SAND2011-0569P

Predicting Performance Margins: Linking the microscale to the macroscale

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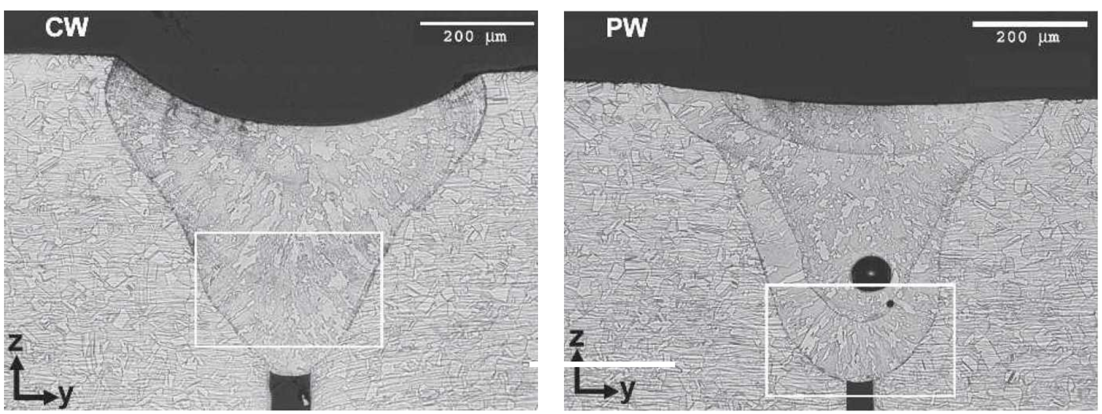
Introduction and Overview

- A series of events led to the creation of this project:
  - In spring and summer 2010, MS&T leadership worked with NW Science campaign leadership to create FY11 material science directed research areas.
  - In August 2010, the Laboratory President, Paul Hommert, requested new, materials science based projects to support Sandia's Annual Assessment Review (AAR).
  - Science and Technology Vice President, Steve Rottler, directed MS&T leadership to develop and support these projects.
  - MS&T leaders scoped the problem area, developed a project plan, assembled a team, and identified funding for an October 1, 2010 start date.
- Overarching project goals:
  - Develop and maintain the MS&T science base and identity.
  - Provide science-based models and data to support engineering judgments in the AAR and the Nuclear Weapons campaigns.
  - Provide growth opportunities for early- and mid-career staff members.

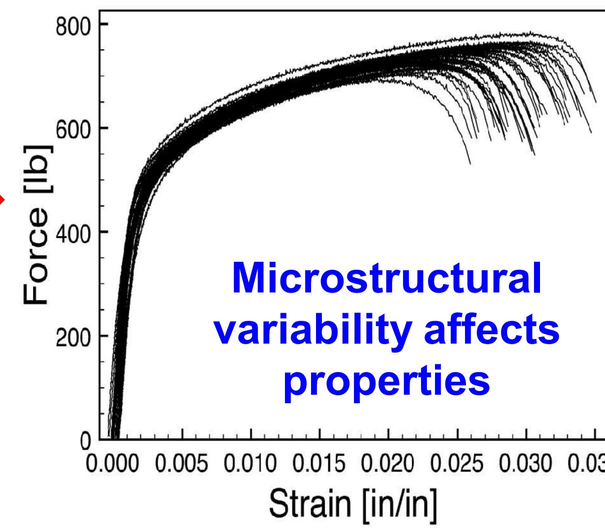
Motivation: Connecting microstructural variability to properties

- Materials are intrinsically inhomogeneous, but the relationship between microstructural variability and property statistics is unknown.
- A science-based, probabilistic underpinning for existing analysis capabilities must include microstructural effects.

