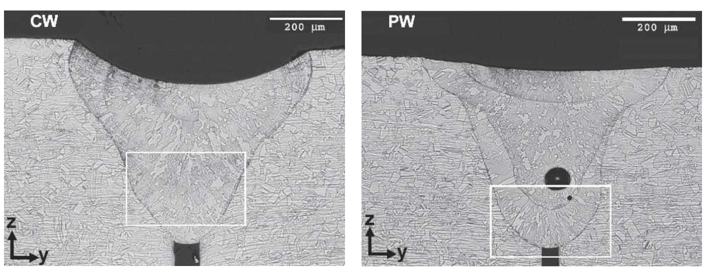




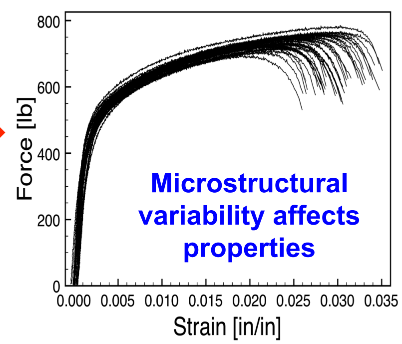
- **Most BCC models are phenomenological, fit from polycrystals**

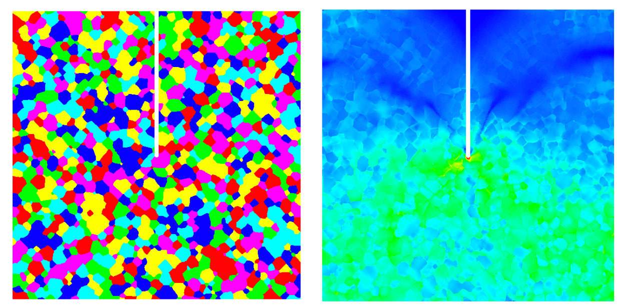
❖ Need capability to include *microstructural variability* in design

- **Connecting microstructural variability to stochastic performance**



Microstructural details vary among 304L stainless steel weldments





CP-FEM simulations

Develop capability for low rate deformation of BCC metals

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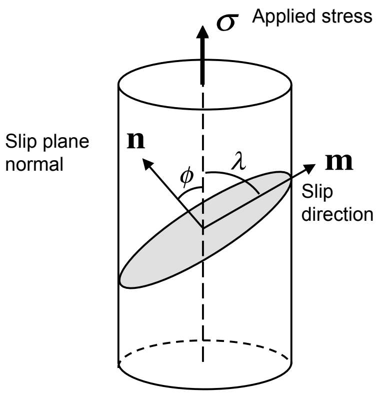
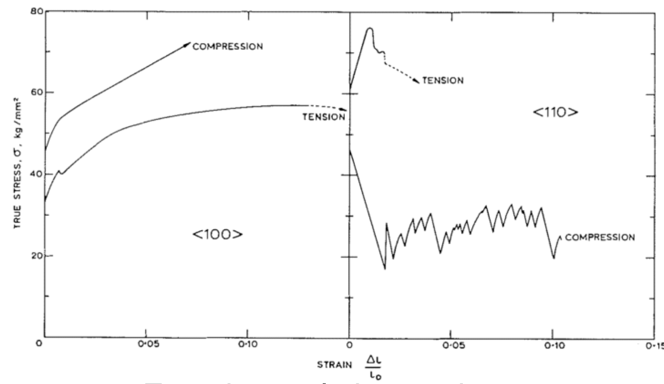
Unusual yield behavior

$$\tau = \sigma \cos\lambda \cos\varphi$$

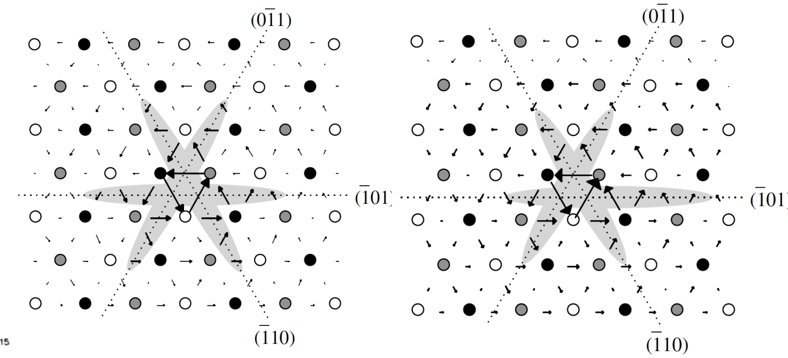


Schmid's law

Non-Schmid yield behavior



Experimental observations:
Tension-Compression Asymmetry in Nb
(Sherwood et.,1967)



Atomistic understanding:
Non-planar crew dislocation cores
(Groger et al., 2008)

$$\tau_{cr}^{\alpha} = \mathbf{P}_{tot}^{\alpha} : \sigma = \mathbf{P}_{S}^{\alpha} : \sigma + \mathbf{P}_{nS}^{\alpha} : \sigma$$

Schmid — Non-Schmid

Generalized non-Schmid yield law

$$\mathbf{P}_{S}^{\alpha} = \frac{1}{2}\left(\mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha} + \mathbf{n}^{\alpha} \otimes \mathbf{m}^{\alpha}\right)$$

$\mathbf{m}$: slip direction
$\mathbf{n}$: slip plane normal
$\mathbf{t} = \mathbf{m} \times \mathbf{n}$

$$\mathbf{P}_{nS}^{\alpha} = c_1 \mathbf{t}^{\alpha} \otimes \mathbf{m}^{\alpha} + c_2 \mathbf{t}^{\alpha} \otimes \mathbf{n}^{\alpha} + c_3 \mathbf{n}^{\alpha} \otimes \mathbf{n}^{\alpha} + c_4 \mathbf{t}^{\alpha} \otimes \mathbf{t}^{\alpha} + c_5 \mathbf{m}^{\alpha} \otimes \mathbf{m}^{\alpha}$$

