SAND2013-7448C

Material Deformation at the Microstructural Scale in BCC Tantalum

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Sandia National Laboratories

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Outline

1. **Motivation**
   - Why do we need to understand grain scale deformation?
2. **Background**
   - Slip in FCC and BCC metals
3. **Relating microstructure to deformation**
   - Schmid factors, etc.
4. **Predicting deformation behavior at the grain scale**
   - Crystal plasticity models
5. **Conclusions**

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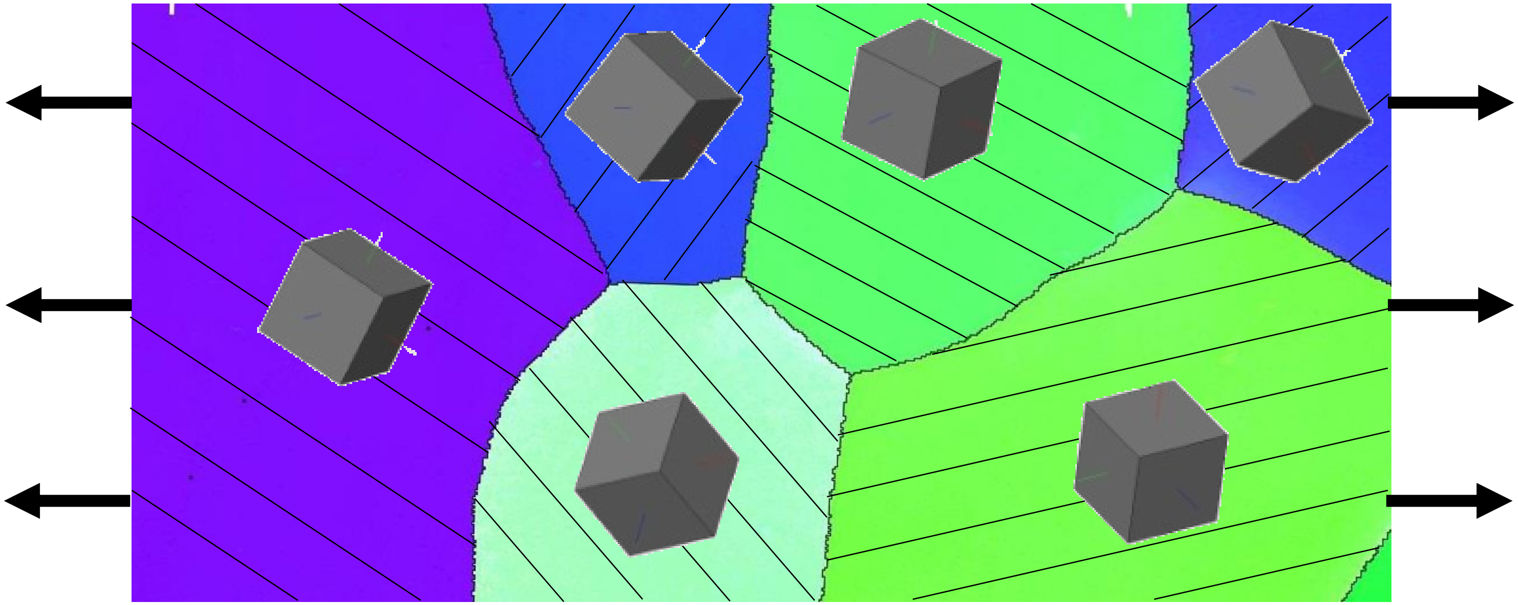
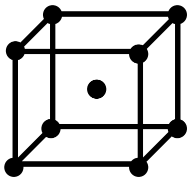
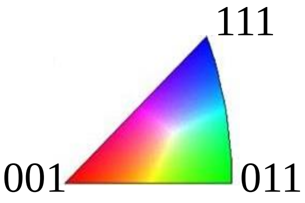
Grains are regions of the material with consistent orientation of the atomic unit cell.

