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A physically-based model for low-temperature plasticity in BCC metals

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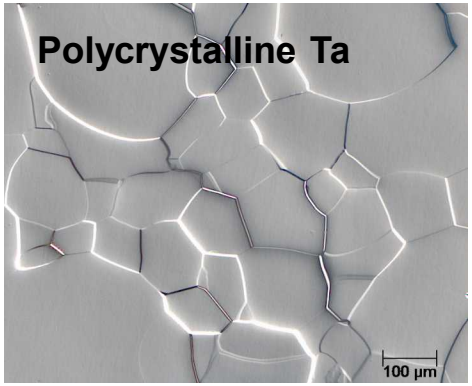
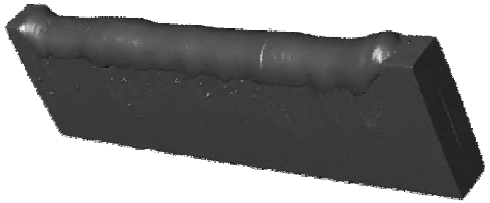
Motivation for developing low-temperature BCC deformation models

- BCC metals are scientifically interesting.
  - Technologically important.
    - *Refractories: W, Mo, Ta*
    - *Steel*
  - Underrepresented in computational materials science studies.
    - *Complex response, compared to FCC*
    - *Most models are phenomenological*
  - Favorable properties for experimental studies.
    - *Can prepare microstructures ranging from single crystal to nanocrystalline.*
    - *Favorable properties for microscopy and EBSD analysis.*

Single-crystal Ta



304L stainless weldment



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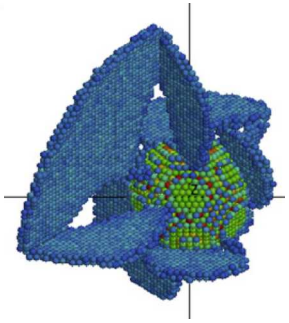
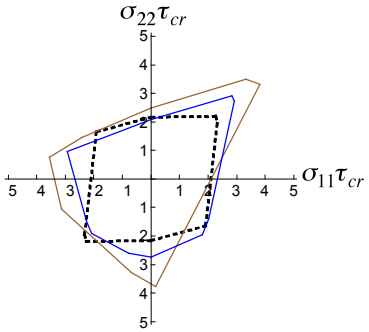
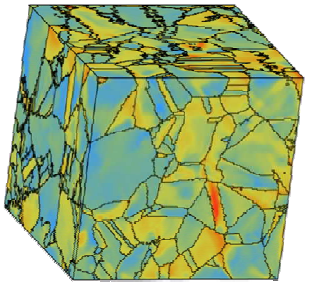
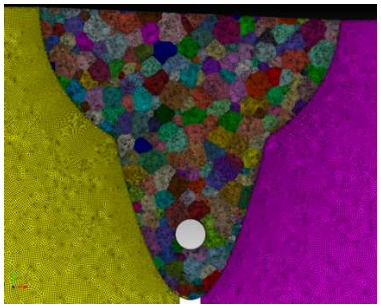
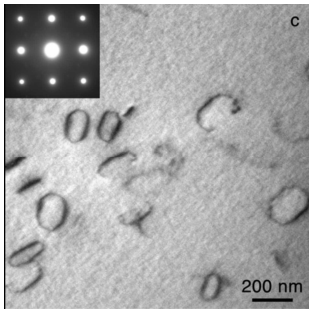
Including microstructure in design and analysis

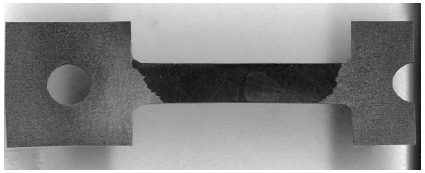


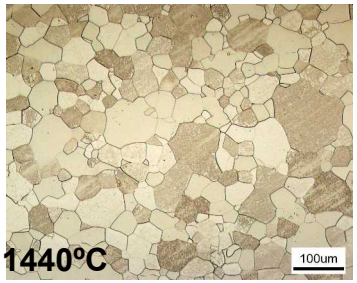


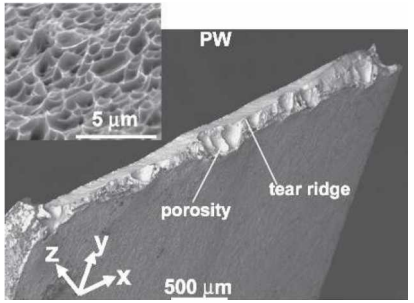












Atomic scale phenomena

Single crystal behavior

Microstructural effects

Material performance

10^{-9} m
10^{-9} s

10^{-6} m
10^{0} s

10^{-3} m
10^{3} s

10^{0} m
10^{6} s

How BCC and FCC crystal plasticity differ

- In BCC metals at low temperatures, slip occurs via the motion of screw dislocations along <111> directions on (110) planes.

The plastic strain rate is given by:

$$\mathbf{D} = \sum_s \dot{\gamma}^{(s)} \mathbf{m}^{(s)}$$

Schmid factor

$$\dot{\gamma}^{(s)} = G\left(\frac{\mathbf{m}^{(s)} : \sigma}{\tau^{(s)}}\right)$$

Note:
FCC slip system: <110>{111}
BCC slip system: <111>{110}
$\therefore$ **m** is the same for BCC and FCC

The lattice resistance on slip system *s* is:

$$\tau^{(s)} = \tau(T, \sigma) = \tau_{\text{obs}} + \tau_{\text{fric}}(T, \sigma)$$

τ_{obs}: Peierls stress

τ_{fric}: Obstacle stress

In FCC metals, $\tau_{\text{obs}} \gg \tau_{\text{fric}}$ $\quad \tau_{\text{fric}} \approx 0$

In BCC metals, $\tau_{\text{fric}} \gg \tau_{\text{obs}}$ $\quad \tau_{\text{obs}} \approx 0$

