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Incorporating Data from Experiments and Atomistic Simulations into Crystal Plasticity Models for BCC Metals

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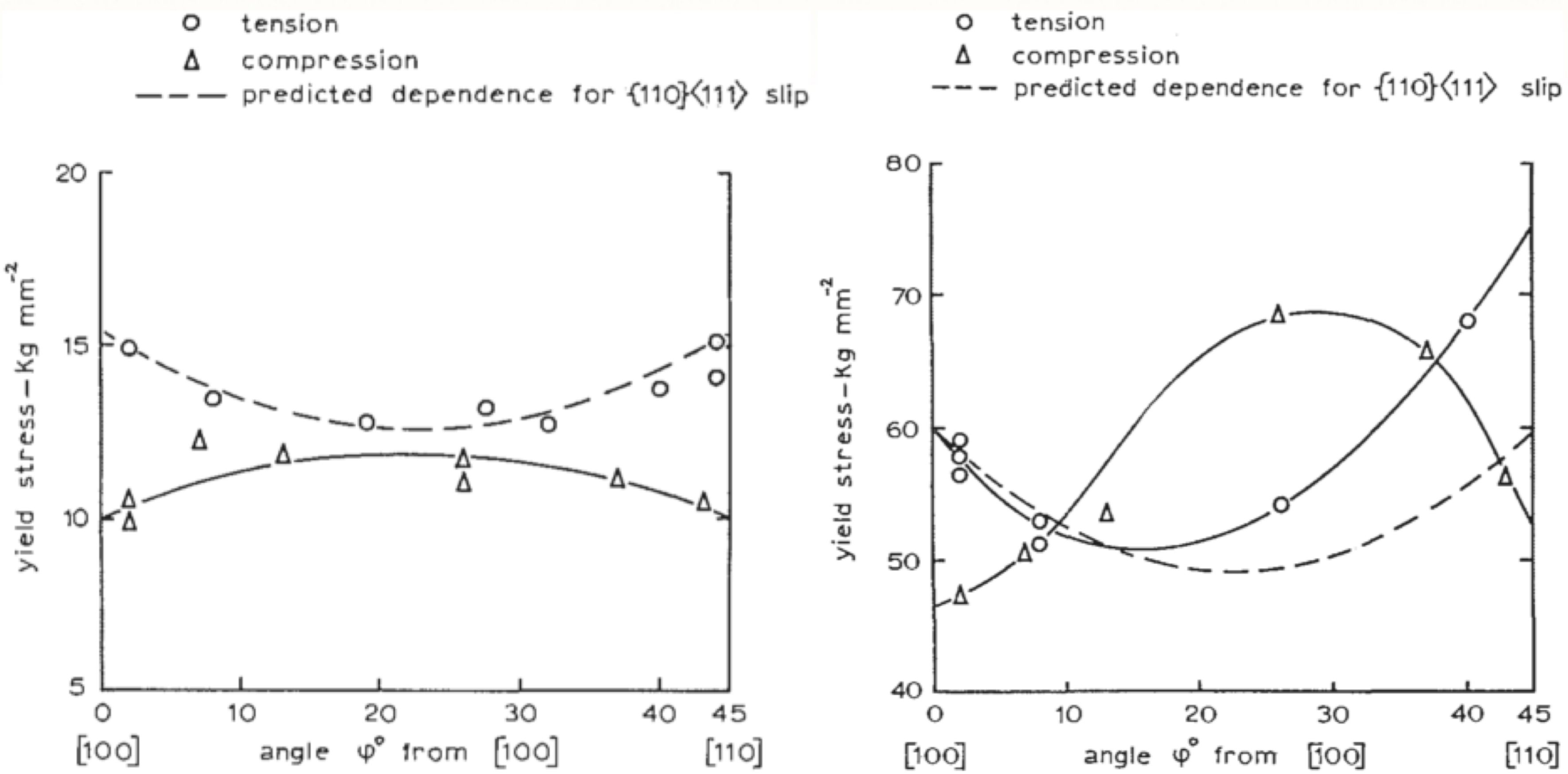
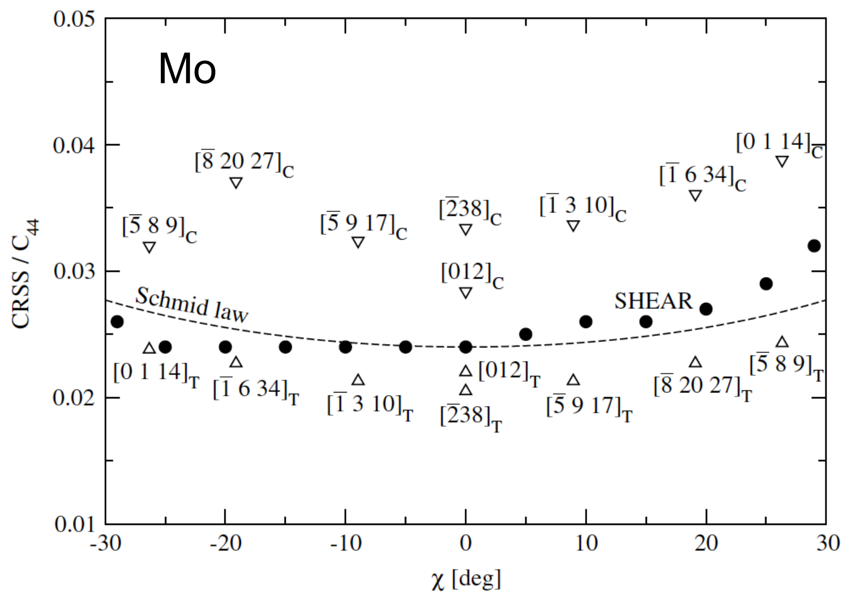
BCC Metals Show Tension/Compression Asymmetry



Hull, Byron, and Noble, *Canadian J. Phys.* **45** (1967) 1091.

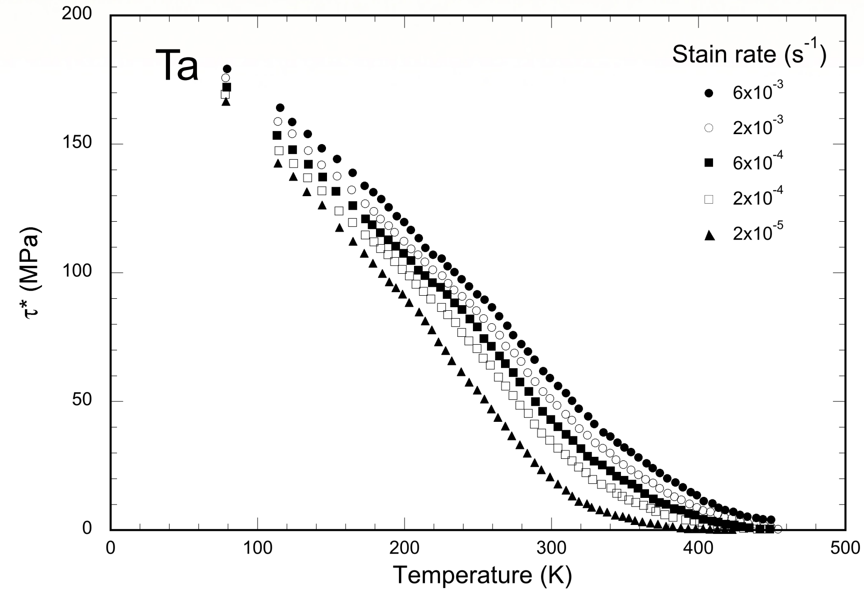
… and Significant Temperature Dependence in Yield

Violations of Schmid law



Gröger et al., Acta Mat. (2008)

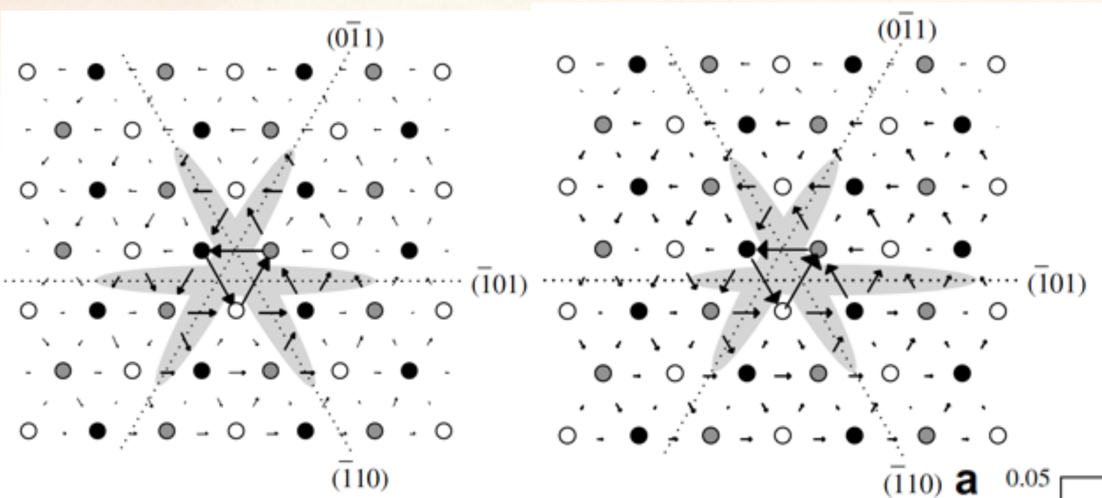
High lattice friction at low T



Werner, Phys. Stat. Sol. (a) (1987)