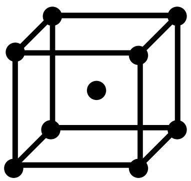




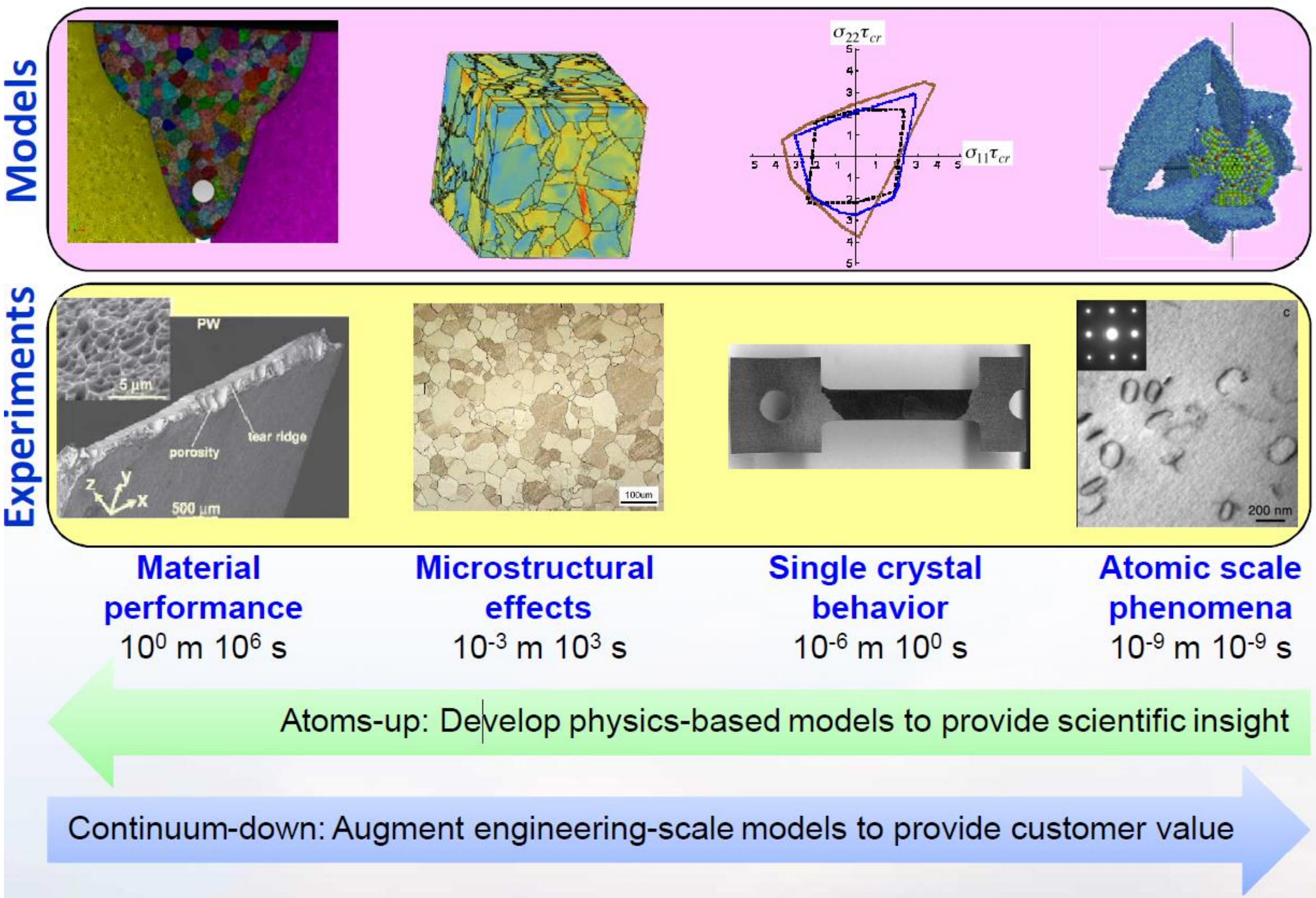


Relate variability in structural behavior to microstructural variability

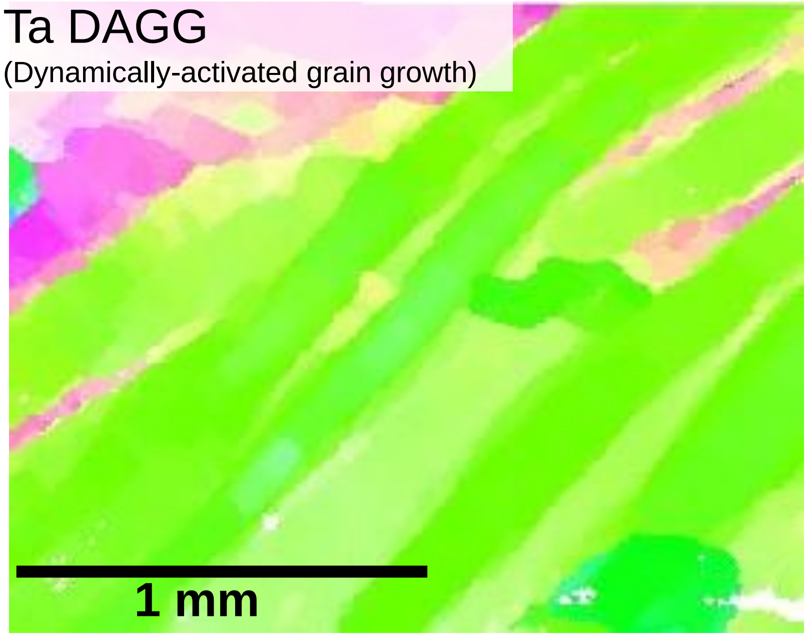
- **Task 3: Predict macroscale variability from microstructural statistical models.**