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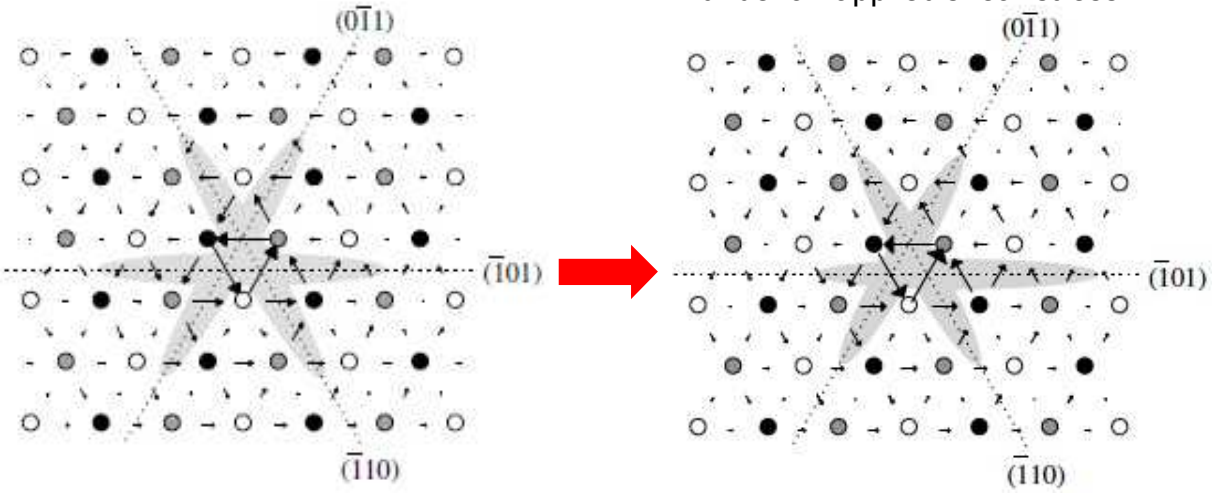
Atomic Scale: Physical model for dislocation motion in BCC metals

- Atomic scale simulations show dislocation core spreading onto adjacent (110) planes in BCC metals.
  - Core spreading creates a significant Peierls barrier to dislocation motion.
  - Because the dislocation spreads onto three planes, motion can be affected by stress components outside the preferred slip plane, i.e. non-Schmid stresses.

[111] zone depiction of a relaxed screw dislocation core in Mo

Distortion of the dislocation core under an applied shear stress



Groger, Vitek et al. *Acta Mat.* **56** (2008) 5412

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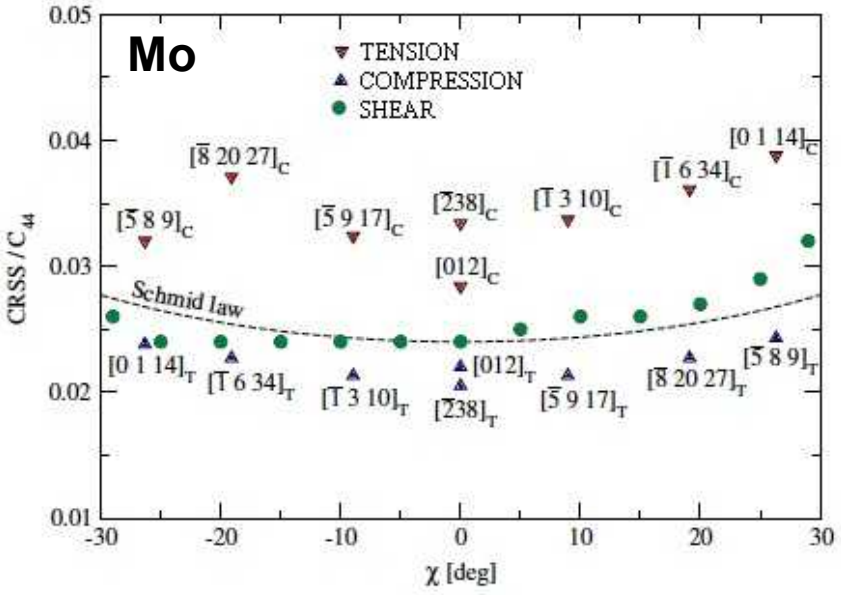
Implications of non-Schmid deformation

- The non-Schmid stress components arise from two causes:
  - Asymmetry within the slip plane (twinning/anti-twinning) is a minor effect.
  - Contributions by stress components outside the slip plane are significant.

"...glide of the 1/2[111] screw dislocation [on the (-101) plane] depends on shear stresses both parallel and perpendicular to the Burgers vector that act not only in the slip plane but also in other {110} planes of the [111] zone."

-Groger, Vitek et al. *Acta Mat.* **56** (2008) 5412.



The non-Schmid stress components cause the widely observed tension-compression asymmetry in BCC metals

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Single crystal behavior: BCC crystal plasticity model

The atomic results can be fit to a yield criterion given by:

$$\sigma_{cr}^{app}\left[a_0\mathbf{m}^{(s)}\mathbf{n}^{(s)}+a_1\mathbf{m}^{(s)}\mathbf{n}^{(s')}+a_2\left(\mathbf{n}^{(s)}\times\mathbf{m}^{(s)}\right)\mathbf{n}^{(s)}+a_3\left(\mathbf{n}^{(s)}\times\mathbf{m}^{(s)}\right)\mathbf{n}^{(s')}\right]=\tau_{cr}$$

applied stress — stress projection tensor, $\mathbf{P}_{\sigma}^{(s)}$ — yield stress

We use this form to derive the generalized stress state on a slip system:

$$\tau^{(s)}=\mathbf{P}_{\sigma}^{(s)}:\sigma^{app}$$

Which leads to a single-crystal constitutive law:

$$\dot{\gamma}^{(s)}=\frac{\tau^{(s)}}{\tau_{cr}}\left|\frac{\tau^{(s)}}{\tau_{cr}}\right|^{\frac{1}{m}-1}$$

Which gives the plastic strain rate:

$$\mathbf{D}=\sum_{s}\dot{\gamma}^{(s)}\mathbf{m}^{(s)}$$

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Material-specific constitutive parameters

- The parameters a_0, a_1, a_2 and a_3 are determined from bond order potential atomistic simulations.

Parameter	FCC	W	Mo	
a_0	1	1	1	Schmid stress
a_1	0	0	0.24	twinning/anti-twinning
a_2	0	0.56	0	out-of-plane effects
a_3	0	0.75	0.35	out-of-plane effects
τ_{cr}	1	1.36	1.26	

- Parameters are normalized such that $\tau_{CRSS} = 1$.

Gap: To develop similar models for other BCC metals, such as Ta and Fe, we need valid interatomic potential functions.