⇒**Current analysis models do not incorporate microstructural variability.**



Microstructural details vary among weldments



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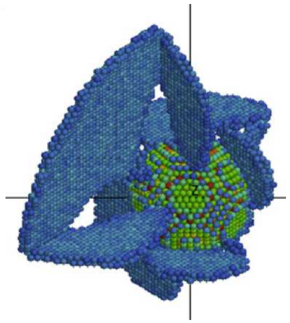
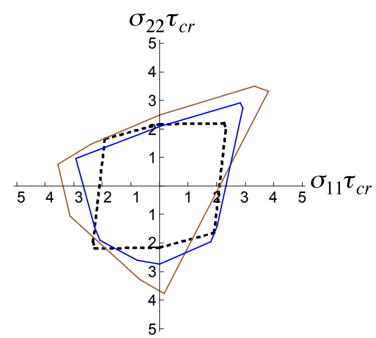
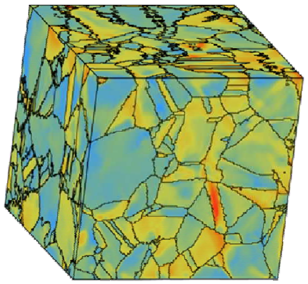
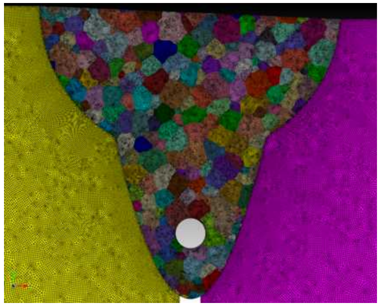
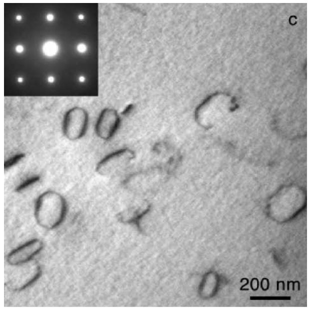
Including microstructure in design and analysis