(Lim et al., 2013)

c_i : non-Schmid constants ⟶ *Atomistic simulations*
Single crystal experiments

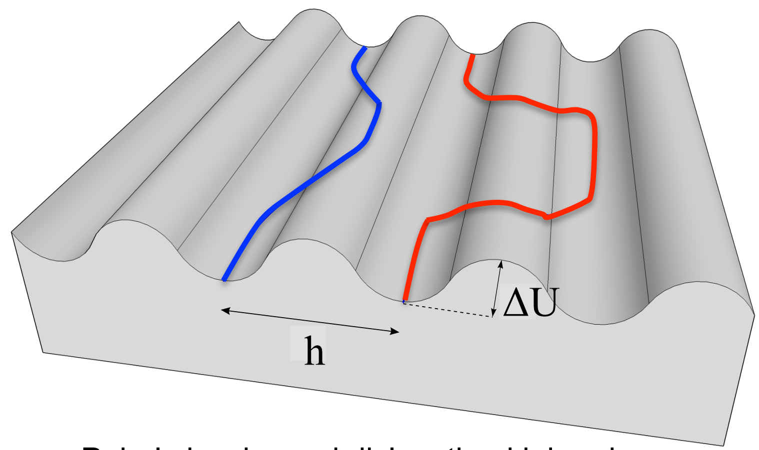
Temperature and strain rate dependent flow

Thermal activation in BCC metals

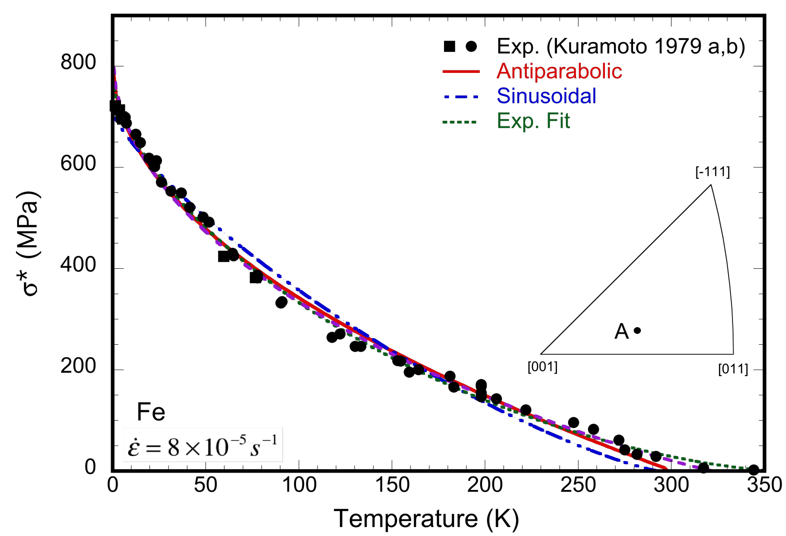
$$\dot{\gamma} = \dot{\gamma}_0 \exp\left(\frac{-\Delta H}{k_B T}\right)$$

$$\Delta H(\tau) = 2H_k \left[1 - \left(\frac{\tau}{\tau_p}\right)^p\right]^q$$

$$\tau = \tau_p \left[1 - \left(\frac{k_B T}{2H_k} \ln\left(\frac{\dot{\gamma}_0}{\dot{\gamma}}\right)\right)^{1/q}\right]^{1/p}$$



Peierls barrier and dislocation kink-pair



Option: Fit Experimental data

p=0.71, q=1.85

Temp & Strain Rate dependence captured

Flow rule incorporating T, ė and Non-Schmid Effect

❖ Non-Schmid yield behavior: scaling law derived from atomistics

$$\frac{\tau^{MRSSP}}{CRSS} = \frac{c_1\mathbf{P}_S : \sigma + c_1\mathbf{P}_{nS}^{mt} : \sigma}{\tau_{cr} - c_2\mathbf{P}_{nS}^{tn} : \sigma - c_3\mathbf{P}_{nS}^{nn} : \sigma - c_4\mathbf{P}_{nS}^{tt} : \sigma - c_5\mathbf{P}_{nS}^{mm} : \sigma}$$

(Hale et al., 2014)

$\mathbf{P}_{nS}^{\alpha,uv} = \mathbf{u}^{\alpha} \otimes \mathbf{v}^{\alpha}$

$\mathbf{m}$: slip direction

$\mathbf{n}$: slip plane normal

$\mathbf{t} = \mathbf{m} \times \mathbf{n}$

❖ Temperature and strain rate dependence: thermally activated flow

$$\frac{\tau^{MRSSP}}{CRSS} = \left(1 - \left(\frac{T}{T_c}\right)^{1/q}\right)^{1/p}$$

$$T_c = \frac{H_0}{k_B \ln\left(\dot{\gamma}_0 / \dot{\gamma}\right)}$$

(Kocks et al., 1975)

H_0 : energy barrier

$\dot{\gamma}_0$: ref. strain rate

p, q : mat. constants

❖ Resolved shear stress

$$\tau^{*\alpha} = B\left(T, \dot{\gamma}^{\alpha}\right)\left[\tau_{cr} - c_2\mathbf{P}_{nS}^{\alpha,tn} : \sigma - c_3\mathbf{P}_{nS}^{\alpha,nn} : \sigma - c_4\mathbf{P}_{nS}^{\alpha,tt} : \sigma - c_5\mathbf{P}_{nS}^{\alpha,mm} : \sigma\right] - c_1\mathbf{P}_{nS}^{\alpha,mt} : \sigma$$

$$B\left(T, \dot{\gamma}^{\alpha}\right) = \left(1 - \left(\frac{k_B T}{H_0} \ln\left(\dot{\gamma}_0 / \dot{\gamma}\right)\right)^{1/q}\right)^{1/p}$$