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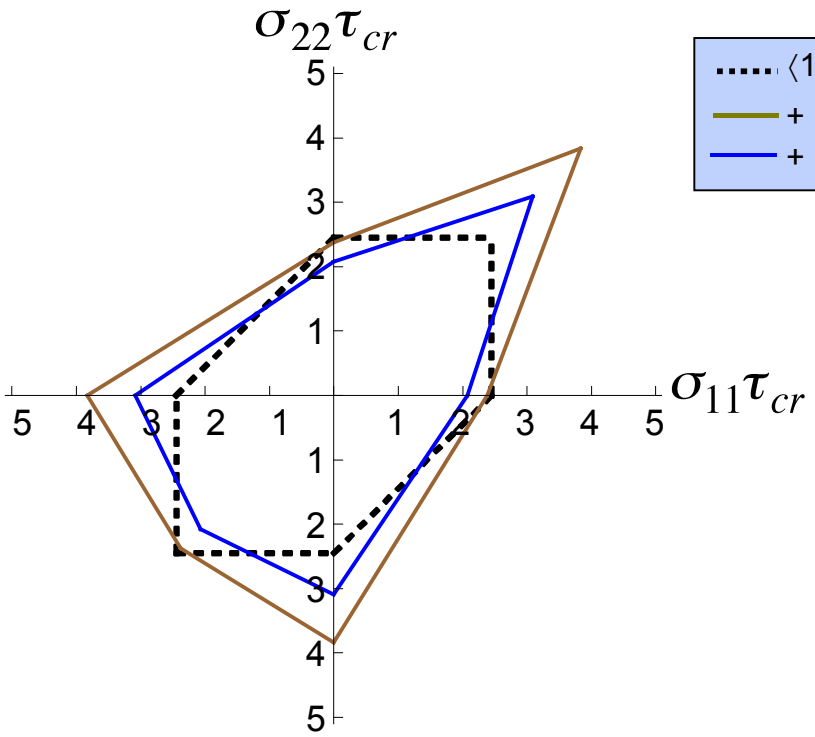
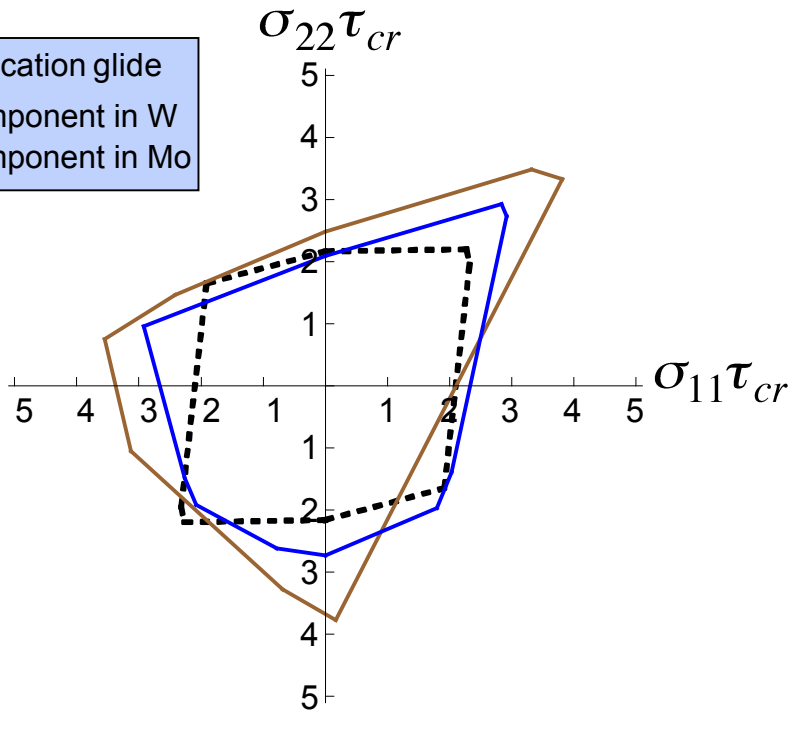
Single Crystal Results: BCC single crystal yield surfaces



⟨100⟩(010) orientation
highly symmetric

⟨111⟩{011} dislocation glide
+ non glide component in W
+ non glide component in Mo



⟨-0.180,0.575,0.798⟩,(0,-0.811,0.585) orientation
asymmetric

- BCC yield surfaces are considerably different from FCC yield surfaces.
- The yield surfaces of W and Mo are quite distinct.
- Tension/compression asymmetry is apparent.