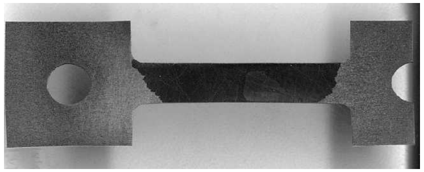


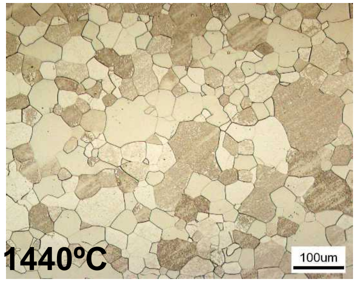


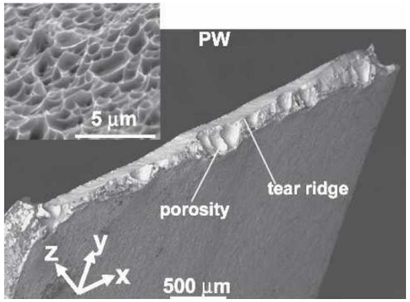






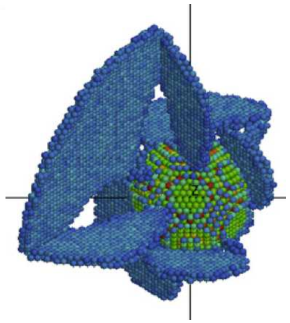


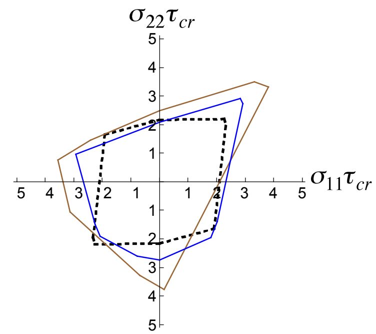


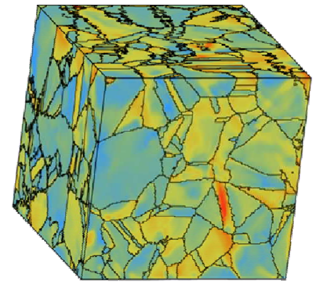


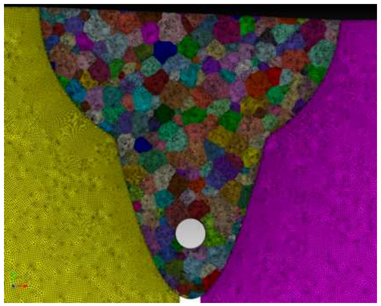
Atomic scale phenomena	Single crystal behavior	Microstructural effects	Material performance
10^{-9} m	10^{-6} m	10^{-3} m	10^{0} m
10^{-9} s	10^{0} s	10^{3} s	10^{6} s

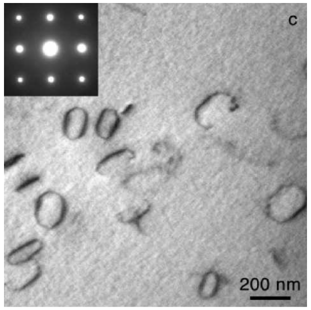
Including microstructure in design and analysis

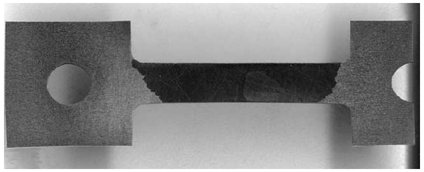


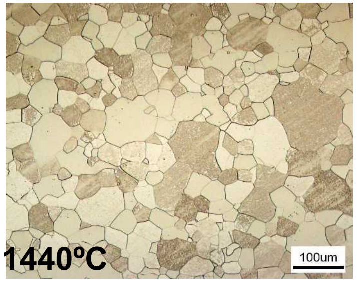


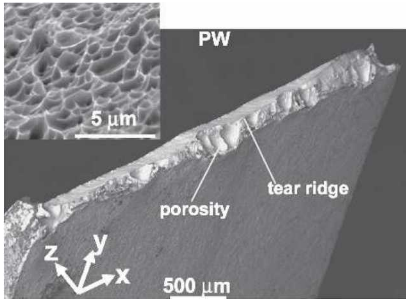












Atomic scale phenomena	**Single crystal behavior**	**Microstructural effects**	**Material performance**
DFT, MD, DD	crystal plasticity	kMC, PPFEM	FEM, QMU
TEM, APT, PAS	XRD, EBSD, µmachining, µtesting	EBSD, FIB, DIC, µmachining, µtesting	mechanical testing, microscopy

Advantages of the microstructural variability approach

- Acknowledges intrinsic materials variability at the **microstructural** scale
- Creates a link between structural variability and **property** variability
- Offers a path to include property statistics in **performance** models
- Provides a **science-based, probabilistic** underpinning for existing analysis capabilities

…. Paradigm shift, from the idealistic view that all parts are created equal, to the realistic view that structure, properties, and performance are probabilistic.

Project team structure enables collaboration, scientific advances, and impact

Task 1: Nanoscale framework for crack initiation and growth in Ta and Ta alloys
[J. Zimmerman (8246), C. Weinberger (1814)]

Task 2: Microscale effects of defect fields in Ta and Ta alloys
[B. Boyce (1831)]

Task 3: Connecting microstructural variability to performance margins in structural metals
[C. Battaile (1814)]

Technical Advisory Council
[S Foiles (1814), D Medlin (8656), J Michael (1822), D Reedy(1526), C Robino (1831), N Moody (8222)]

Customer Advisory Council
[B Paulsen (2211) (chair), T Mattsson (1641), D Balch (8224), S Whalen (2547), E Fang (1524), S Harris (2141), B Oetken (8224), J McLaughlin (0425)]

External Collaborators
[LLNL, LANL, UT Austin, Georgia Tech, Michigan State University, Cal Tech, Carnegie Mellon, etc.]