- **Task 2: Microscale effects on deformation behavior.**
- **Task 1: Atomic/nanoscale defects and dislocation effects.**



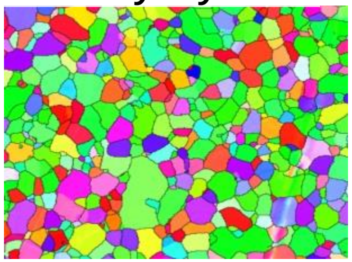
BCC
Ta

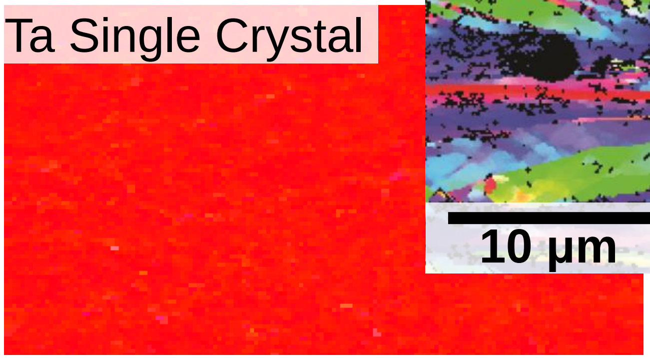


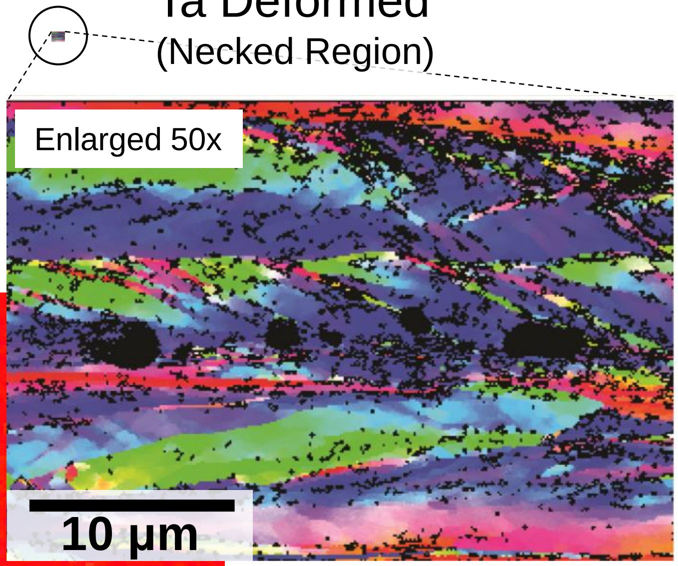
Grain structure strongly depends on the material's history.