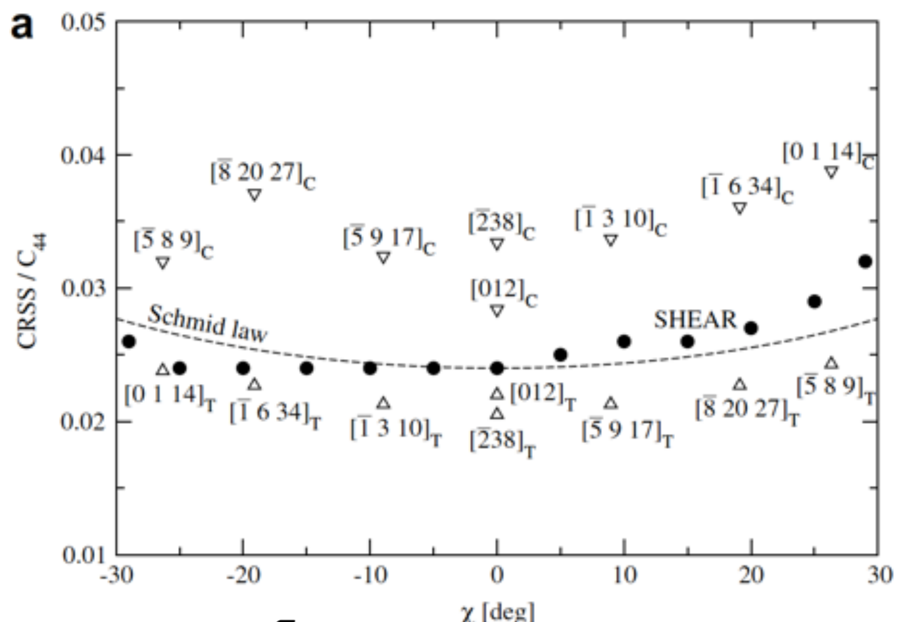
Ambiguity of the operating slip system: {110}, {112}, {123} planes

Screw Dislocation Core Structure is Important



Screw dislocation cores are non-planar, leading to high lattice friction.

Twinning / anti-twinning asymmetry is weak by comparison.



Shear stress perpendicular to the core is important.

$$\mathbf{M}^{(s)} : \sigma + \mathbf{P}^{(s)}_{\mathrm{ns}} : \sigma = \tau_{\mathrm{cr}}$$

$$\mathbf{m}^s \cdot \sigma \mathbf{n}^s + a_1 \mathbf{m}^s \cdot \sigma \mathbf{n}_1^s + a_2(\mathbf{n}^s \times \mathbf{m}^s) \cdot \sigma \mathbf{n}^s + a_3(\mathbf{n}_1^s \times \mathbf{m}^s) \cdot \sigma \mathbf{n}_1^s = \tau_{\mathrm{cr}}$$

Gröger, Bailey, an Vitek, *Acta Mater.* **56** (2008) 5401.

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Generalized Yield Law Incorporating Non-Schmid Effect

The resistance to slip on a slip system α:

$$\tau_{\mathrm{cr}}^{\alpha} = \mathbf{P}_{\mathrm{tot}}^{\alpha} : \boldsymbol{\sigma} = \mathbf{P}_{\mathrm{s}}^{\alpha} : \boldsymbol{\sigma} + \mathbf{P}_{\mathrm{ns}}^{\alpha} : \boldsymbol{\sigma}$$

$$\mathbf{P}_{\mathrm{s}}^{\alpha} = c_0 \frac{1}{2} \left(\mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha} + \mathbf{n}^{\alpha} \otimes \mathbf{m}^{\alpha} \right)$$

$\mathbf{m}^{\alpha}$: slip direction

$\mathbf{n}^{\alpha}$: slip plane normal

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

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

Representation of various yield criteria

Ref.	Structure	c_o	c_1	c_2	c_3	c_4	c_5
Qin and Bassanni (1992)	FCC	$1+\frac{\sqrt{3}}{3}B$	$\frac{\sqrt{6}}{3}B$	0	0	0	0
Steinmann et al. (1998)	FCC	α^{sm}	α^{cm}	α^{mm}	0	0	0
Qin and Bassanni (1992)	$L1_2$	$1+\frac{\sqrt{3}}{3}B$	$\frac{\sqrt{6}}{3}B$	$-A-\frac{7}{9}Ak$	$\frac{2\sqrt{2}}{9}Ak$	$-\frac{2\sqrt{2}}{9}Ak$	0
Dao and Asaro (1993)	$L1_2$	1	$2\eta^0_{zs}$	$2\eta^0_{mz}$	$2\eta^0_{mm}$	$2\eta^0_{zz}$	$2\eta^0_{ss}$
Gröger et al. (2008)	BCC	$1+\frac{1}{2}a_1$	$\frac{\sqrt{3}}{2}a_1$	$-a_2+\frac{1}{2}a_3$	$\frac{\sqrt{3}}{4}a_3$	$-\frac{\sqrt{3}}{4}a_3$	0
Yalcinkaya et al. (2008)	BCC	1	η_2	η_3	η_4	η_5	η_1

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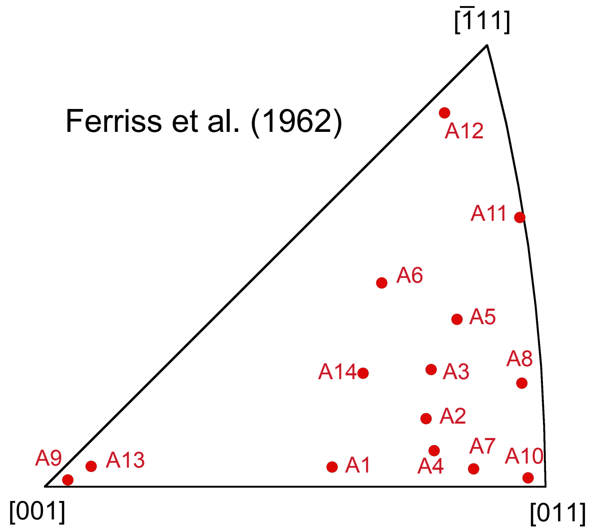
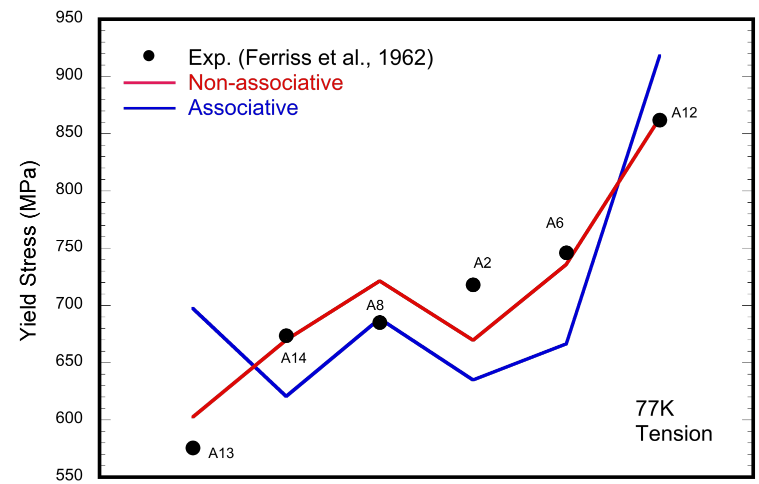
Yield Stress Prediction for Ta Single Crystals

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

$$\boldsymbol{\sigma}_y = \frac{\tau_{cr} + \tau_{obs}^{\alpha}}{P_{tot}^{T}} \quad \text{(Tension)} \qquad \boldsymbol{\sigma}_y = -\frac{\tau_{cr} + \tau_{obs}^{\alpha}}{P_{tot}^{C}} \quad \text{(Compression)}$$





Ta single crystal tests

Temp.	c_1	c_2	c_3	c_4	τ_{cr}	Std. dev. (A)	Std. dev. (NA)
77 K	-0.35	0.12	-0.79	0.53	383	75.3 MPa	27.4 MPa
300 K	-1.18	0.70	0.12	0.08	57	10.9 MPa	7.7 MPa

Best-fit Parameters

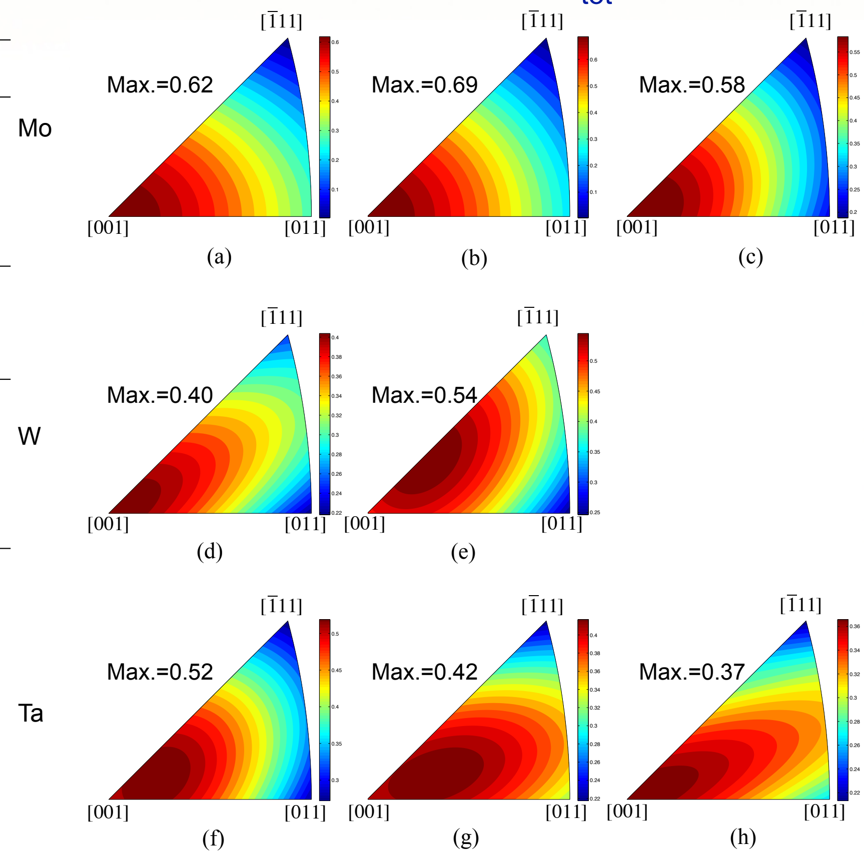
Yield Stress Prediction for Mo, W and Ta Single Crystals