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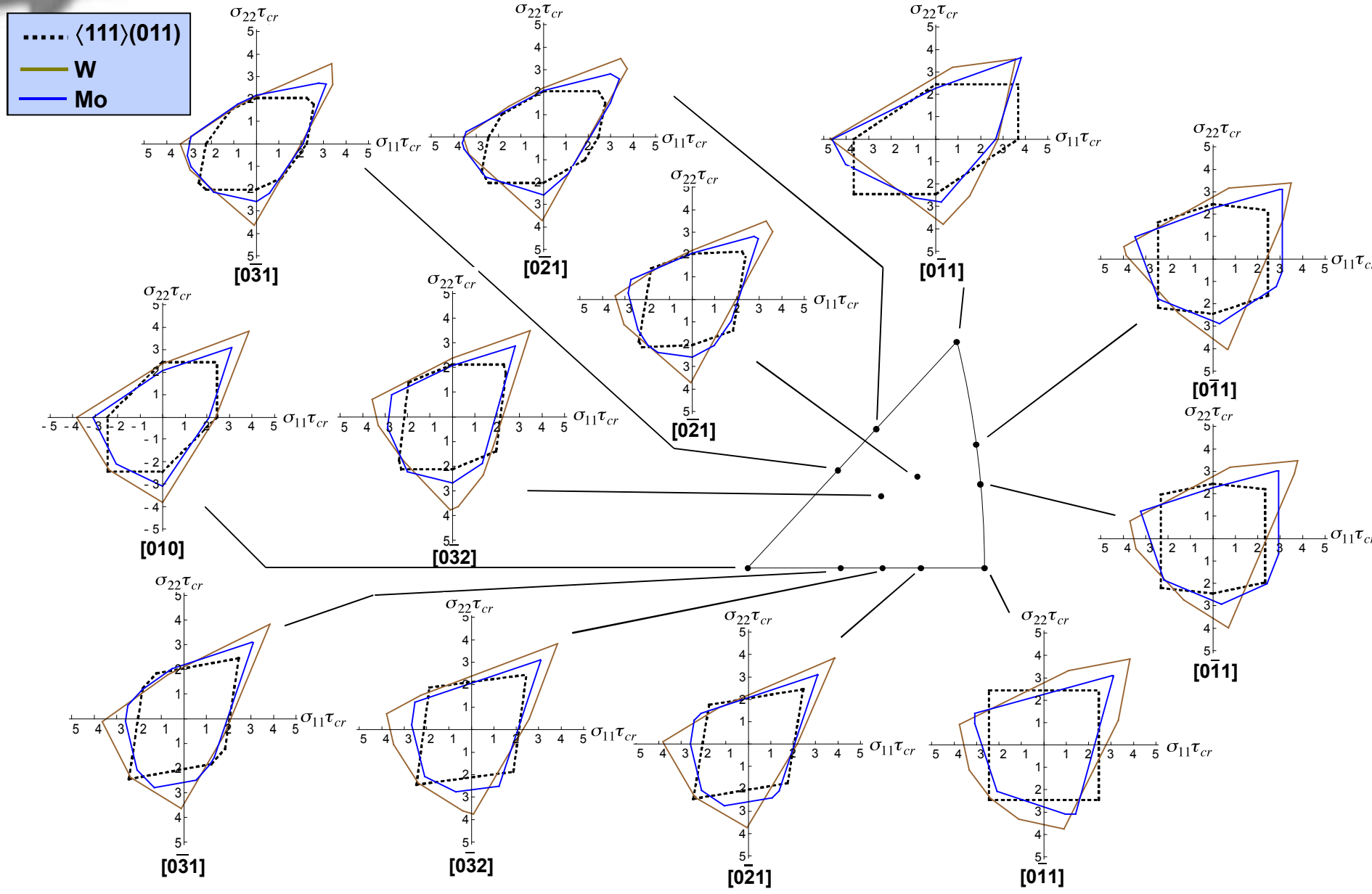
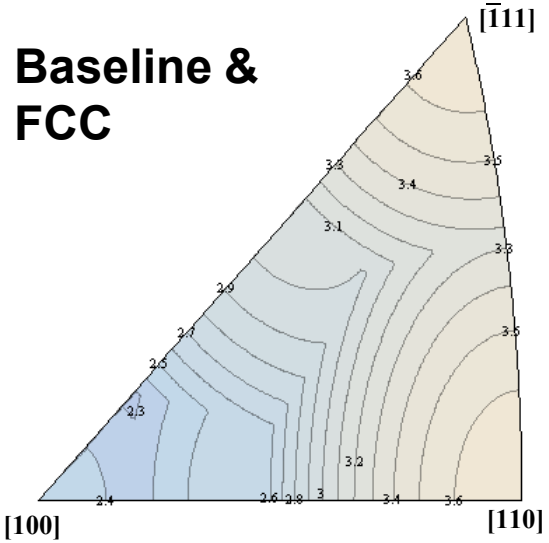
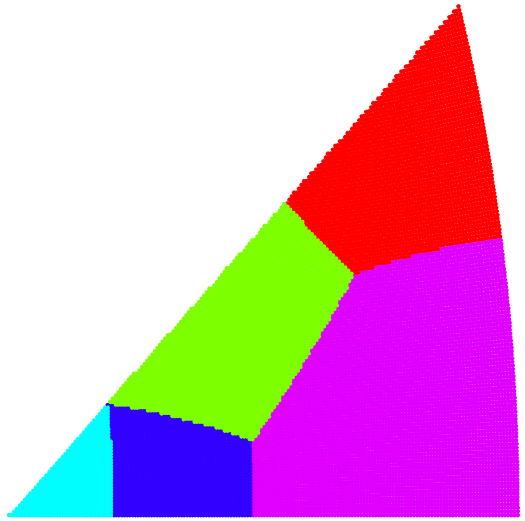
There is significant biaxial tension-compression asymmetry in BCC yield surfaces



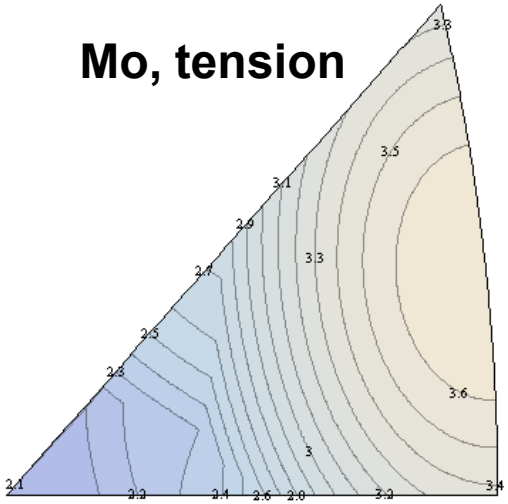
Non-Schmid stresses significantly alter the Taylor factor landscape in BCC metals