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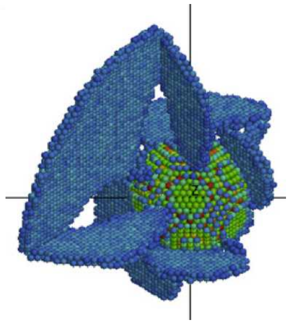
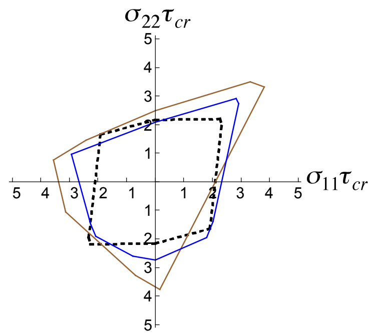
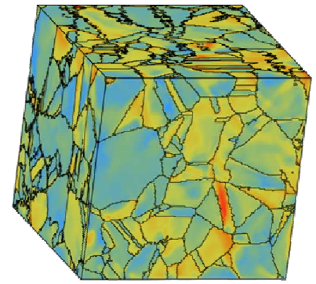
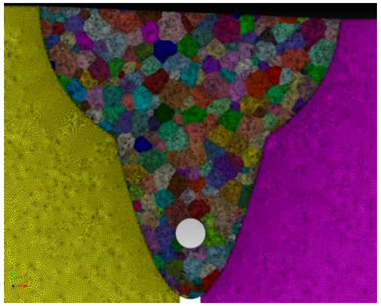
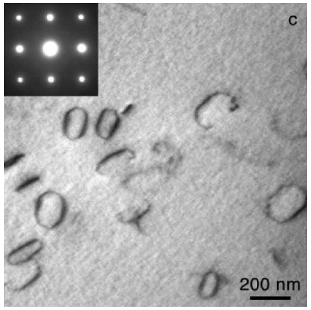
Including microstructure in design and analysis