Best-fit non-Schmid constants

Material	c_1	c_2	c_3	c_4	τ_{cr}	Ref.
Mo (a)	0.11	0.70	0.04	-0.04	208	Sherwood et al. (1967)
Mo (b)	0.31	0.70	0.11	-0.11	215	Guiu and Pratt (1966)
Mo (c)	0.42	0.23	0.13	-0.02	147	Irwin et al. (1974)
W (d)	0.15	0.05	-0.01	0.26	325	Rose et al. (1962)
W (e)	0.36	-0.09	0.23	-0.01	293	Argon and Maloof (1966)
Ta (f)	0.30	0.04	0.11	0.01	173	Sherwood et al. (1967)
Ta (g)	-0.11	0.19	-0.03	0.16	225	Hull et al. (1967)
Ta (h)	-0.07	0.15	-0.08	0.29	211	Ferriss et al. (1962)

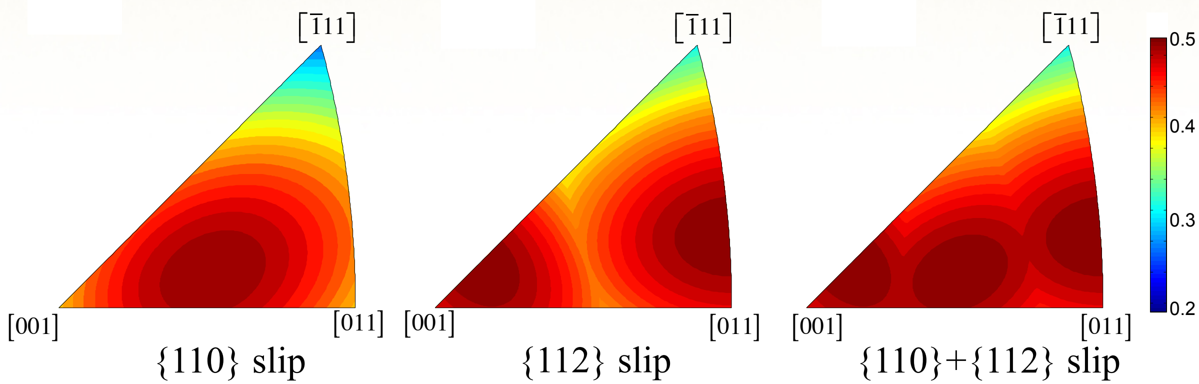
T= 77 K, $\dot{\varepsilon} = 10^{-4}\ s^{-1}$

Predicted P_{tot}



{110} vs. {112} Slip

Predicted P_{tot}



Standard deviation (MPa) between predicted and measured yield stresses

	Baseline model			Non-Schmid model			References
	{110}	{112}	{110}+{112}	{110}	{112}	{110}+{112}	
Mo	311	311	311	**105**	211	188	Sherwood (1967)
	388	310	297	**12**	109	114	Guiu (1966)
	185	185	185	**1**	170	123	Irwin (1974)
W	322	318	314	**47**	68	67	Rose (1962)
	344	344	344	**1**	83	39	Argon (1966)
Ta	135	135	135	**1**	45	29	Sherwood (1967)
	101	101	101	**1**	1	1	Hull (1967)
	104	105	95	**20**	66	23	Ferriss (1962)
	107	112	103	74	69	**63**	Byron (1968)

BCC CP-FEM Formulation

Slip rate: $\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \left(\frac{\tau^{\alpha}}{g^{\alpha}} \right)^{1/m}$ (Hutchinson, 1976)

24 <111>{110} slip systems

Slip resistance: $g^{\alpha} = \max\left(\tau_{\text{cr}}^{\alpha} - \tau_{\text{ns}}^{\alpha}, 0\right) + \tau_{\text{obs}}^{\alpha}$ (Weinberger, 2012)

$\tau_{\text{obs}}^{\alpha}$ → Obstacle stress

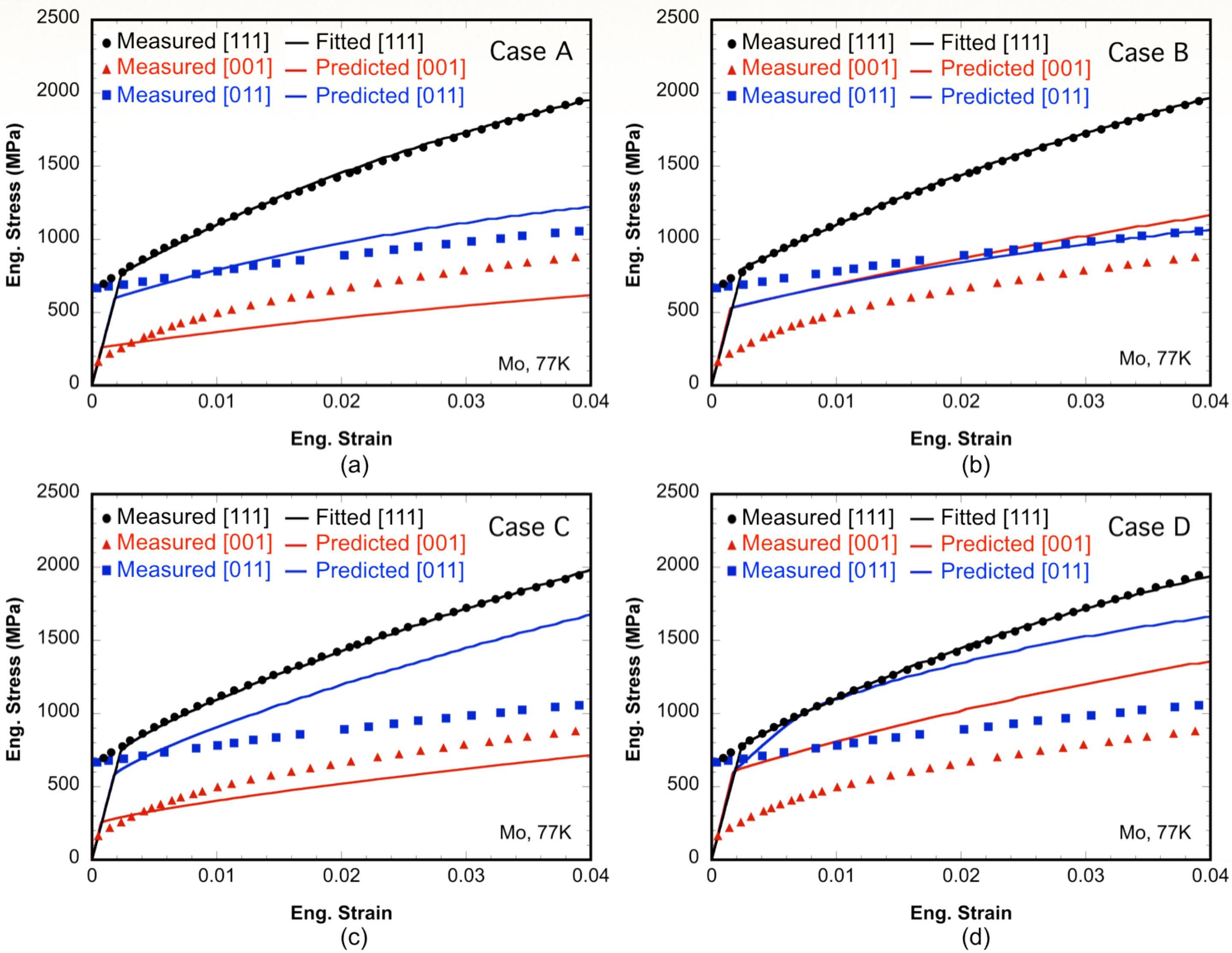
$\tau_{\text{ns}}^{\alpha}$ → Lattice friction

Obstacle stress: $\tau_{\text{obs}}^{\alpha} = \alpha \mu \mathrm{b} \sqrt{\sum_{\beta=1}^{NS} \rho^{\beta}}$ (Taylor, 1934)

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

Single Crystal Stress-Strain Predictions for Mo

Orientation dependent stress-strain curve is most accurately predicted in Case A.