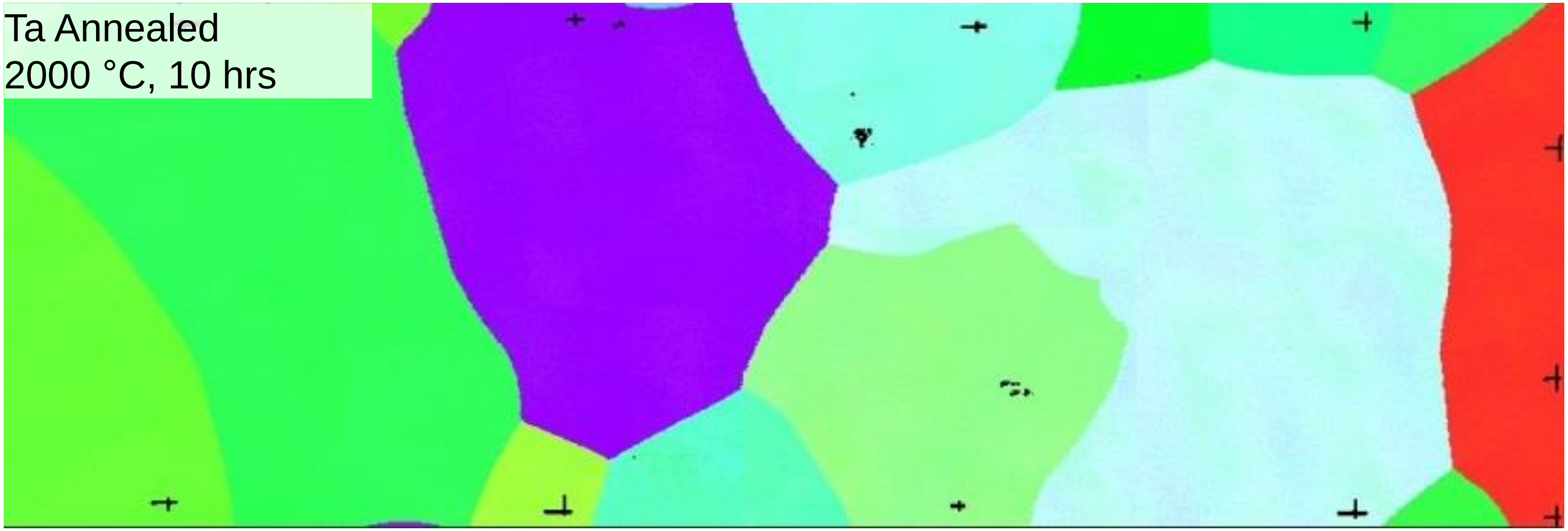


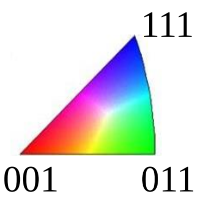
Ta Polycrystal