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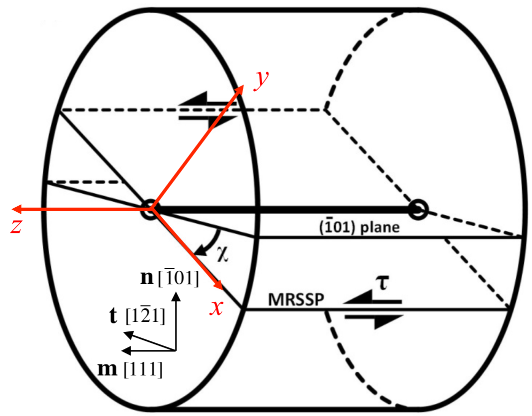
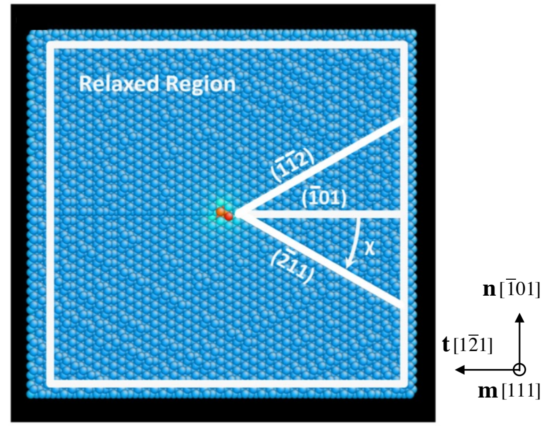
Atomistic simulations

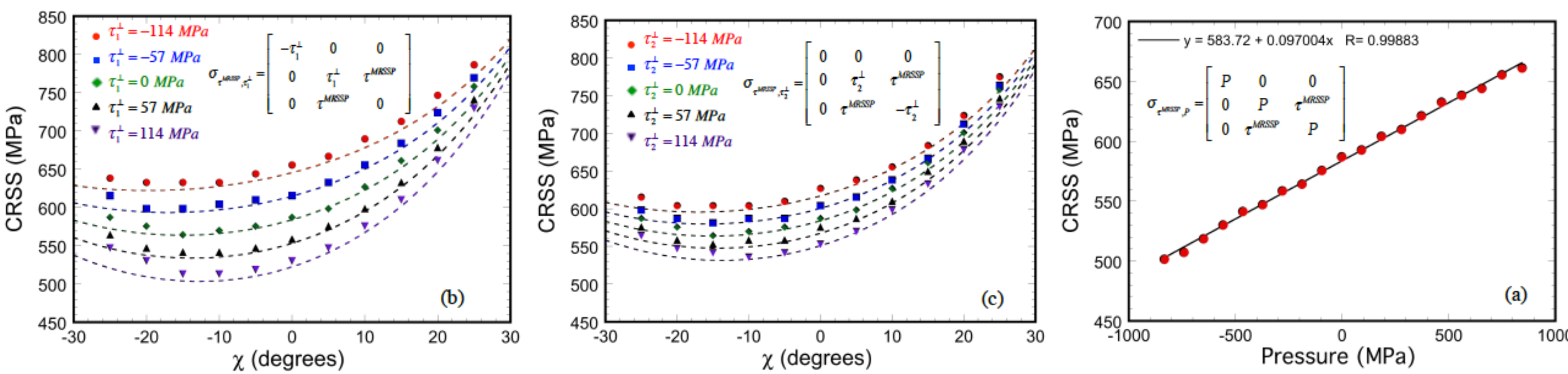
- LAMMPS
- Chamanti's potential
- 552,960 atoms

$24a[\bar{1}2\bar{1}]\times 40a[\bar{1}01]\times 48a[111]$





❖ **Parameterization:** $\tau_{cr} = \mathbf{m}\cdot\sigma\mathbf{n} + c_1\mathbf{m}\cdot\sigma\mathbf{t} + c_2\mathbf{n}\cdot\sigma\mathbf{t} + c_3\mathbf{n}\cdot\sigma\mathbf{n} + c_4\mathbf{t}\cdot\sigma\mathbf{t} + c_5\mathbf{m}\cdot\sigma\mathbf{m}$