(a) Case A
Non-associative model
{110} slip
Taylor hardening

(b) Case B
Associative model
{110} slip
Taylor hardening

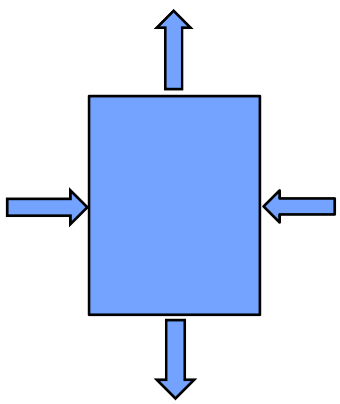
(c) Case C
Non-associative model
{110} slip
Power-law hardening

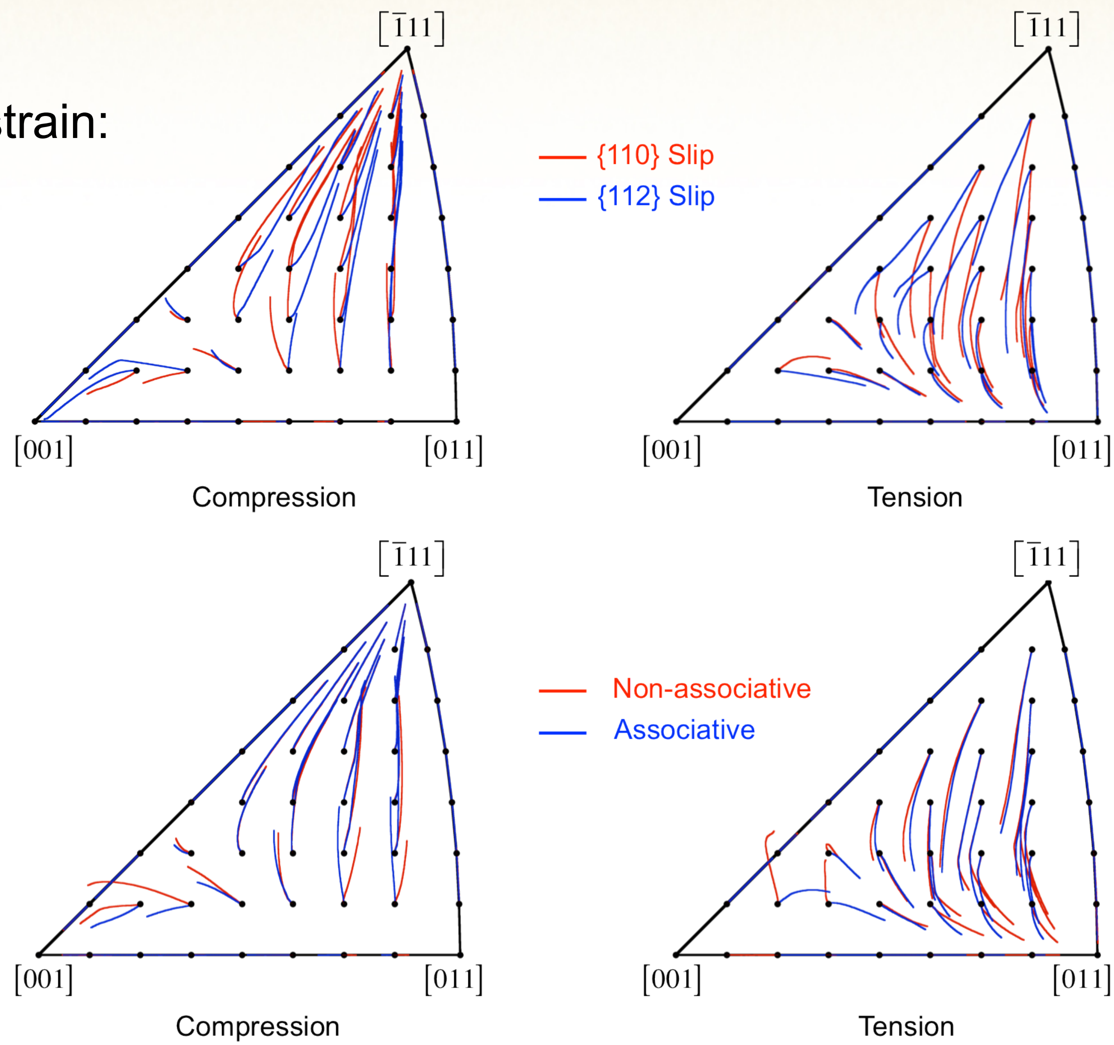
(d) Case D
Non-associative model
{112} slip
Taylor hardening

Texture Evolution in Mo

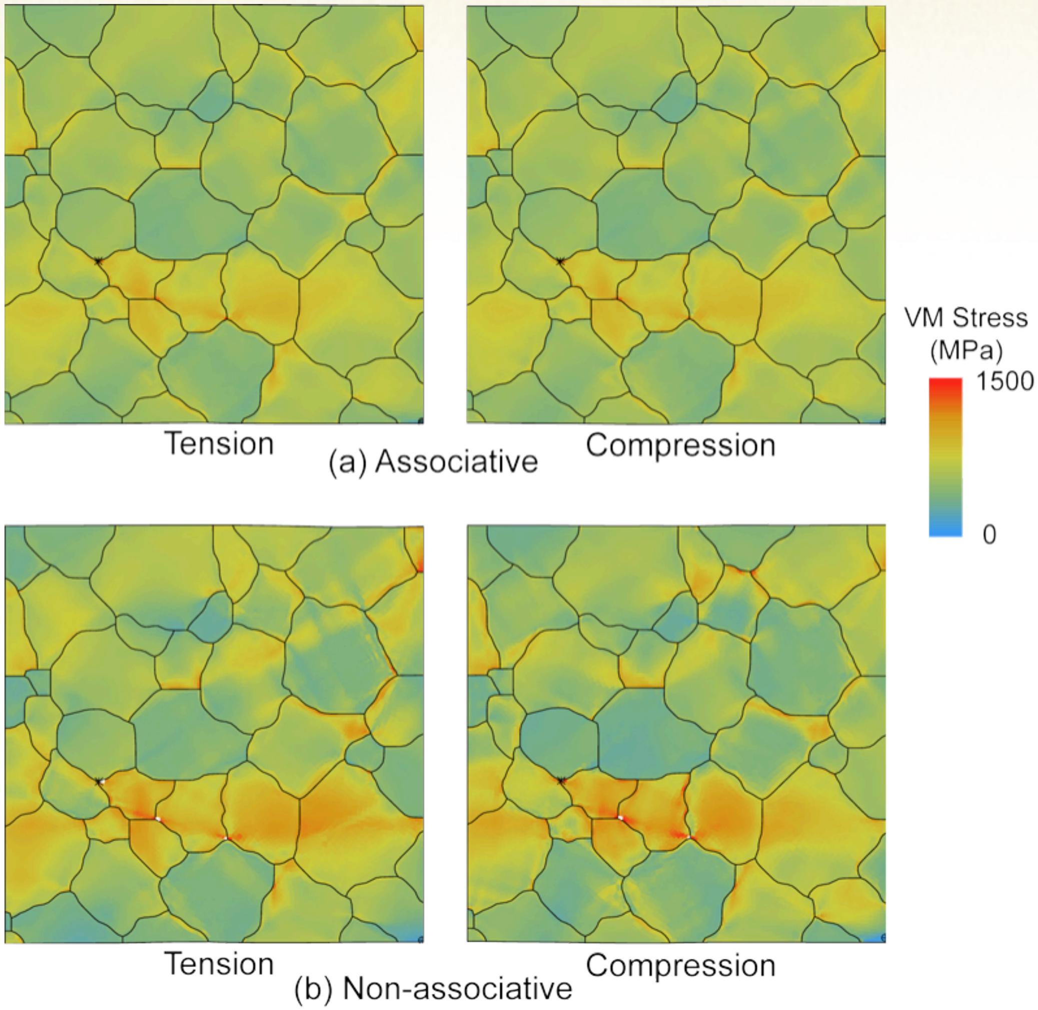
Isochoric deformation to 20% strain:

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





Stress Maps in Mo



Similar Stress Distributions

Non-Associative Model has higher and more localized stresses, greater tendency for failure