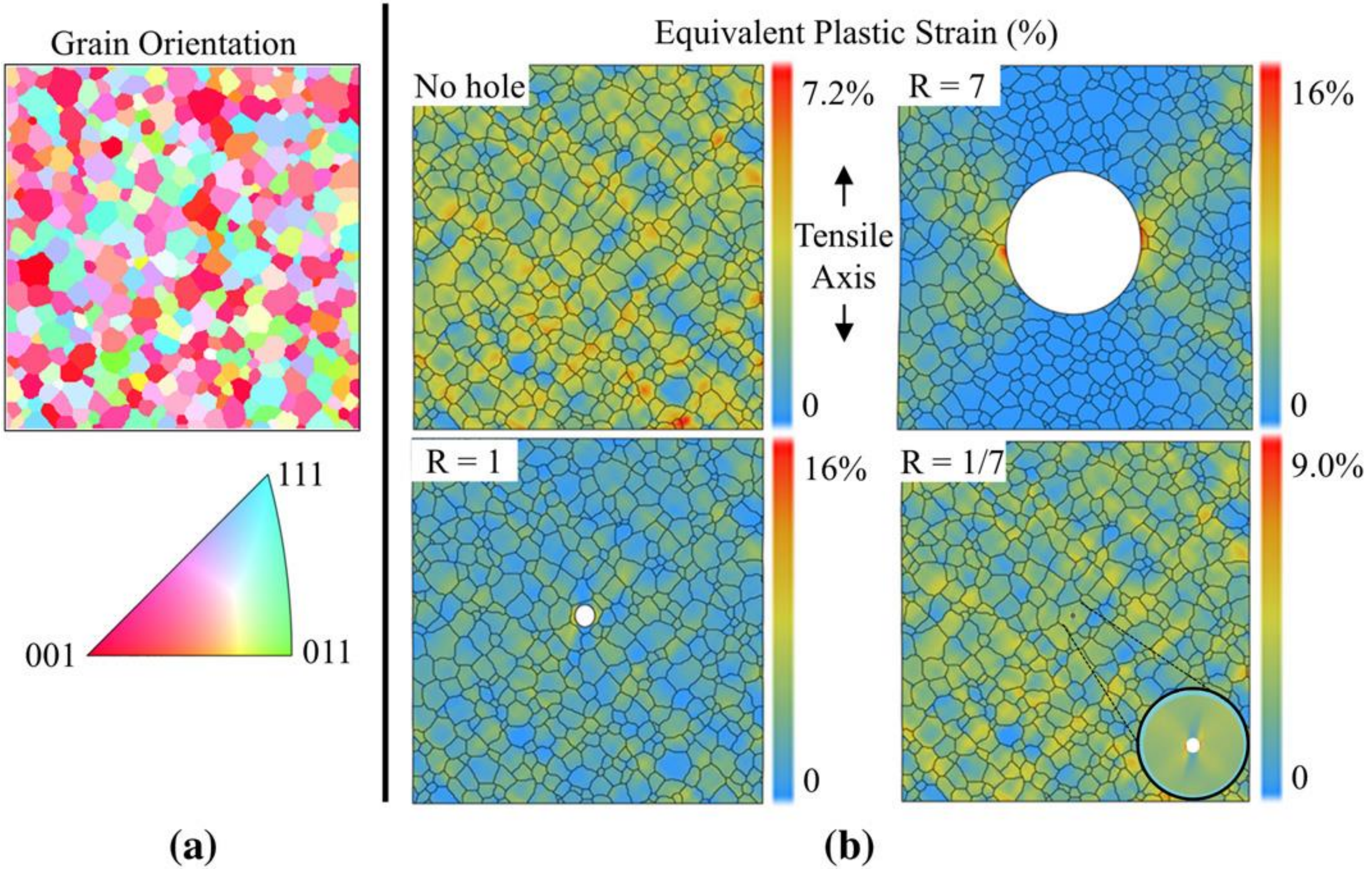






For small features, microstructure can be more important than the stress concentrator.