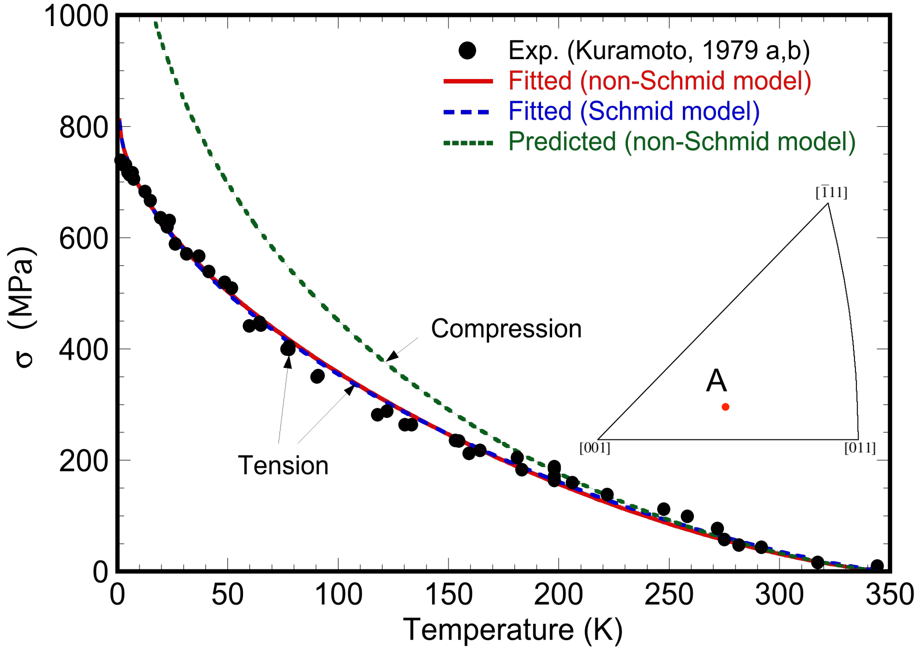
Best-fit c_i and τ_{cr} from atomistics

c_1	c_2	c_3	c_4	c_5	τ_{cr}
0.27	0.15	0.31	-0.23	0.02	584 MPa

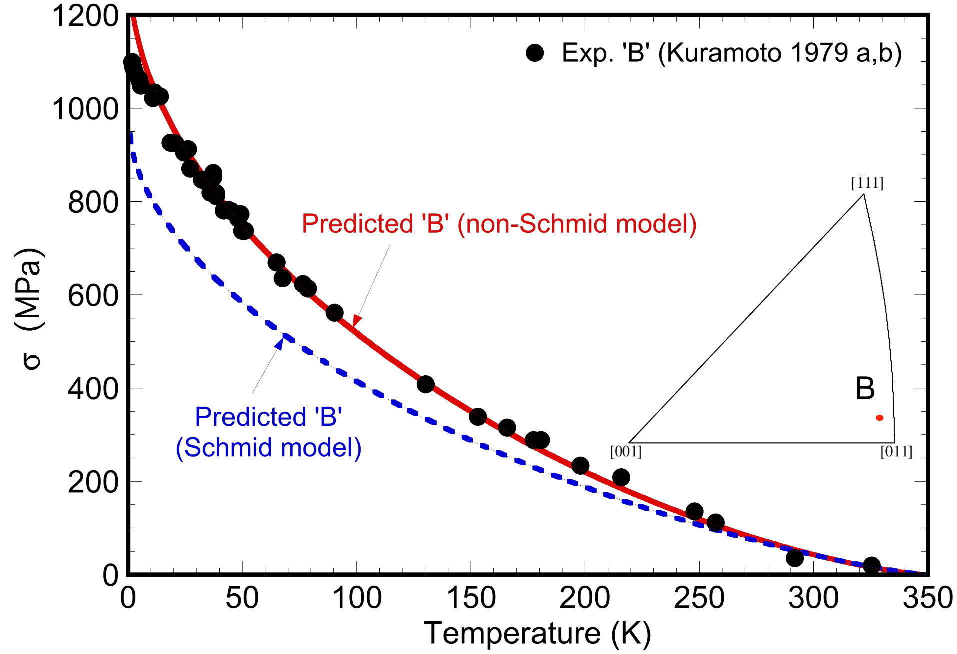
(Fellinger et al., 2010)

Flow stress predictions: α-Fe single crystals

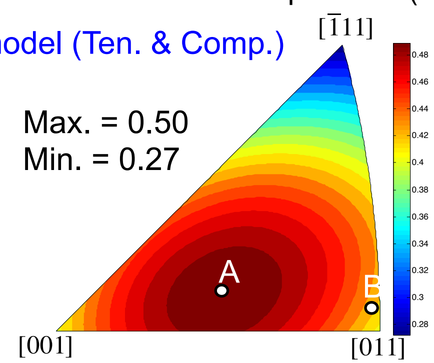
Temperature dependence



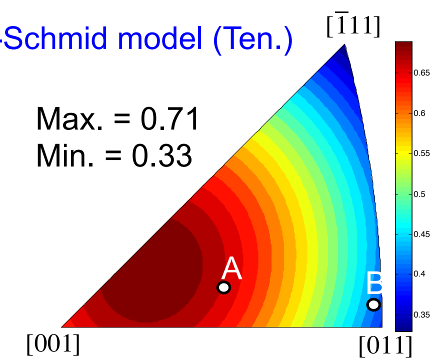
Crystal orientation dependence



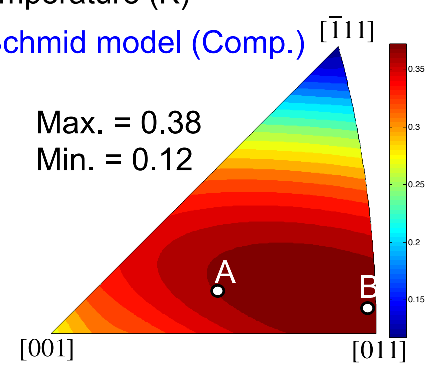
Schmid model (Ten. & Comp.)



Non-Schmid model (Ten.)