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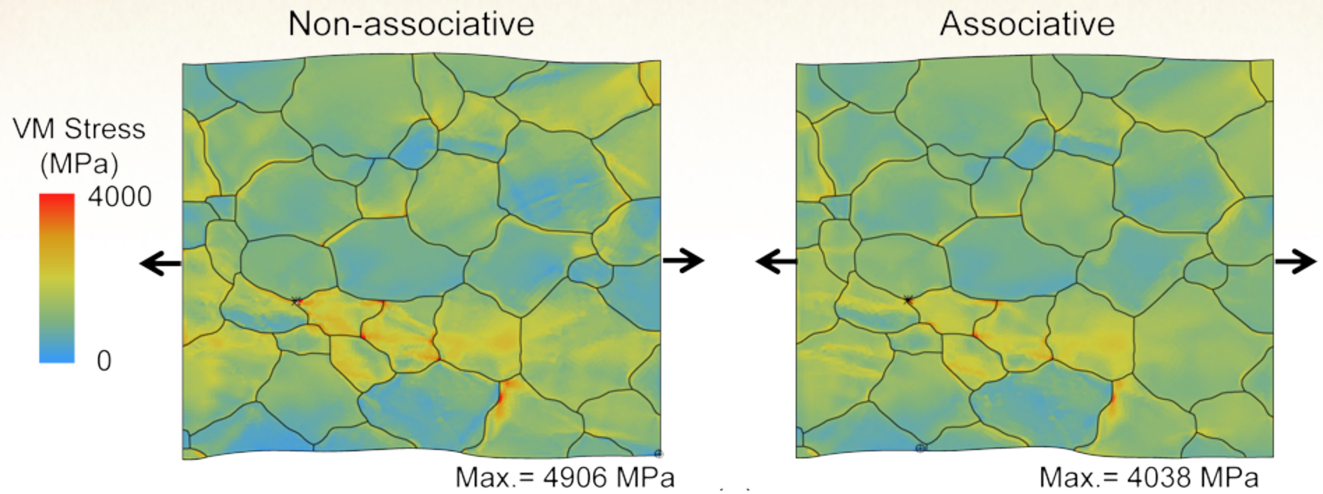
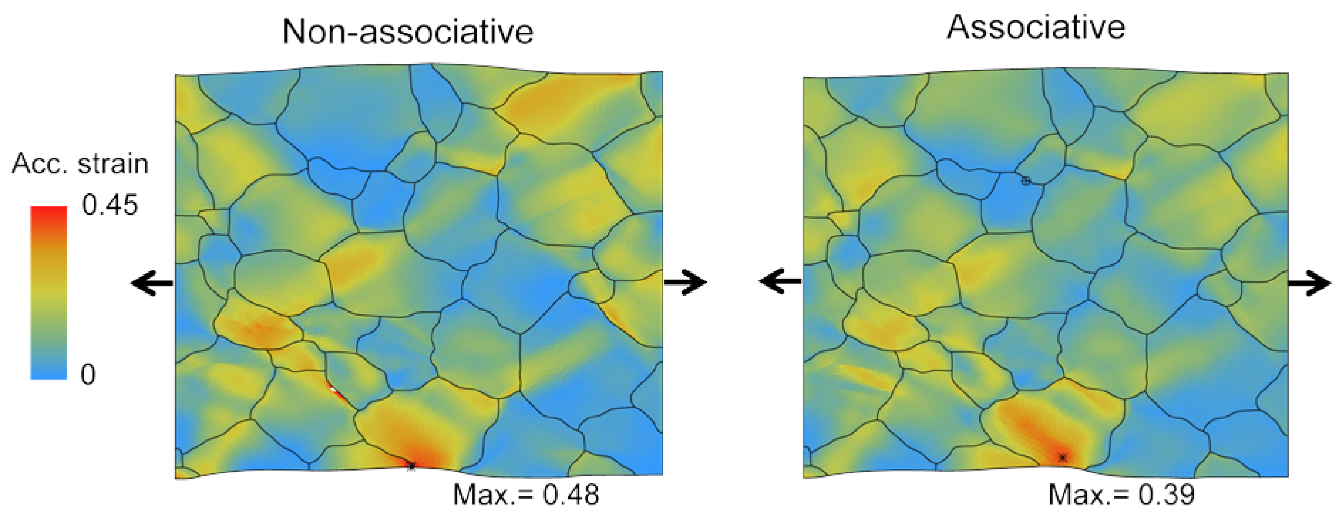
Stress and Strain Maps in Mo