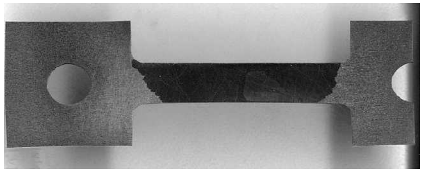


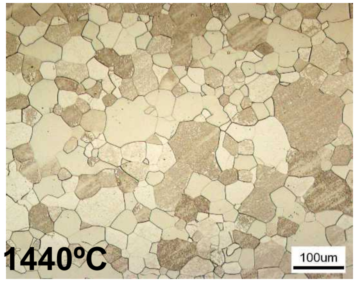


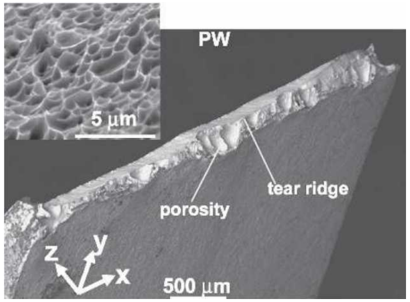












Atomic scale phenomena

Single crystal behavior

Microstructural effects

Material performance

Task 1

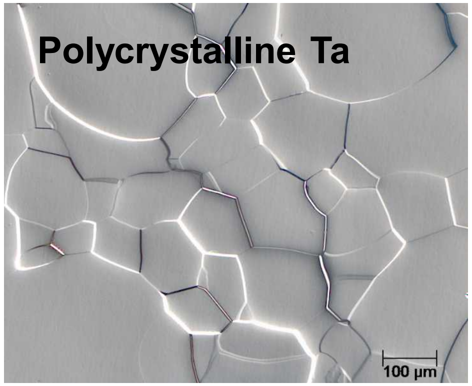
Task 2

Task 3

Proof-of-principle: Plasticity in BCC metals

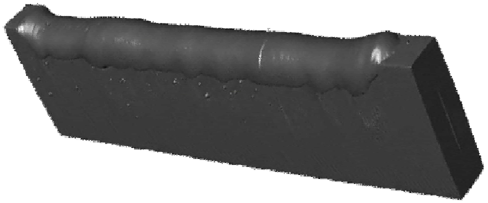
- BCC metals provide a platform for microstructural variability studies
  - Technologically important.
    - *Refractories: W, Mo, Ta*
    - *High energy applications: W, Ta*
    - *Steel*
  - Underrepresented in computational materials science studies.
    - *Complex response, compared to FCC*
    - *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



Polycrystalline Ta

304L stainless weldment



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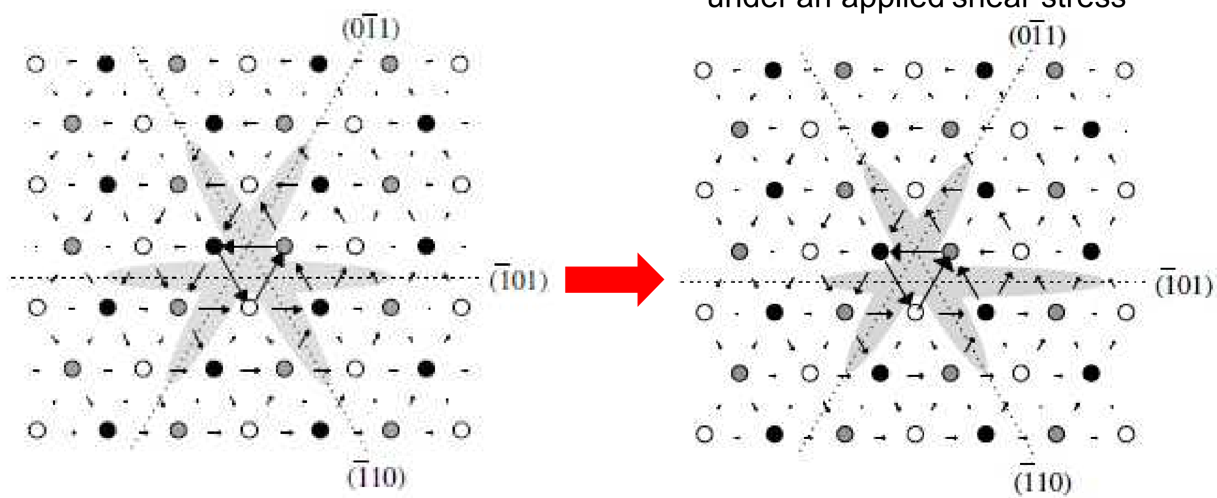
Atomic Scale: Physical model for dislocation motion in BCC metals

- 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

Single crystal behavior: BCC crystal plasticity model

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

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

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:

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

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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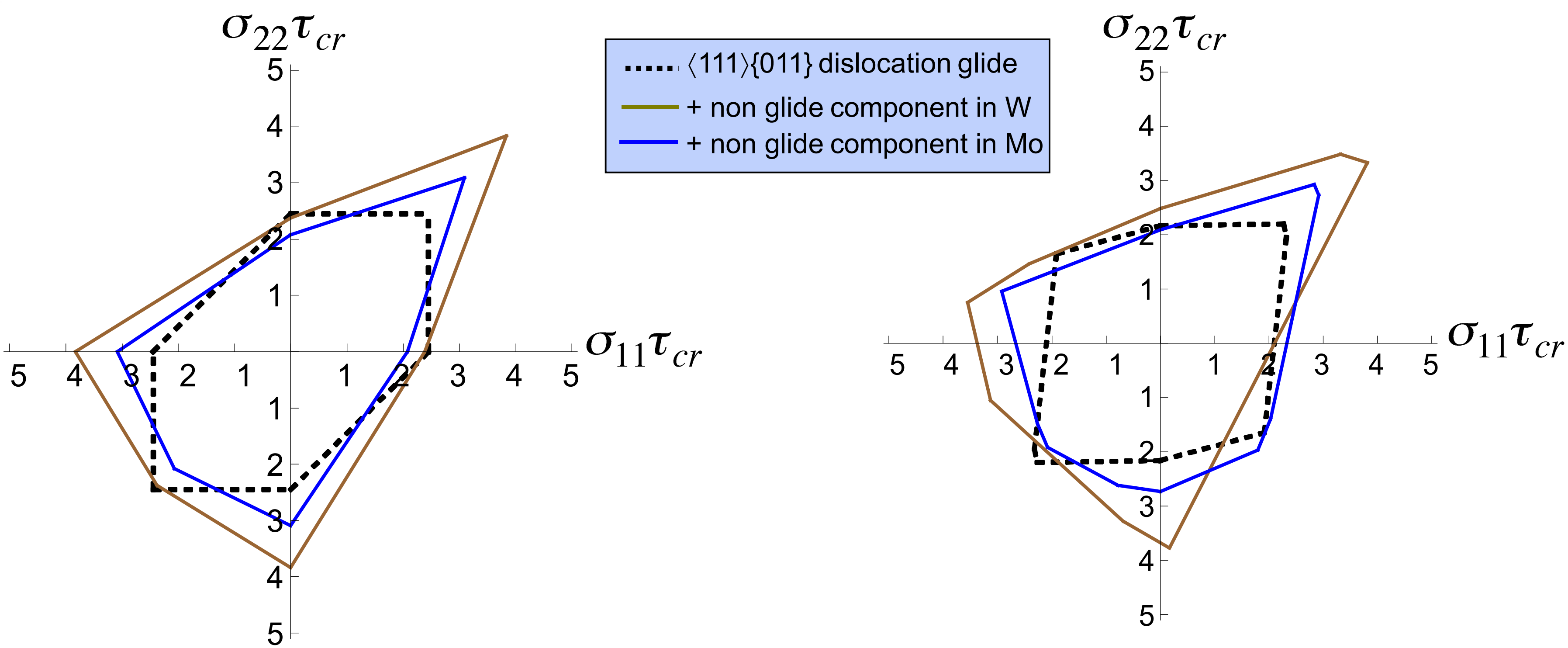
Single Crystal Results: BCC single crystal yield surfaces



⟨100⟩(010) orientation
highly symmetric

⟨-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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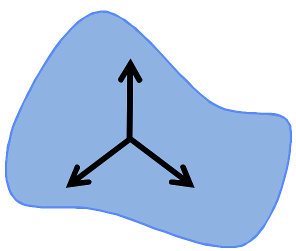
Extending single crystal behavior to capture microstructural effects