- **Model predictions**

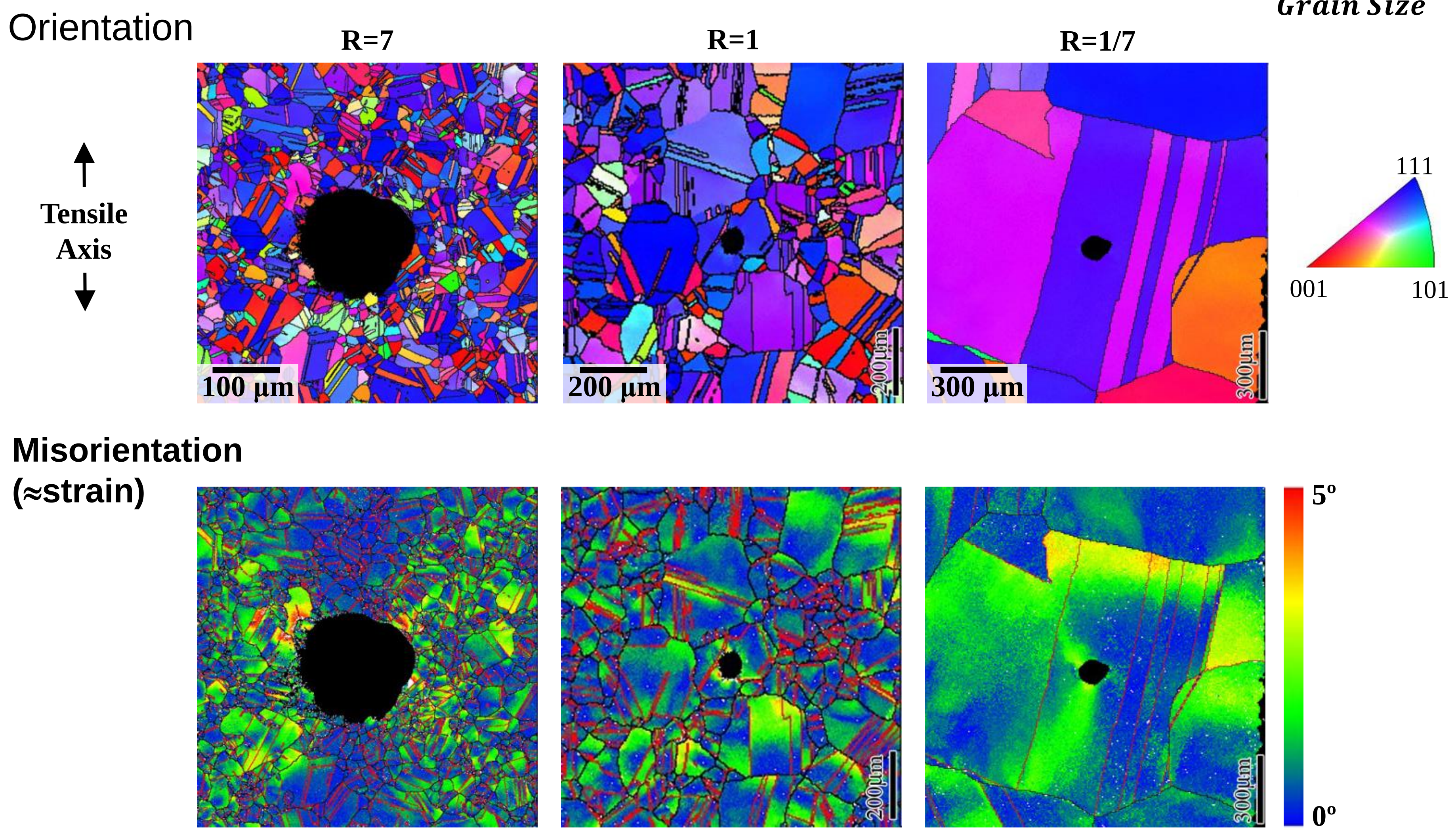


Carroll J.D., Brewer L.N., Battaile C.C., Boyce B.L., Emery J.M., Int. J. Plasticity, v. 39 (2012).

For small features, microstructure can be more important than the stress concentrator.