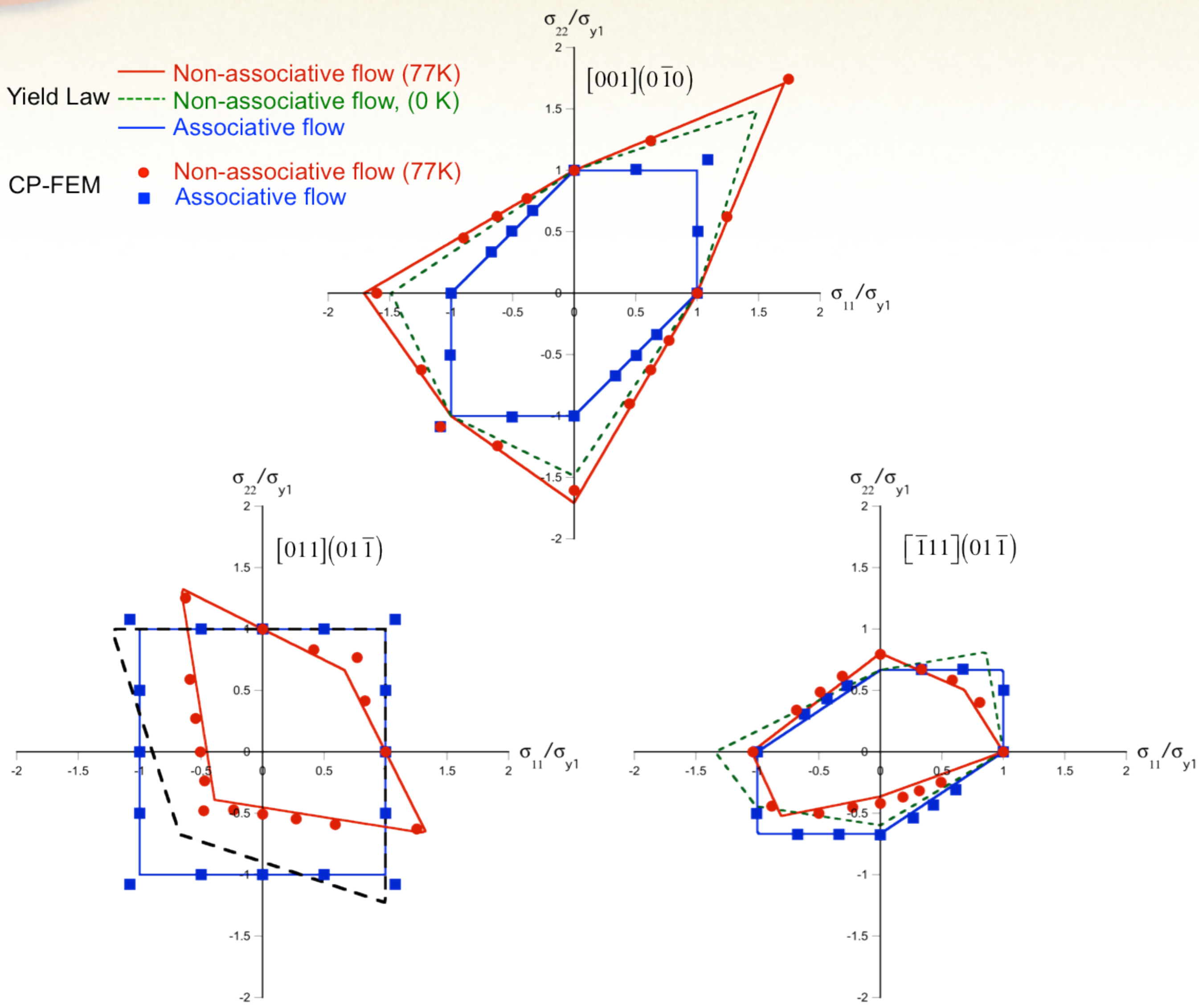


Von Mises Stress Distribution

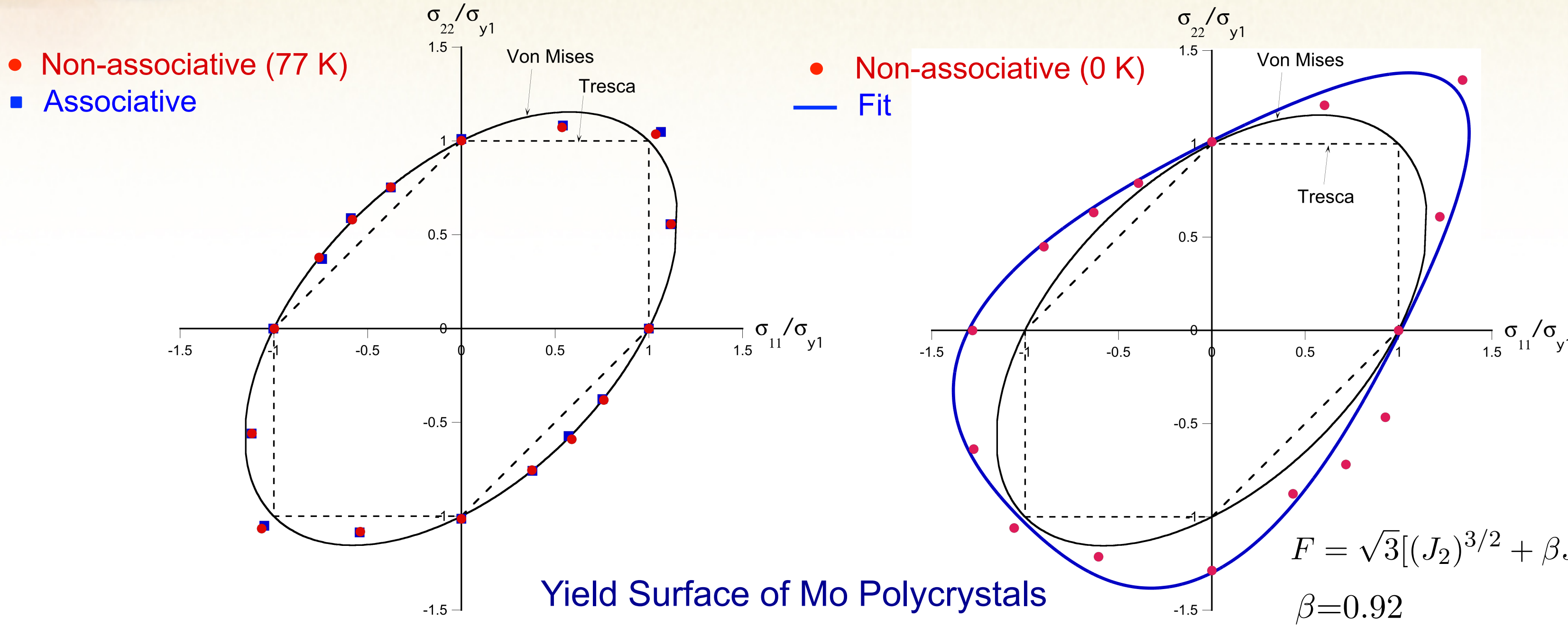


Accumulated Strain Distribution

Yield Surface Predictions: Mo Single Crystals



Yield Surface Predictions: Mo Polycrystals

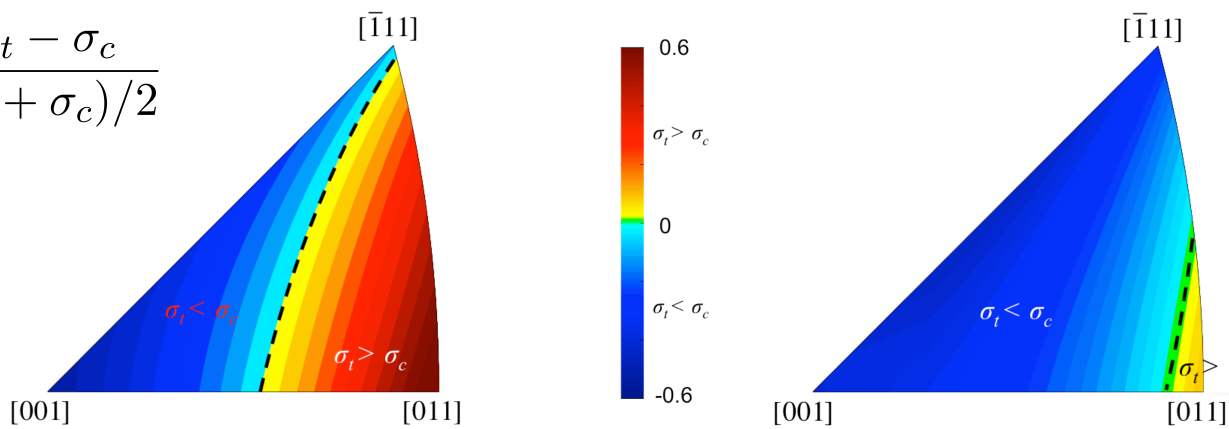


$$F = \sqrt{3}[(J_2)^{3/2} + \beta J_3]^{1/3}$$

$$\beta = 0.92$$

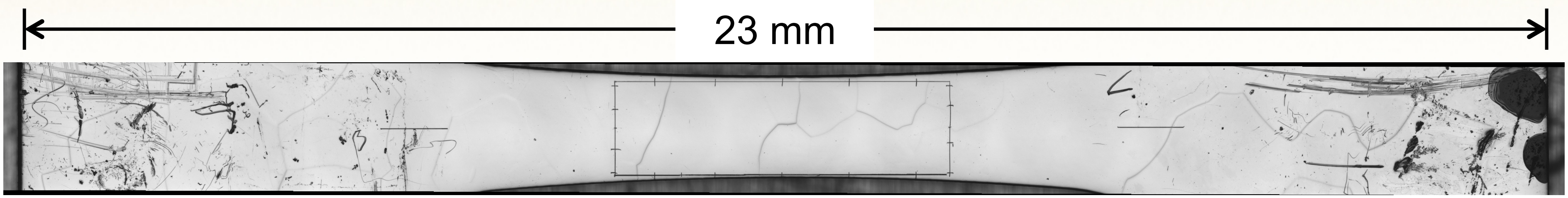
Yield Surface of Mo Polycrystals

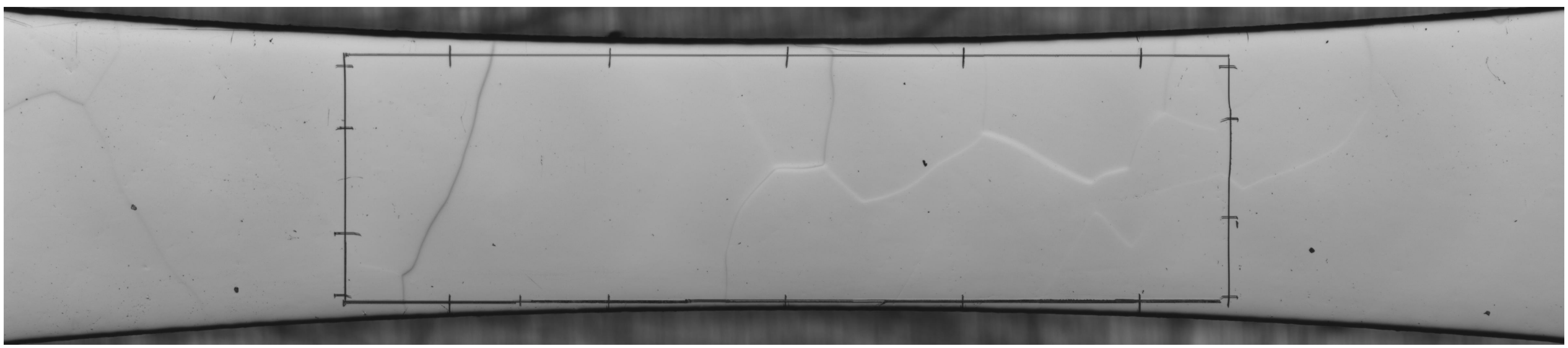
$$\mathrm{SD} = \frac{\sigma_t - \sigma_c}{(\sigma_t + \sigma_c)/2}$$

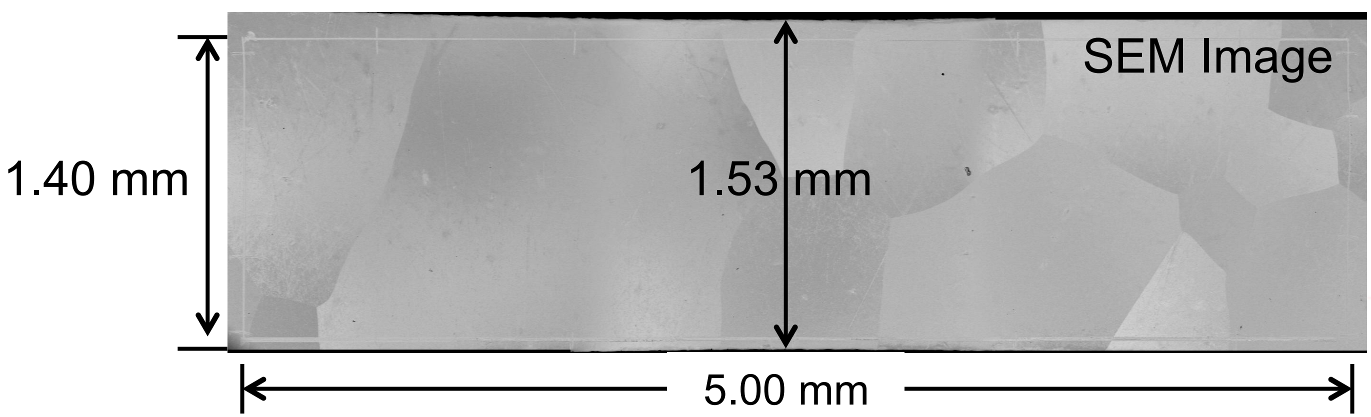


Strength differential (SD) predictions

Digital Image Correlation of Ta Oligocrystal







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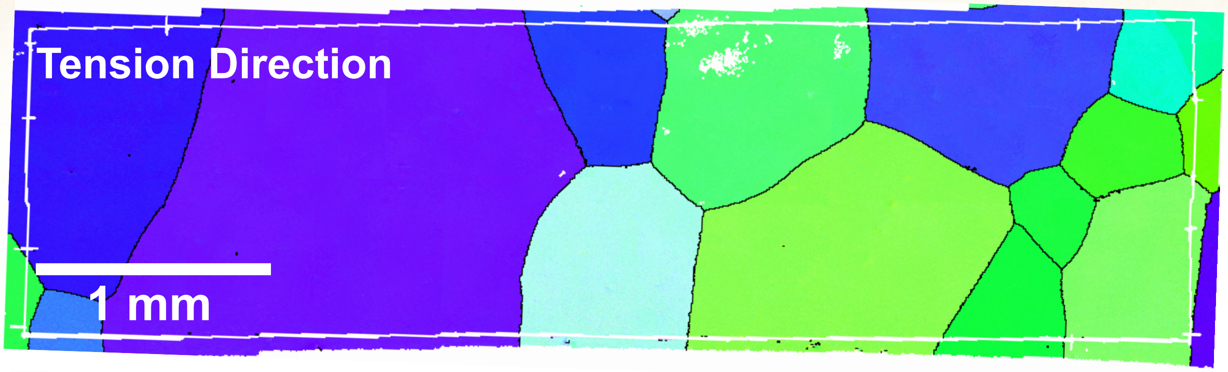
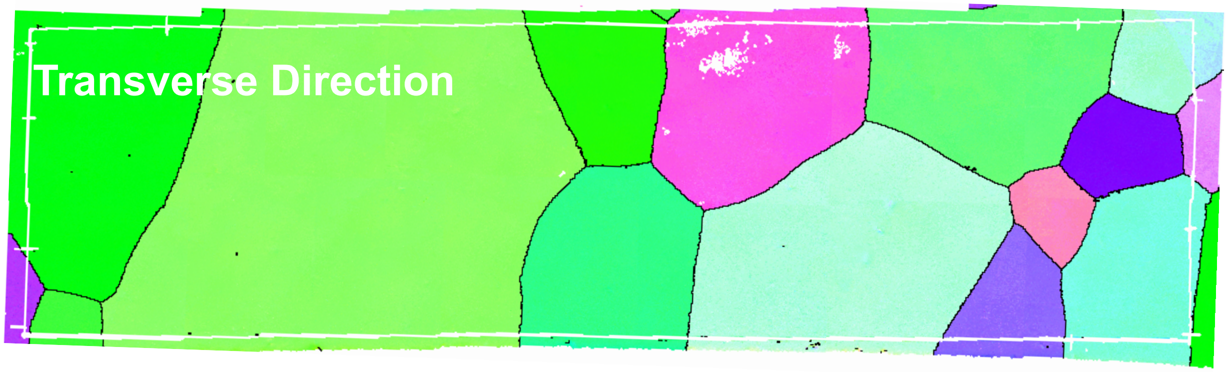
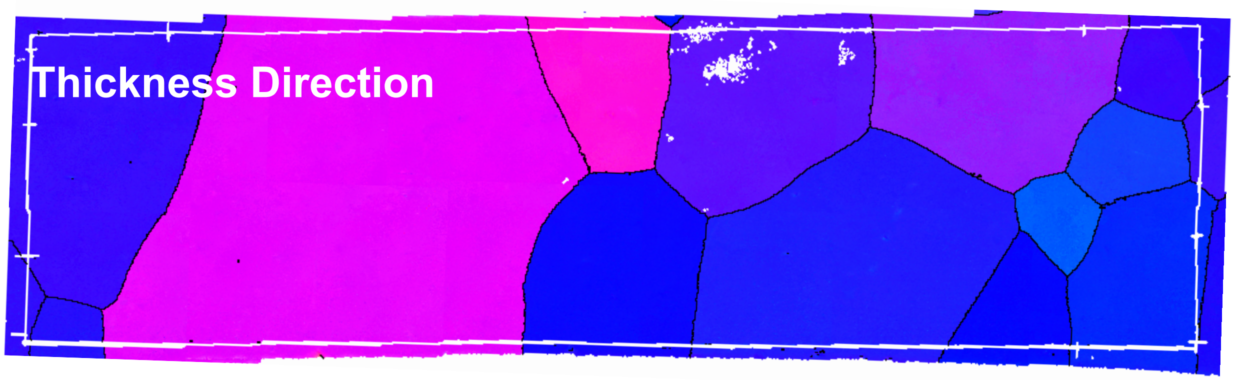
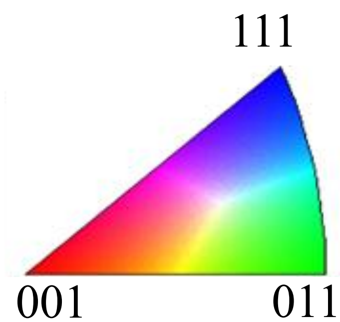
Electron Backscatter Diffraction Maps