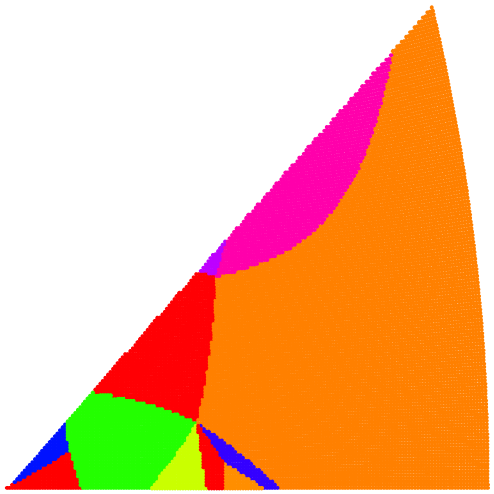
Baseline & FCC



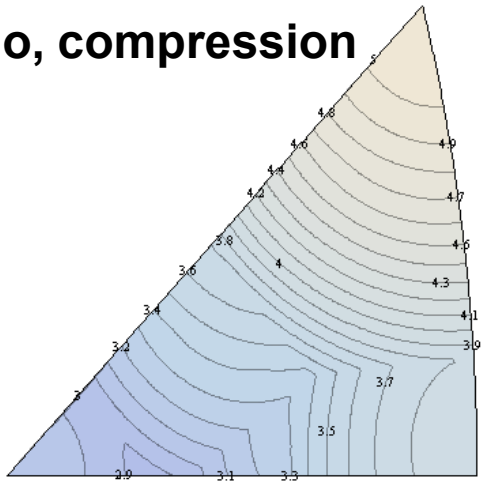


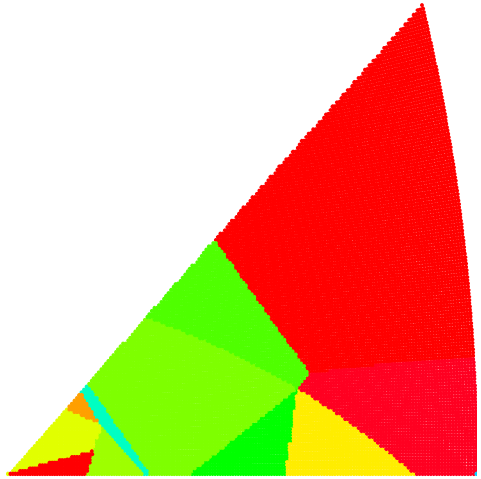
Mo, tension



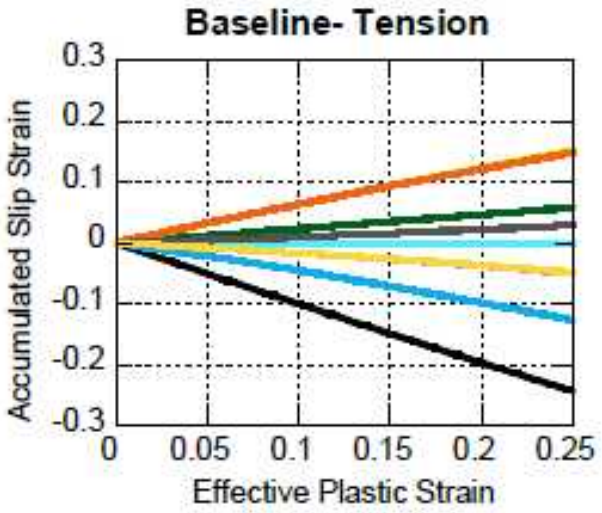


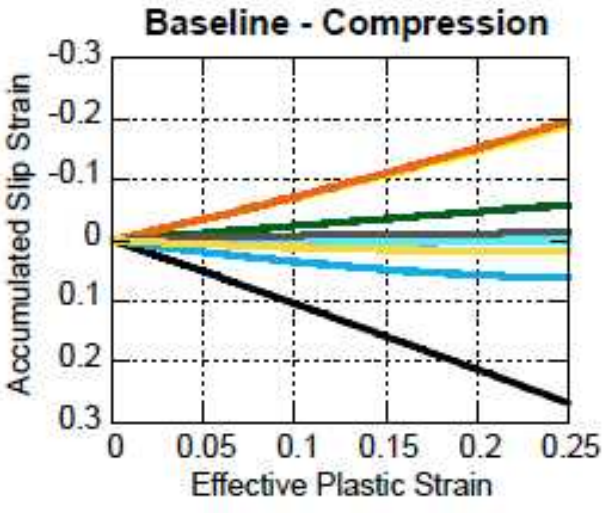
Mo, compression

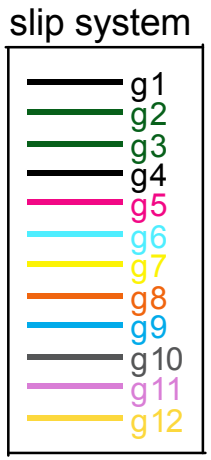




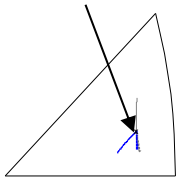
Non-Schmid stresses significantly alter slip system activity in BCC metals

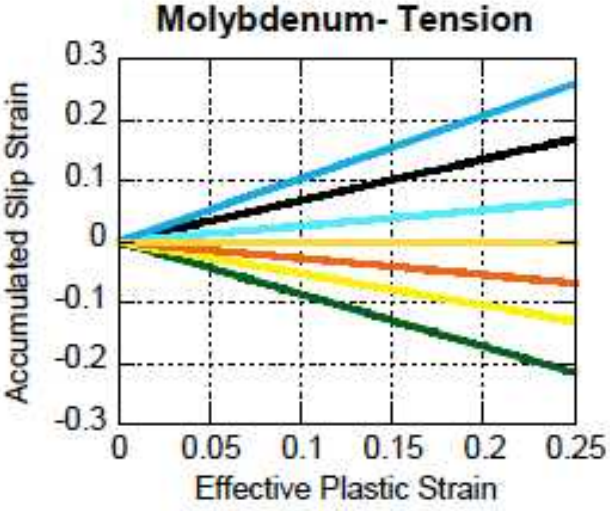


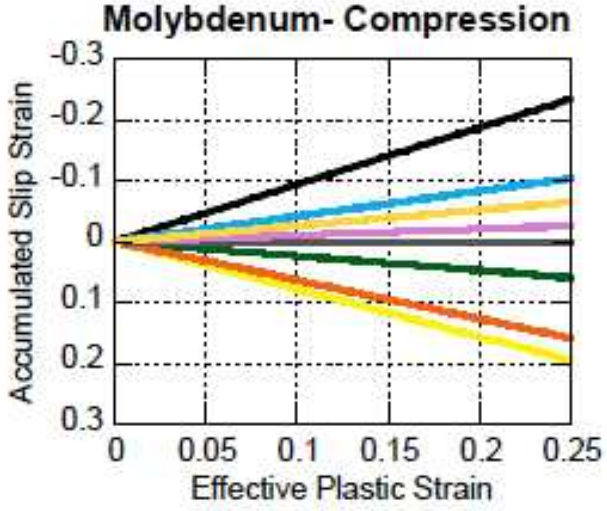




crystal orientation:
[-.180, 0.575,0.798]







- Baseline is the same in tension and compression.
- Mo differs in tension and compression.
- Mo differs from baseline in tension and compression.