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

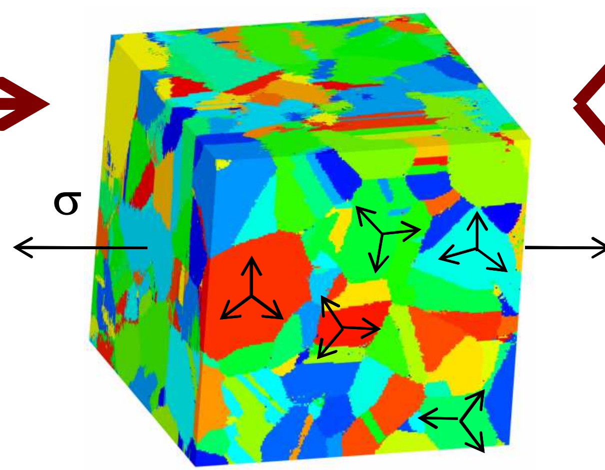
Single crystal plasticity



Constitutive law

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

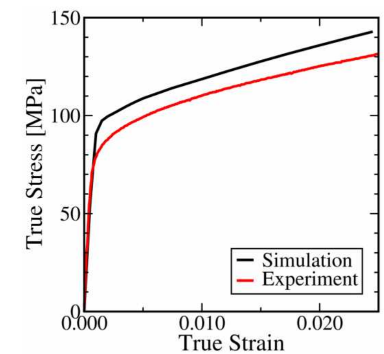
Polycrystal plasticity



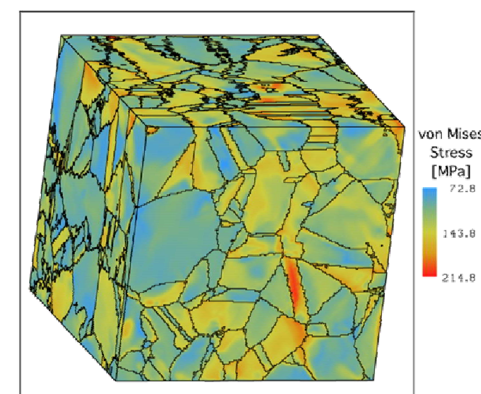
Each grain responds via the orientation-dependent constitutive law

Results

Overall mechanical response

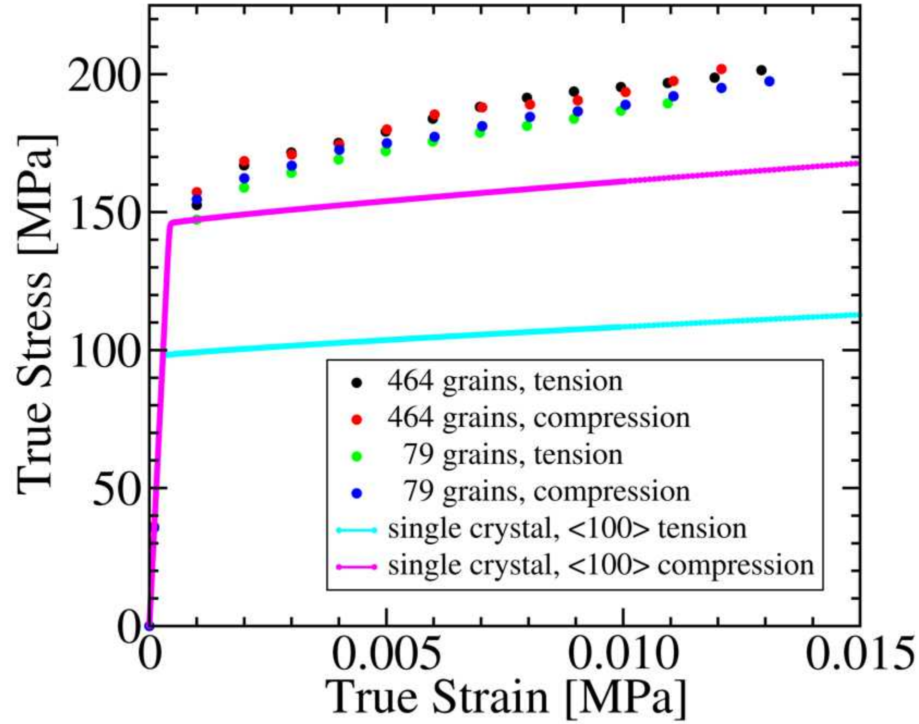


Individual grain response (rotation, stress, etc.)