- **Experimental measurements**

$$R = \frac{Hole\ Size}{Grain\ Size}$$



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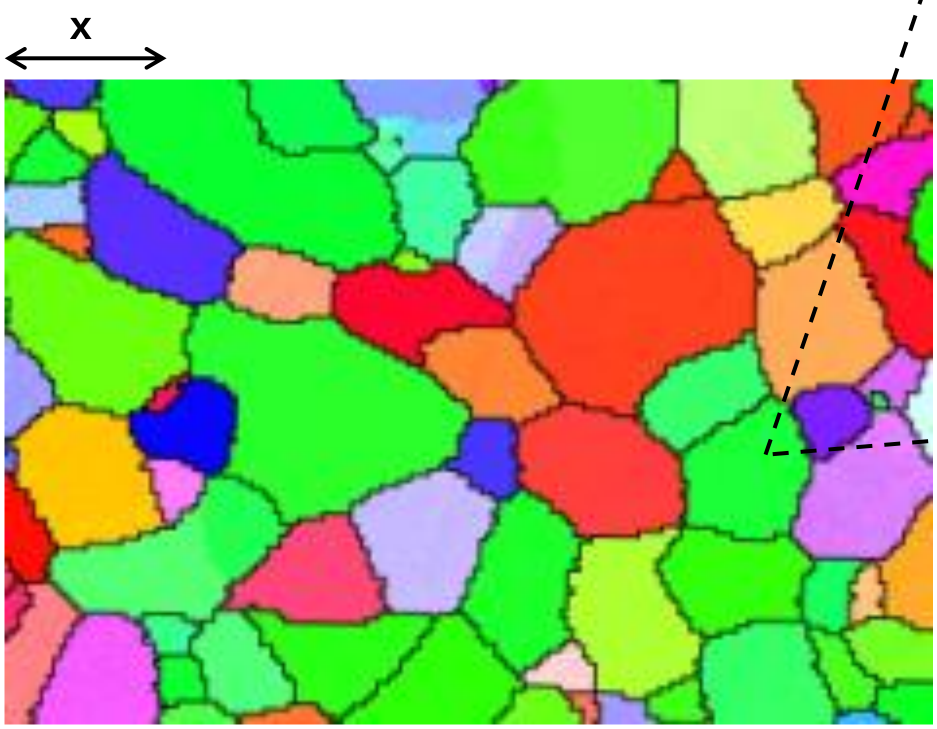
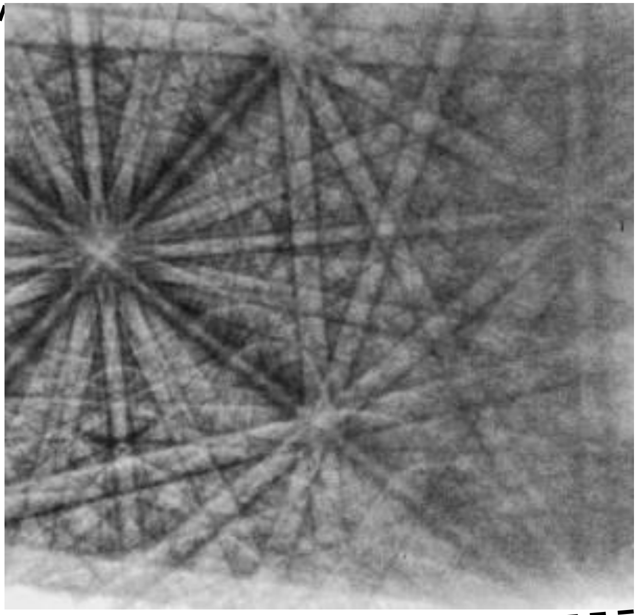
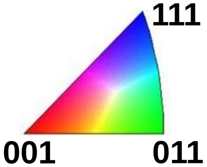
Electron Backscatter Diffraction (EBSD) measures local grain orientation.

- **Capture an image of Kikuchi diffraction bands.**
- **Compare angles of bands to a lookup table to find the crystal orientation.**
- **Repeat for all pixels in the map.**