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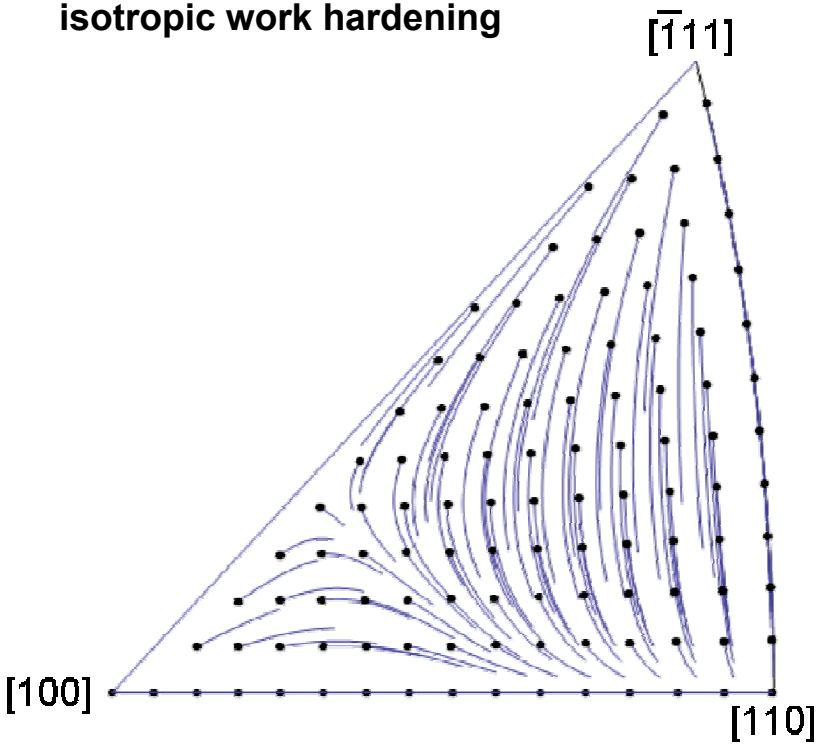
Non-Schmid stresses significantly alter crystal rotations in BCC metals

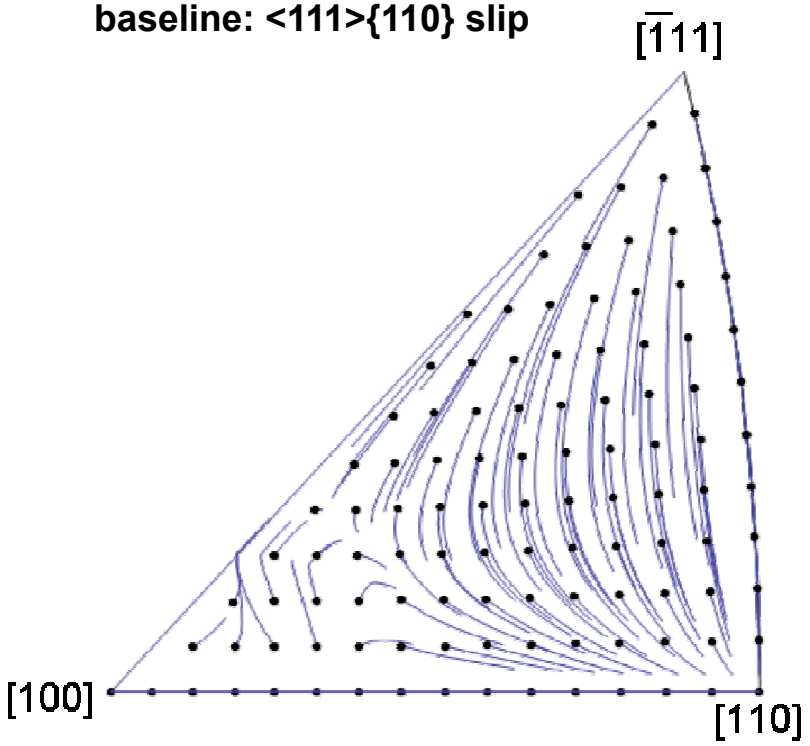
Isochoric Deformation to 50% strain:

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

FCC crystal plasicity model with isotropic work hardening



BCC crystal plasticity baseline: <111>{110} slip



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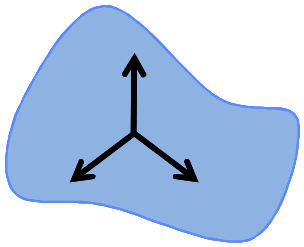
Extending single crystal behavior to capture microstructural effects

•Polycrystal plasticity models reveal how individual grains to take part in polycrystalline deformation

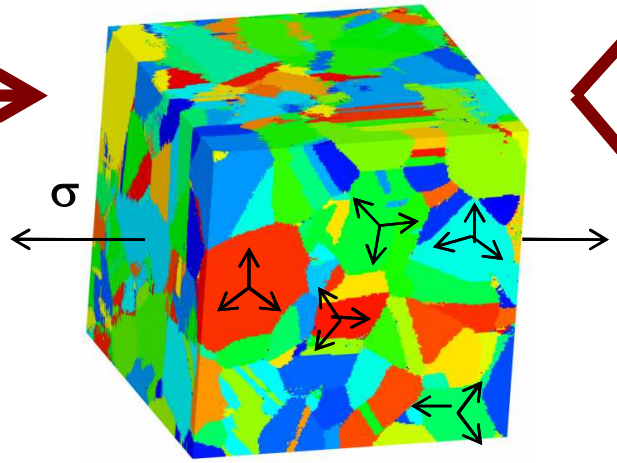
Single crystal plasticity



Constitutive law

$$\dot{\gamma}^{(s)} = \frac{\tau^{(s)}}{\tau_{cr}} \left| \frac{\tau^{(s)}}{\tau_{cr}} \right|^{\frac{1}{m}-1}$$

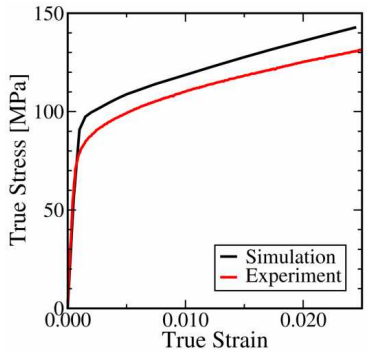
Polycrystal plasticity



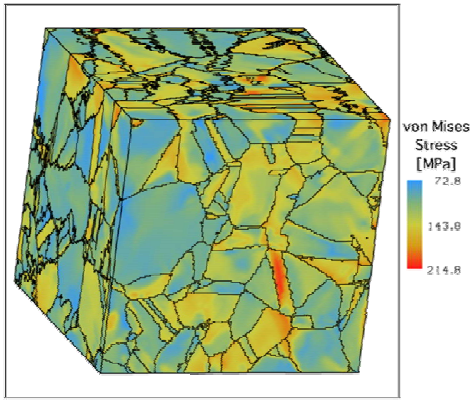
Each grain responds via the orientation-dependent constitutive law