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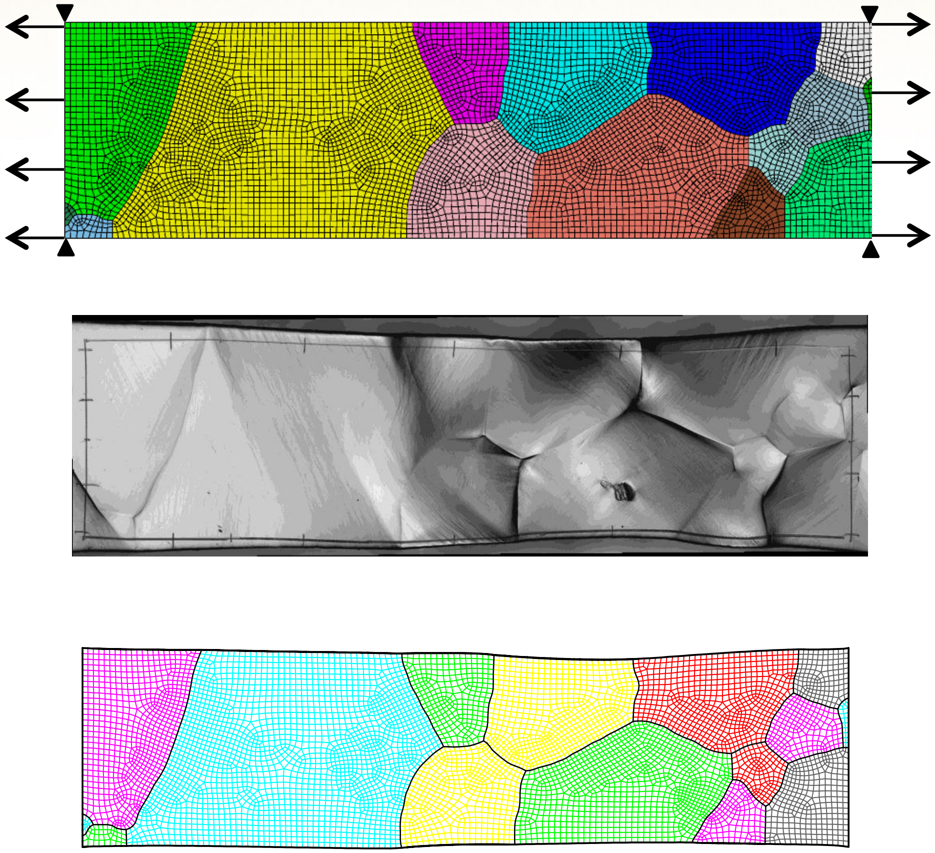
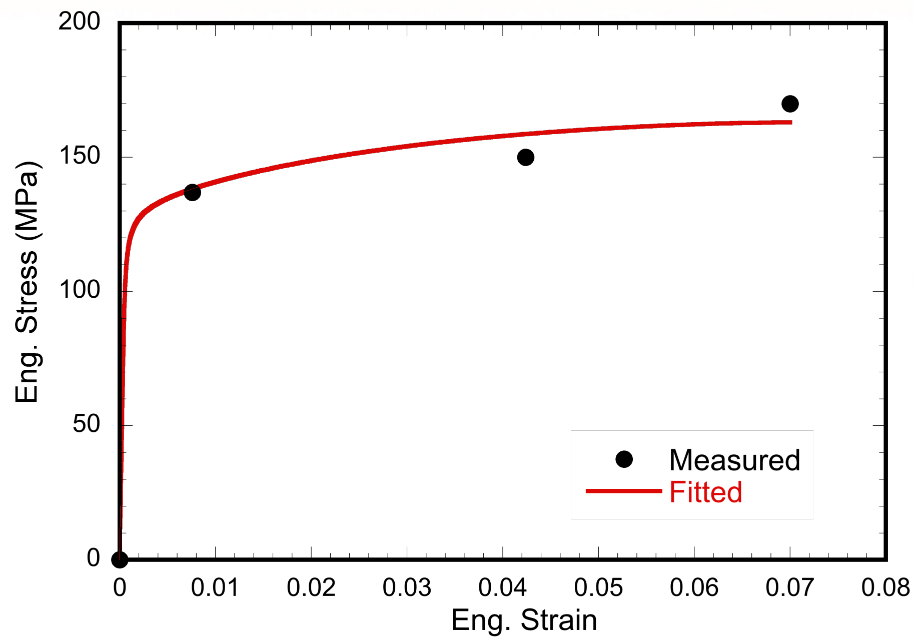
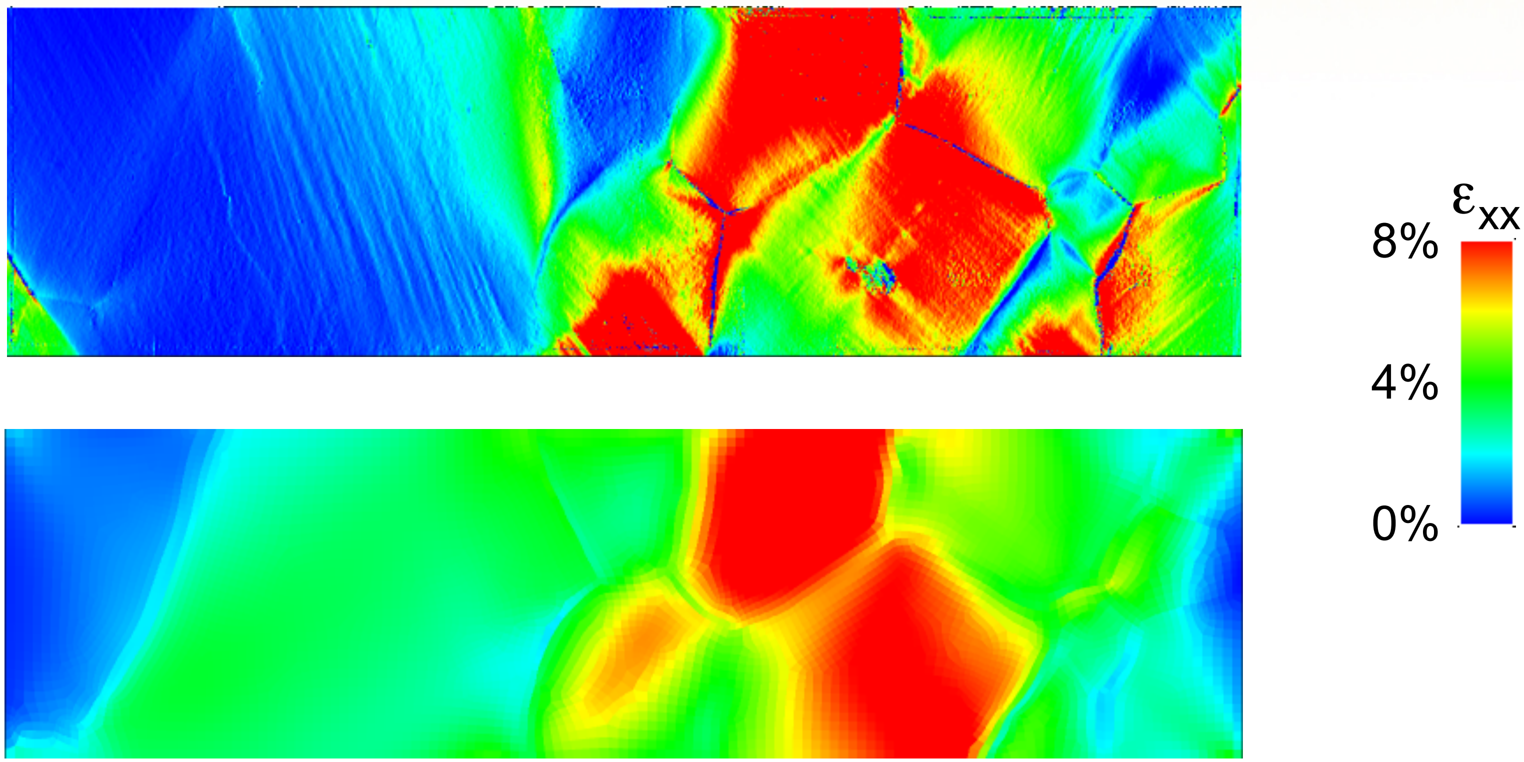
Finite Element Mesh