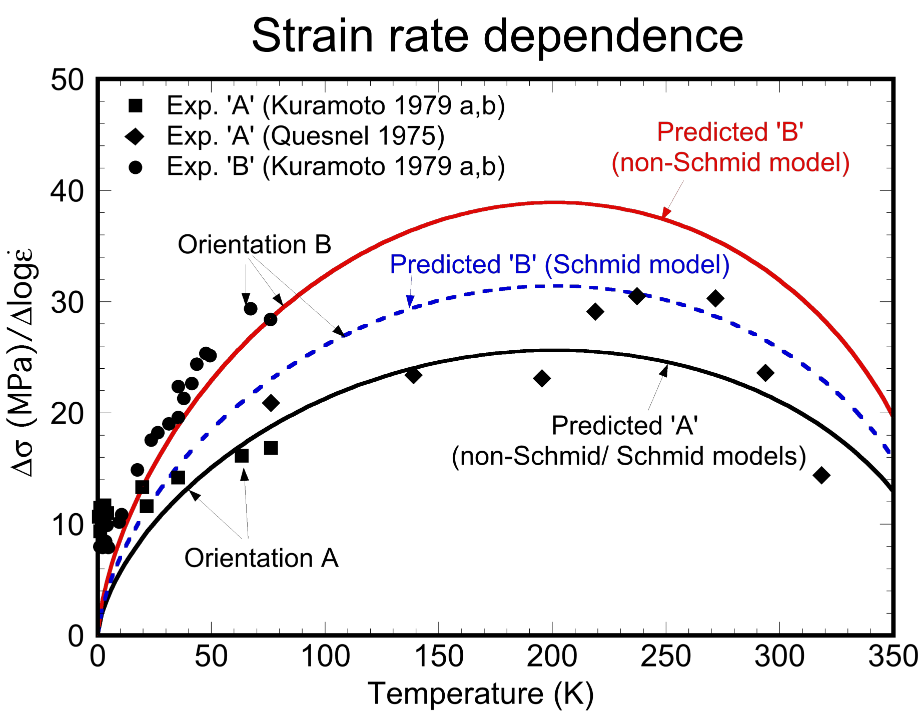


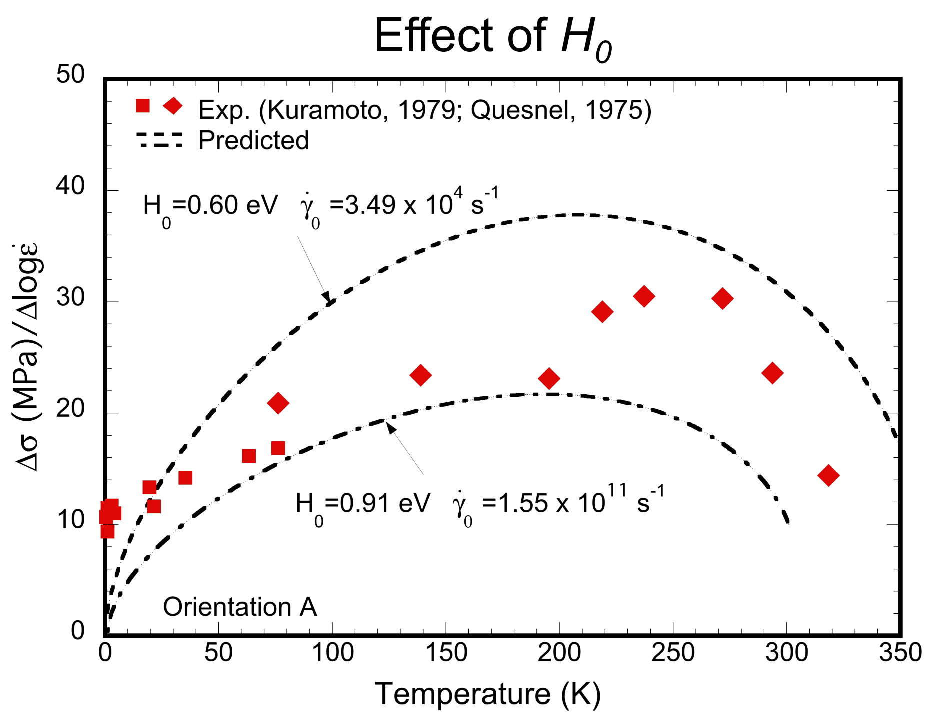
Non-Schmid model (Comp.)



Orientation dependent yield behavior is accurately predicted by non-Schmid model

Strain rate dependence: α-Fe single crystal





$$\tau^{*\alpha} = B\left(T,\dot{\gamma}^{\alpha}\right)\left[\tau_{cr} - c_2\mathbf{P}_{nS}^{\alpha,tn}:\sigma - c_3\mathbf{P}_{nS}^{\alpha,nn}:\sigma - c_4\mathbf{P}_{nS}^{\alpha,tt}:\sigma - c_5\mathbf{P}_{nS}^{\alpha,mm}:\sigma\right] - c_1\mathbf{P}_{nS}^{\alpha,mt}:\sigma$$

$$B\left(T,\dot{\gamma}^{\alpha}\right) = \left(1-\left(\frac{k_B T}{H_0}\ln\left(\dot{\gamma}_0/\dot{\gamma}\right)\right)^{1/q}\right)^{1/p}$$

$$0.60\,eV \le H_0 \le 0.91\,eV$$

Brunner and Diehl, 1991a,b; Proville et al., 2013

Strain rate dependent yield behavior is accurately predicted by non-Schmid model

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BCC CP-FEM model

- Solid mechanics code developed at Sandia National Laboratories (JAS-3D)
- 24 {110}<111> slip systems
- Slip rate: $\dot{\gamma}^{\alpha} = \dot{\gamma}^{0} \left(\frac{\tau^{\alpha}}{g^{\alpha}} \right)^{1/m}$ (Hutchinson, 1976)
- Slip resistance: $g^{\alpha} = \sqrt{(\tau^{*\alpha})^2 + (\tau^{\alpha}_{obs})^2}$

$(\tau^{*\alpha})$ → Lattice friction; (τ^{α}_{obs}) → Obstacle stress

Lattice friction: $\tau^{*\alpha} = B\left(T, \dot{\gamma}^{\alpha}\right)\left[\tau_{cr} - c_2 \mathbf{P}^{\alpha}_{tn} : \sigma - c_3 \mathbf{P}^{\alpha}_{nn} : \sigma - c_4 \mathbf{P}^{\alpha}_{tt} : \sigma - c_5 \mathbf{P}^{\alpha}_{mm} : \sigma\right] - c_1 \mathbf{P}^{\alpha}_{mt} : \sigma$