Results

Overall mechanical response

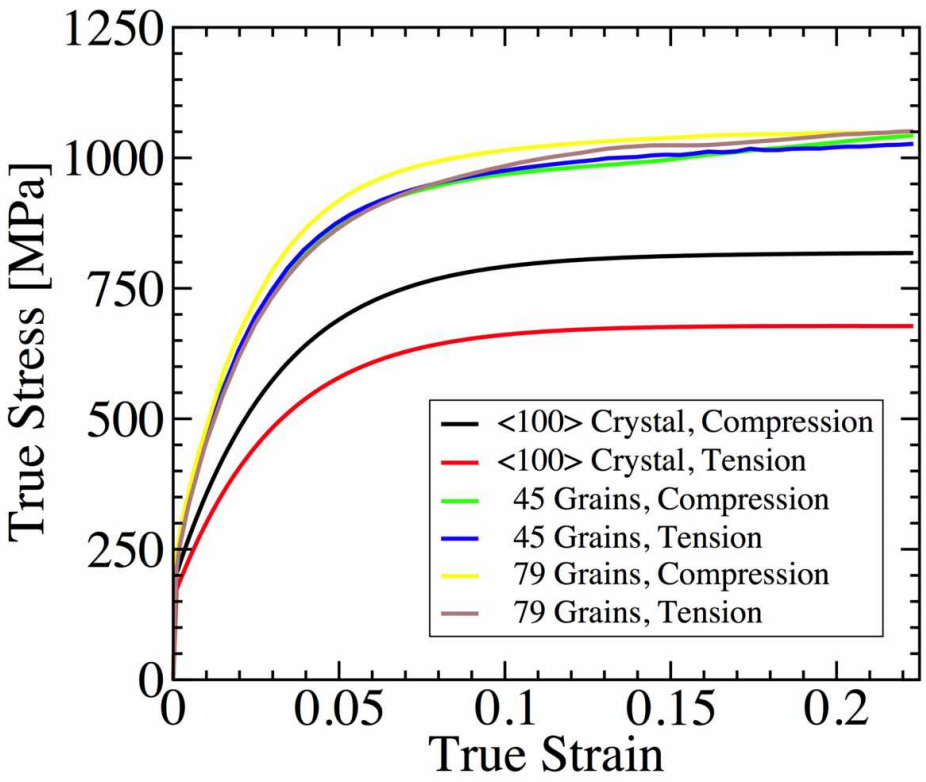


Individual grain response (rotation, stress, etc.)



Microstructural Results: Continuum response of BCC polycrystals

- In plasticity simulations of single- and polycrystalline Mo:
  - *Single crystal and polycrystal response differ considerably.*
  - *Single crystals show considerable tension/compression asymmetry.*
  - *Polycrystals do not exhibit tension/compression asymmetry.*
  - *There is no grain size dependence in this model.*



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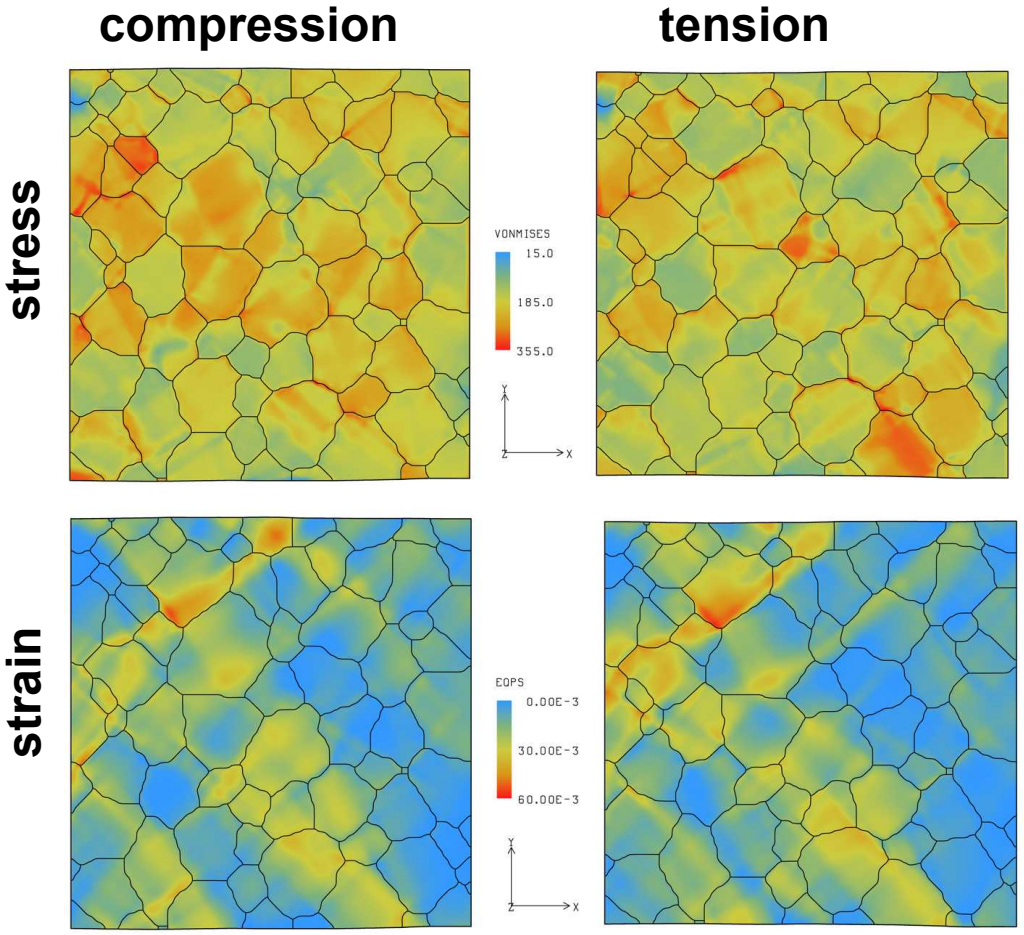
Microstructural Results: Grain scale stress and strain partitioning

- At the grain scale, tension/compression asymmetry affects local stress distribution.
- Grain structure influences the distribution of local strains, but tension/compression asymmetry does not.
- Local strains are partitioned to accommodate global deformation.

➢ Grain-scale stresses adjust to produce the required local strain.

Polycrystal plasticity reveals the complex interdependence of local stress and strain in BCC metals.