Microstructural Results: Continuum response of BCC polycrystals

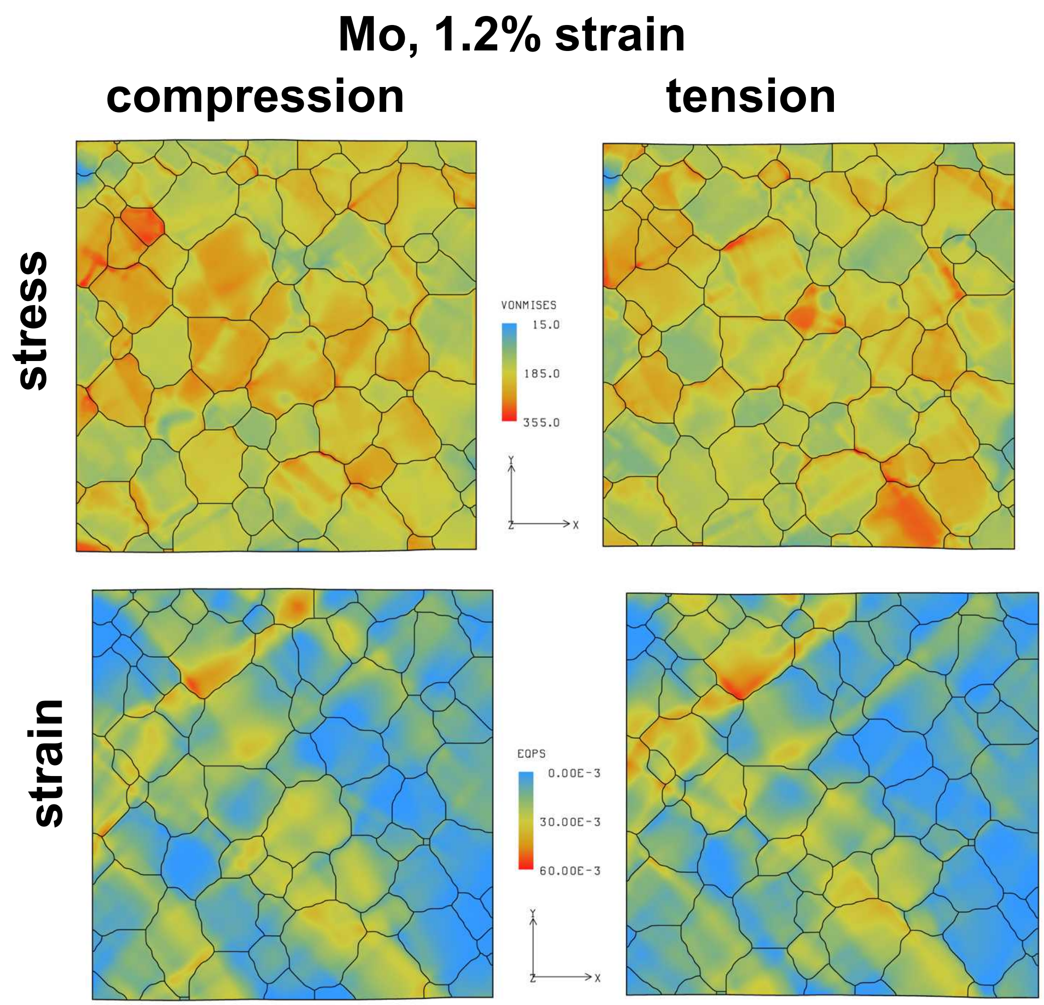
- In plasticity simulations of single- and polycrystalline Mo:
  - *Single crystal and polycrystal response differ considerably.*
  - *Single crystals show considerable tension/compression asymmetry.*
  - *Polycrystals do not exhibit tension/compression asymmetry.*
  - *There is no grain size dependence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



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.

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Summary and Conclusions

- We have recently developed and commenced a new project to connect microscale variability to performance uncertainty in BCC metals.
  - Science-based effort spanning length and time scales.
  - Project team includes staff, customers, and external collaborators.

- Early results illustrate the value of the multiscale, multidisciplinary approach.
  - Plasticity in BCC metals depends on atomic, single crystal, and microstructural variables.
  - Traditional continuum approaches cannot capture deformation physics.

- The long-term goal of the project is to integrate these results into a probabilistic model for component deformation and failure.