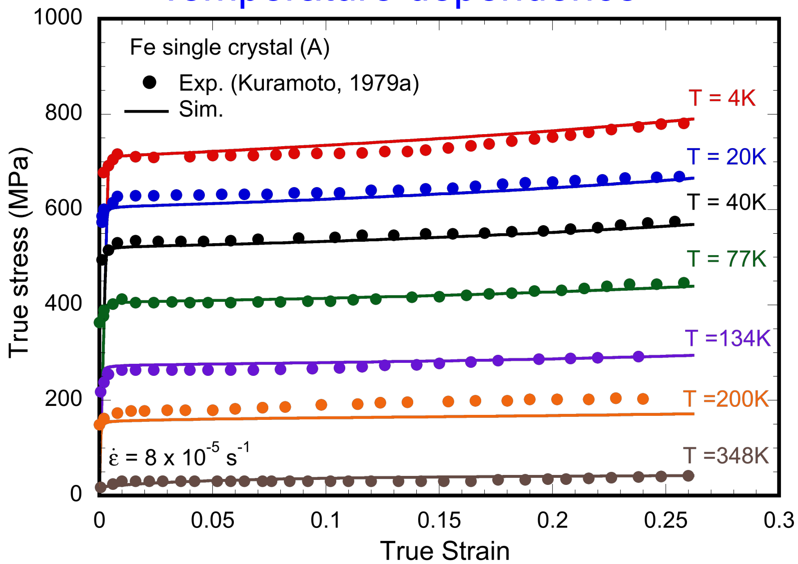
$$B(T, \dot{\gamma}) = \left(1 - \left(\frac{k_B T}{H_0} \ln\left(\dot{\gamma}_0 / \dot{\gamma}\right) \right)^{1/q} \right)^{1/p}$$

Obstacle stress: $\tau^{\alpha}_{obs} = A \mu b \sqrt{\sum_{\beta=1}^{24} \rho^{\beta}}$ (Taylor, 1934)

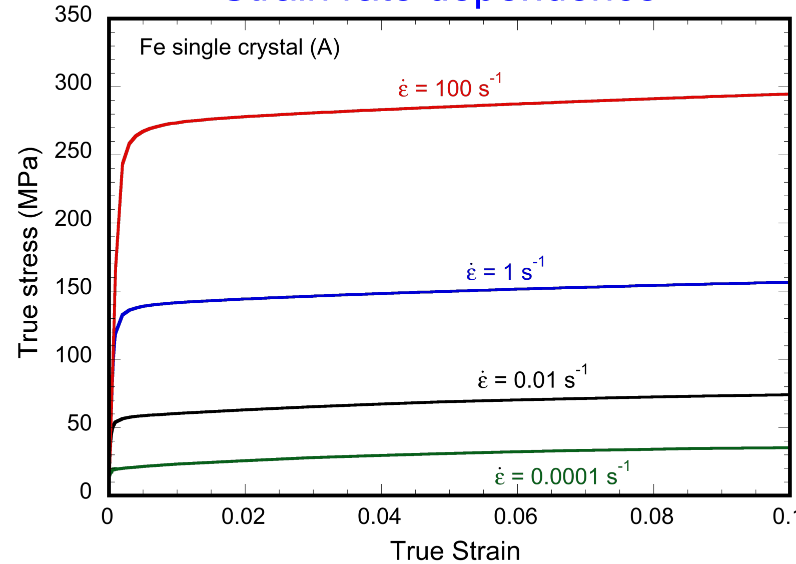
$$\dot{\rho}^{\alpha} = \left(\kappa_1 \sqrt{\sum_{\beta=1}^{\mathrm{NS}} \rho^{\beta}} - \kappa_2 \rho^{\alpha} \right) \cdot |\dot{\gamma}^{\alpha}|$$ (Kocks, 1976)

CP-FE simulations: α-Fe single crystals

Temperature dependence



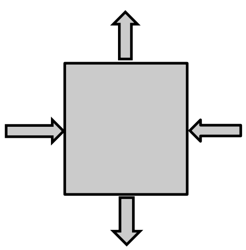
Strain rate dependence

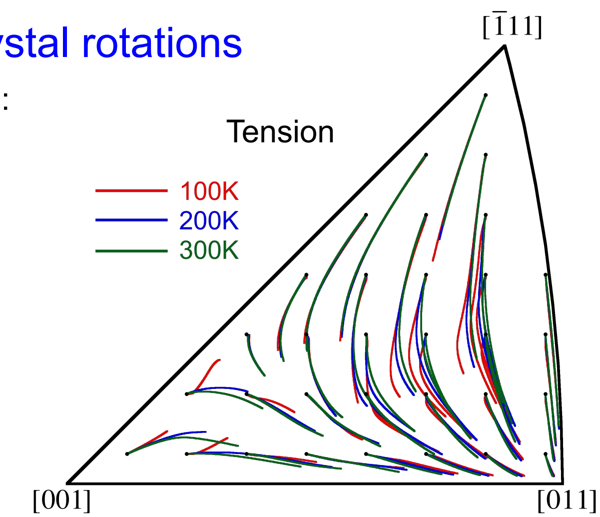


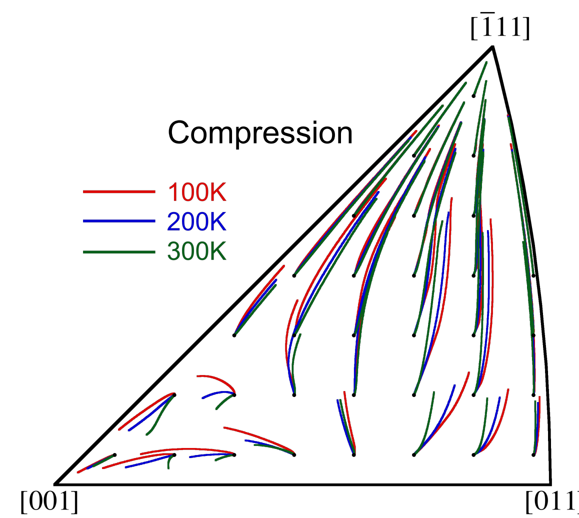
Crystal rotations

Isochoric deformation to 20% strain:

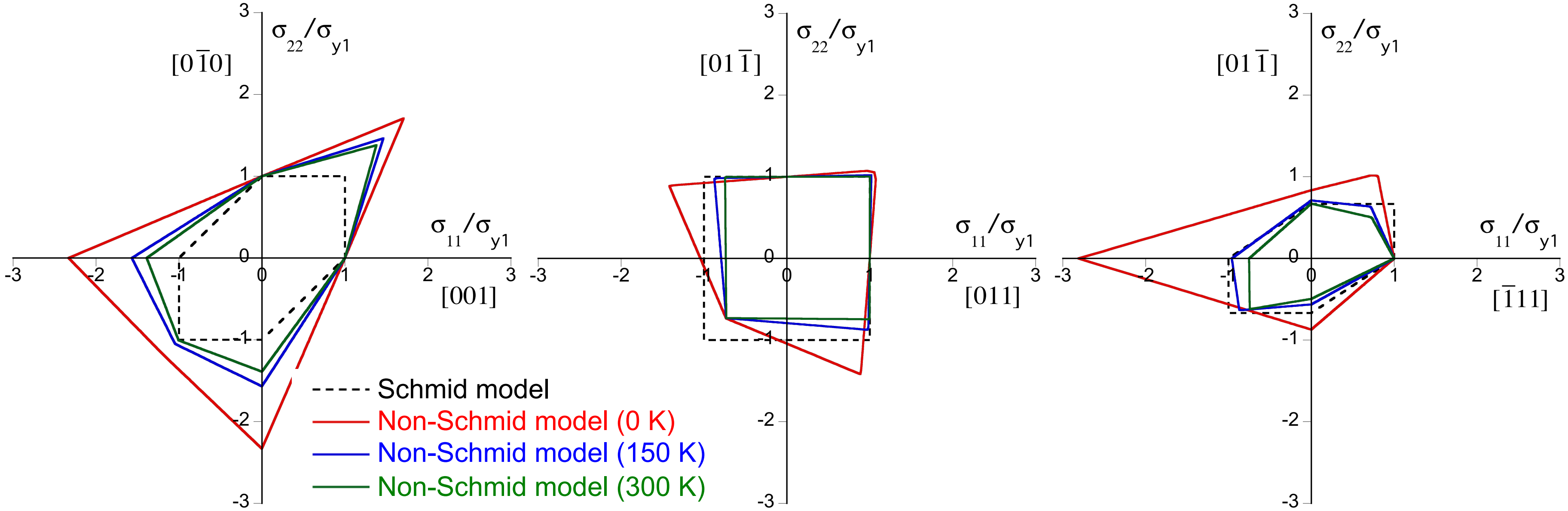
$$\dot{\varepsilon} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1/2 & 0 \\ 0 & 0 & -1/2 \end{pmatrix} dt$$