Mo, 1.2% strain



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Summary and Conclusions

- **BCC plasticity differs fundamentally from FCC plasticity**
- **A physically-based model captures key elements of BCC plasticity**
  - *Tension/compression asymmetry and yield surfaces*
  - *Differences in Taylor factor, slip system activity, crystal rotation*
- **Polycrystal plasticity reveals how single-crystal properties interact in realistic grain structures**
  - *Tension/compression asymmetry is maintained*
  - *Significant stress concentrations occur*

Supplementary Slides

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Polycrystal plasticity model

Cauchy stress resolved on each slip system: $\tau = \sigma : (\mathbf{s} \otimes \mathbf{m})$

Cauchy stress **from** FE solver

Slip rate on each system: $\dot{\gamma} = \dot{\gamma}_o \left| \frac{\tau}{\tau_{CRSS}} \right|^{\frac{1}{m}} \text{sign}(\tau)$

Plastic velocity gradient: $\hat{\mathbf{L}}_p = \dot{\gamma}(\hat{\mathbf{s}} \otimes \hat{\mathbf{m}})$

Plastic deformation gradient: (Cayley-Hamilton theorem[1])

$$\dot{\mathbf{F}}_p = \hat{\mathbf{L}}_p \bullet \mathbf{F}_p \Rightarrow \begin{cases} \mathbf{F}_p = \exp\left(\hat{\mathbf{L}}_p \Delta t\right) \mathbf{F}_p \\ \exp\left(\hat{\mathbf{L}}_p \Delta t\right) = I + \frac{\sin\phi}{\phi} \hat{\mathbf{L}}_p \Delta t + \frac{1 - \cos\phi}{\phi^2} \left(\hat{\mathbf{L}}_p \bullet \hat{\mathbf{L}}_p\right) \Delta t^2 \\ \phi = \Delta t \sqrt{\frac{1}{2}\left(\hat{\mathbf{L}}_p : \hat{\mathbf{L}}_p\right)} \end{cases}$$

Elastic deformation gradient and strain: $\mathbf{F}_e = \mathbf{F} \bullet \left(\mathbf{F}_p\right)^{-1} \Rightarrow \hat{\mathbf{E}}_e = \frac{1}{2}\left[\left(\mathbf{F}_e\right)^T \bullet \mathbf{F}_e - \mathbf{I}\right]$

2nd Piola-Kirchhoff stress (hyper-elasticity): $\hat{\sigma}_{PK2} = \mathbf{C} : \hat{\mathbf{E}}_e$

Updated Cauchy stress: $\sigma = \frac{1}{J^{\mathbf{F}_e}} \left[\mathbf{F}_e \bullet \hat{\sigma}_{PK2} \bullet \left(\mathbf{F}_e\right)^T\right]$

Cauchy stress **to** FE solver

Updated crystallographic orientation: $\mathbf{F}_e = \mathbf{U}_e \bullet \mathbf{R}_e \Rightarrow \mathbf{R}_{lattice} = \mathbf{R}_e \bullet \mathbf{R}_h$

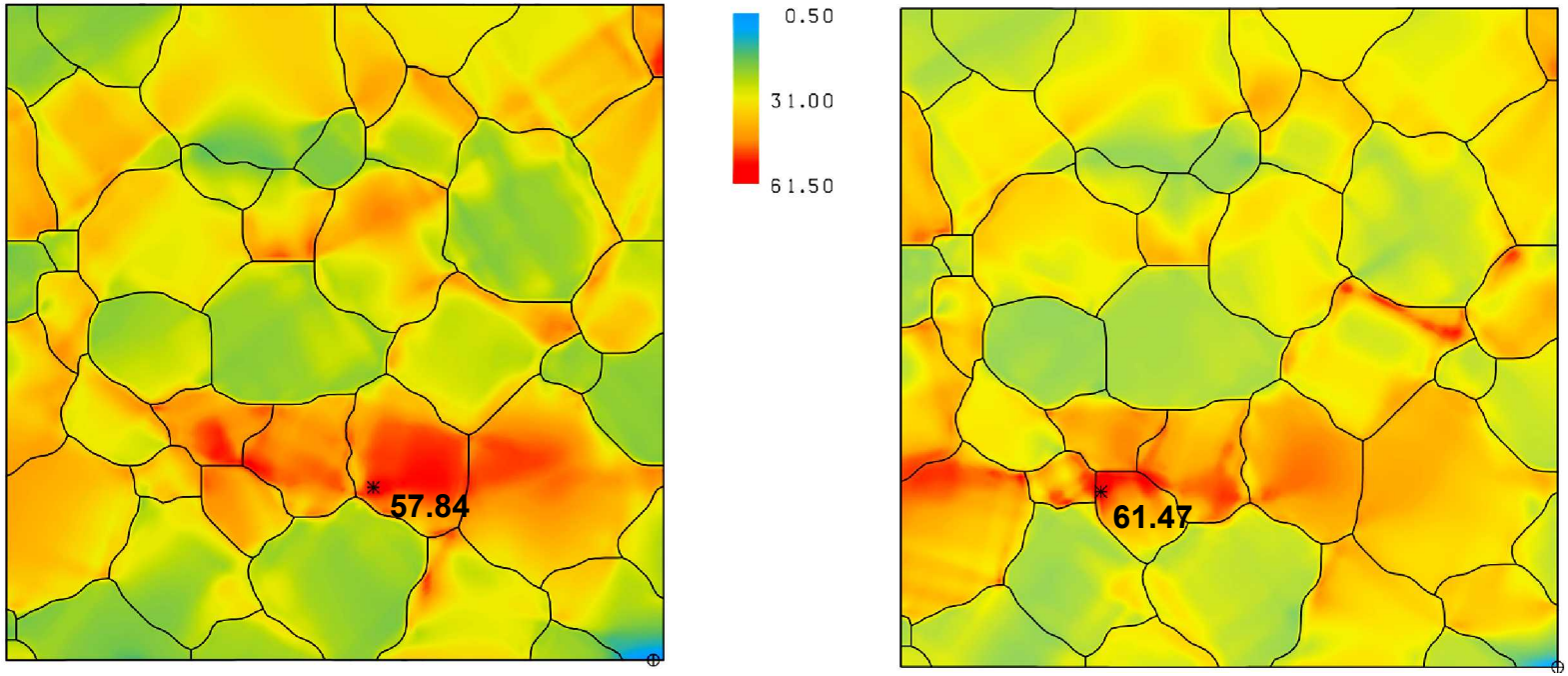
Effective plastic strain: $\bar{\varepsilon}_p = \sqrt{\frac{2}{3} \mathbf{E}_p : \mathbf{E}_p}$

Updated "hardness" (CRSS): $\tau_{CRSS} = \tau_o + A \exp\left(-\frac{n}{A} \bar{\varepsilon}^p\right)$

1. M.F. Atiyah and I.G. MacDonald, Introduction to Commutative Algebra, Westview Press, 1969, ISBN 0-201-40751-5.

Local stress concentrations are more severe prior to yielding

Von-Mises Stress Distribution in Mo (0.1% Strain)



Tension **Compression**

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