Validating CP-FEM Simulations w/ DIC Experiments

Experiment

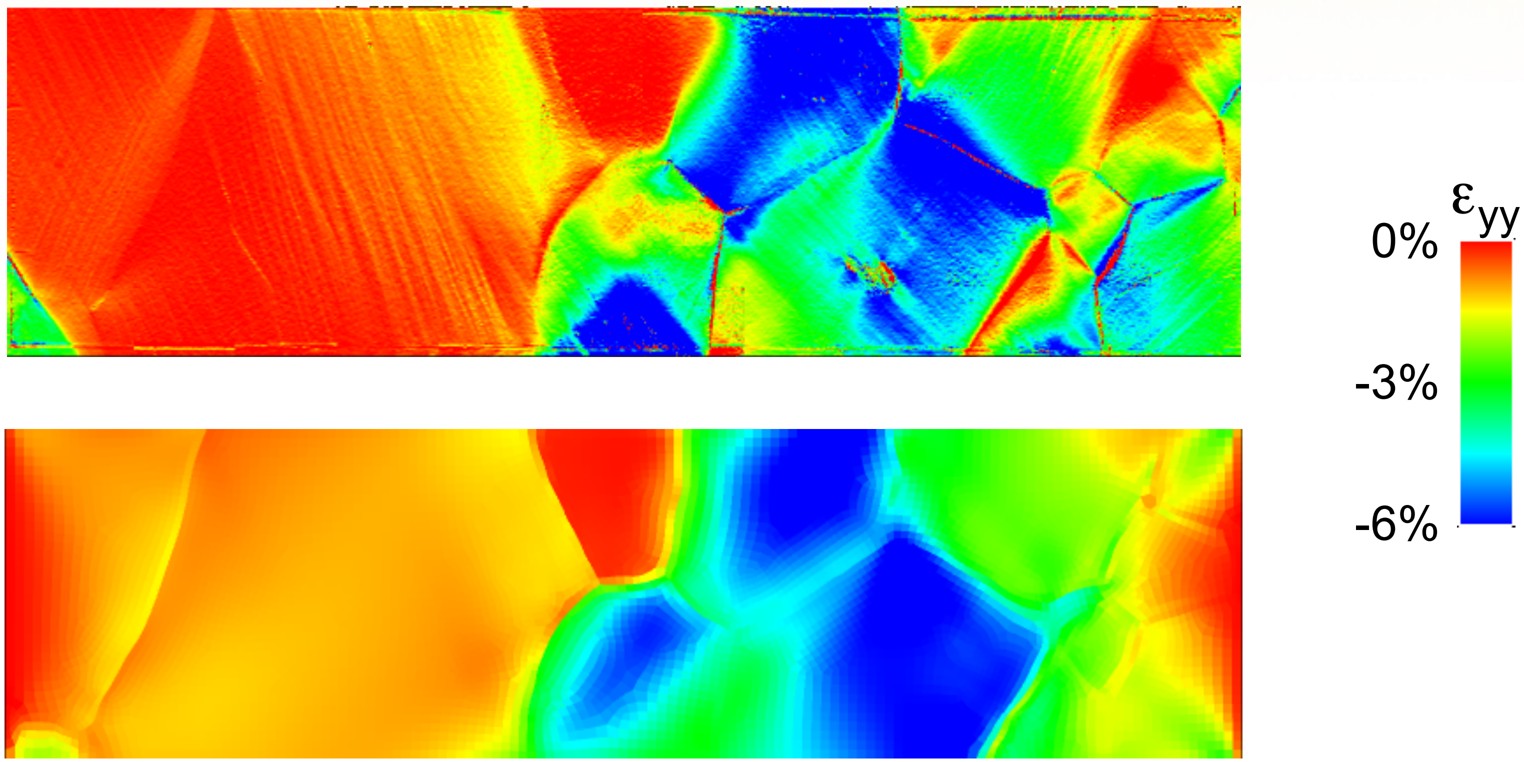


CP-FEM Simulation

4.2% Applied Strain

Validating CP-FEM Simulations w/ DIC Experiments

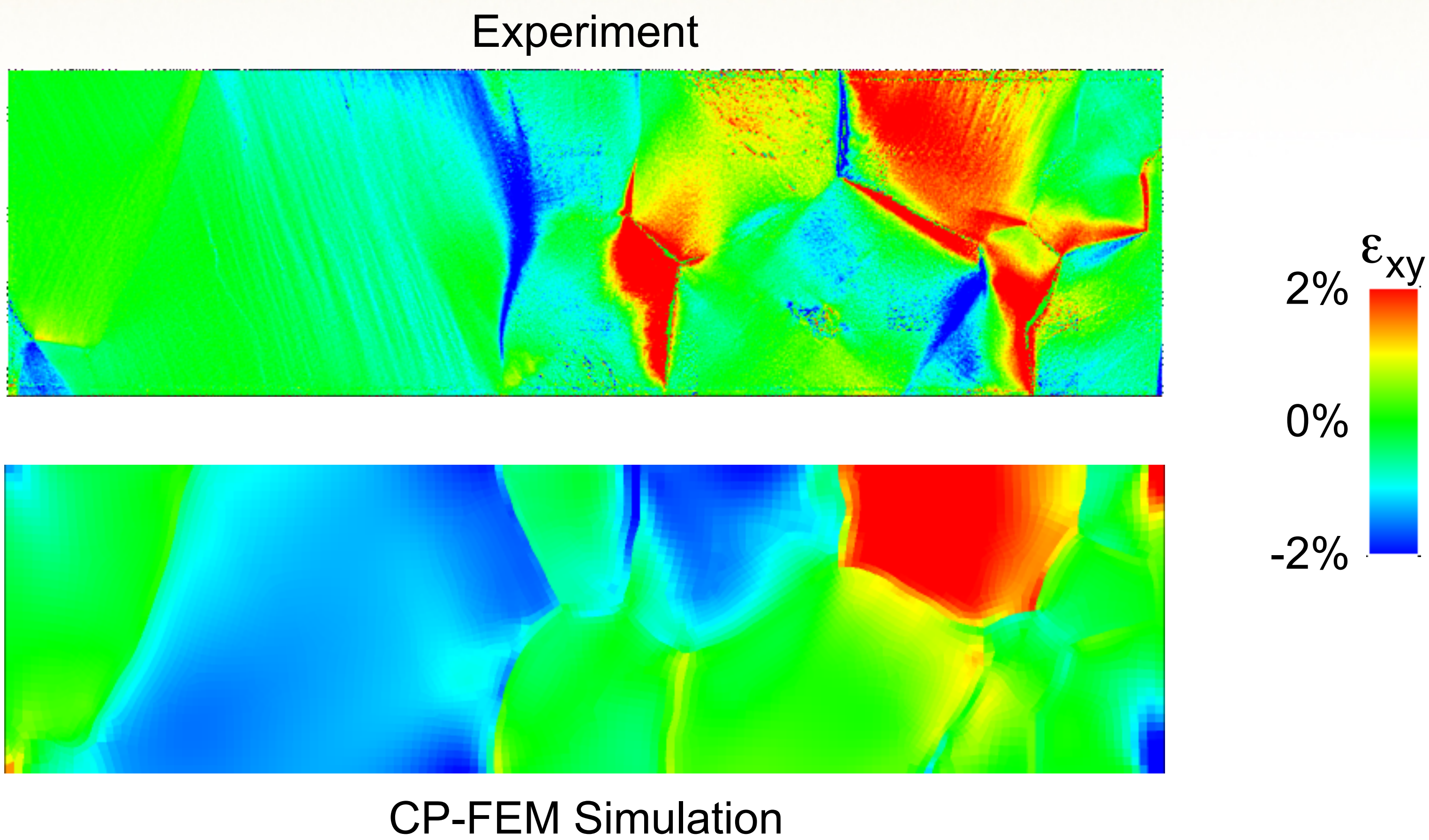
Experiment



CP-FEM Simulation

4.2% Applied Strain

Validating CP-FEM Simulations w/ DIC Experiments



4.2% Applied Strain

Summary

- Dislocation plasticity in BCC metals (and most materials, for that matter) is significantly more complex than in FCC.
- We have developed a generalized yield criterion for BCC transition metals, and implemented it into a BCC CP-FEM model.
- Yield criteria are calibrated to single crystal experiments on Mo, Ta, and W.
- Non-Schmid effects are clearly reflected in the stress-strain response, texture evolution, damage localization, and yield surfaces of single and polycrystals.
- Early CP-FEM predictions show good qualitative agreement with digital image correlation experiments on Ta oligocrystals.