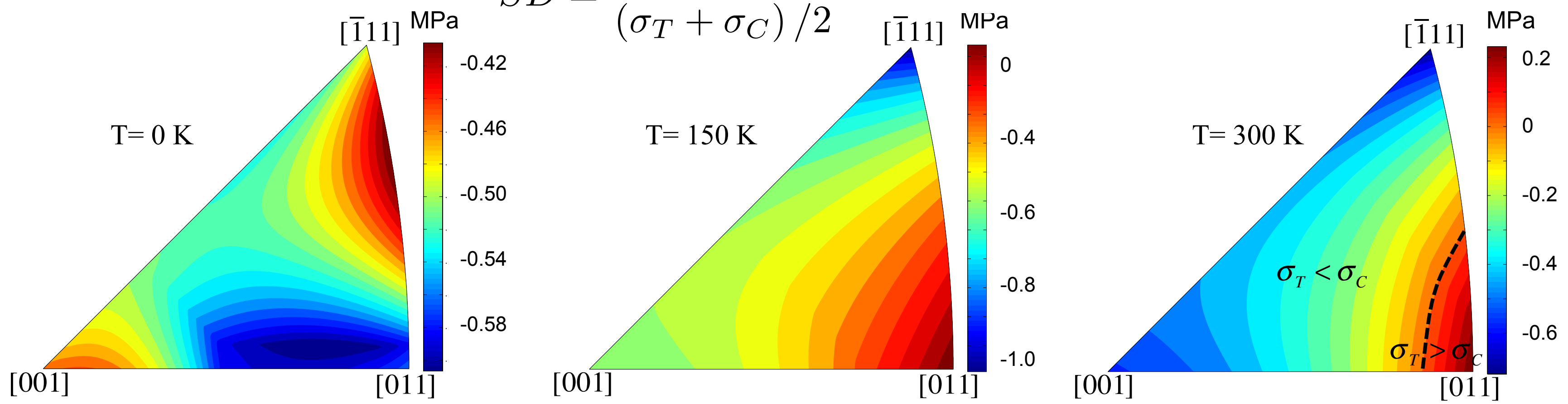




Single crystal deformations

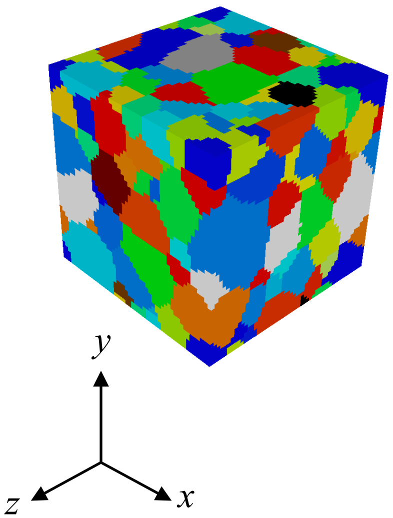


$$SD = \frac{\sigma_T - \sigma_C}{(\sigma_T + \sigma_C)/2}$$

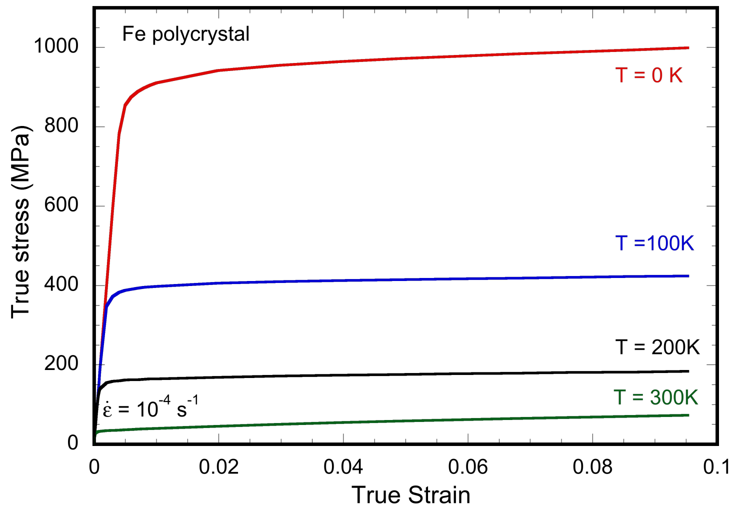


Polycrystal deformations

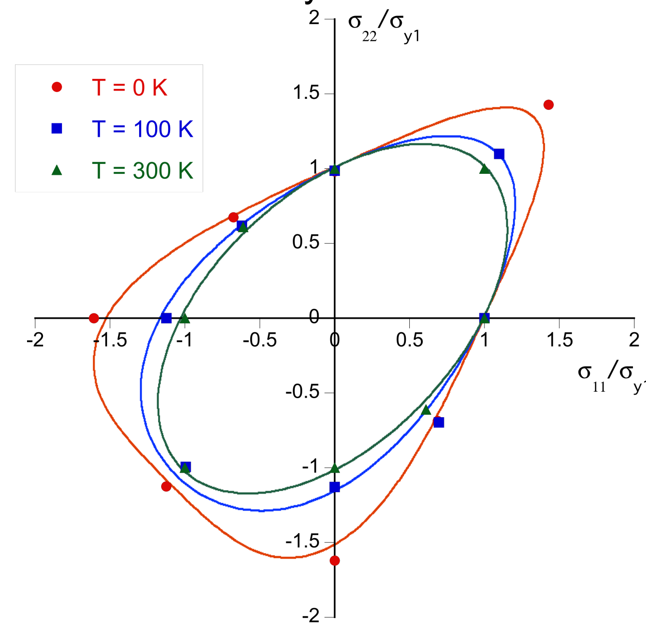
3-D FE model

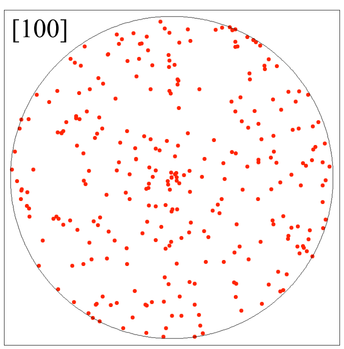


Uniaxial tension: temperature dependence

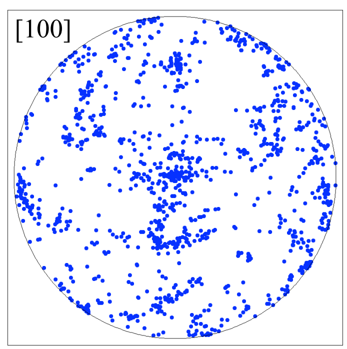


Bi-axial yield surface

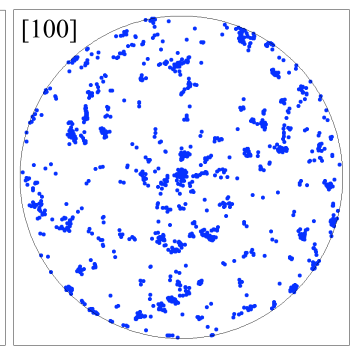




Initial



Deformed (0 K)



Deformed (300 K)

$$f(I_1, J_2, J_3) = \underbrace{\alpha_1 I_1}_{\text{'P dep.'}} + \underbrace{\left(J_2^{3/2} + \alpha_2 J_3\right)}_{\text{'Shape'}}{}^{1/3}$$

I_1 : 1st stress invariant
J_2 : 2nd invariant of deviatoric stress
J_3 : 3rd invariant of deviatoric stress

The model captures temperature dependent stress-strain responses & texture evolution

Summary

- A new BCC plasticity model incorporating temperature, strain rate and non-Schmid effects for bcc iron is proposed.

- Atomistically-informed CP-FE model more accurately predicts temperature and strain rate effects as well as crystal orientation dependent yield stresses.

- Non-Schmid stresses affect stress-strain responses as well as texture evolutions. Non-Schmid effects are more significant at low temperatures and high strain rates.

- Proposed computational method provides a convenient and direct link from the fundamental dislocation physics to the continuum-scale plastic deformation of BCC metals at the grain scale.

THANK YOU !

hnlim@sandia.gov