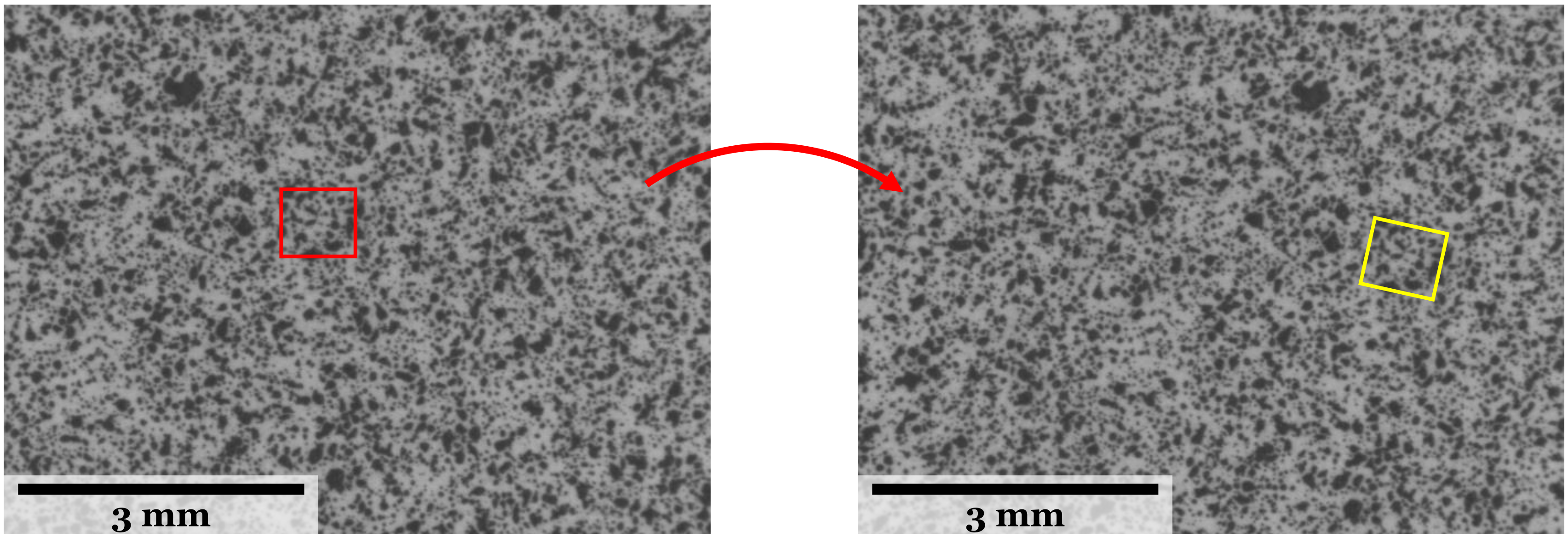


- J.A. Small, J.R. Michael, Journal of Microscopy-Oxford, v. 201 (2001).



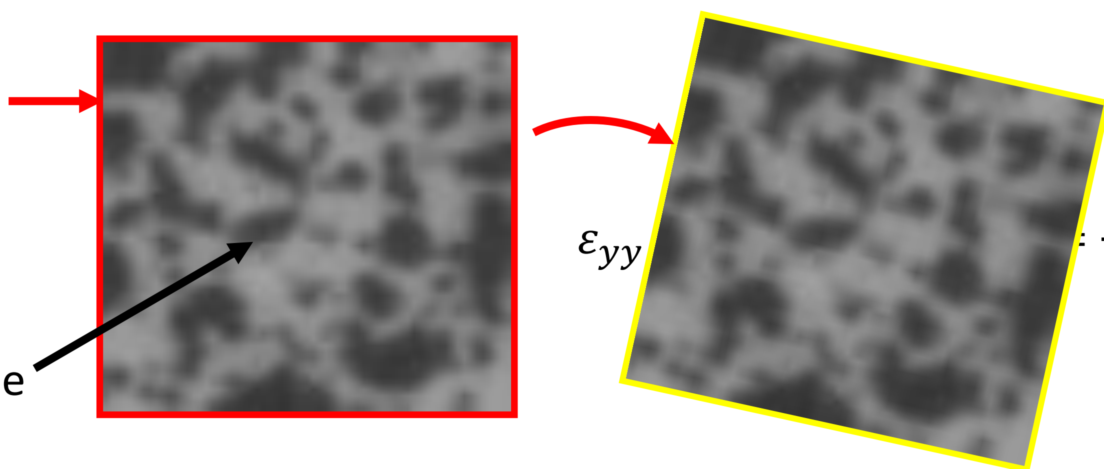
Digital image correlation (DIC) measures full field displacements and strains by tracking speckles.

Reference | Deformed



Subset

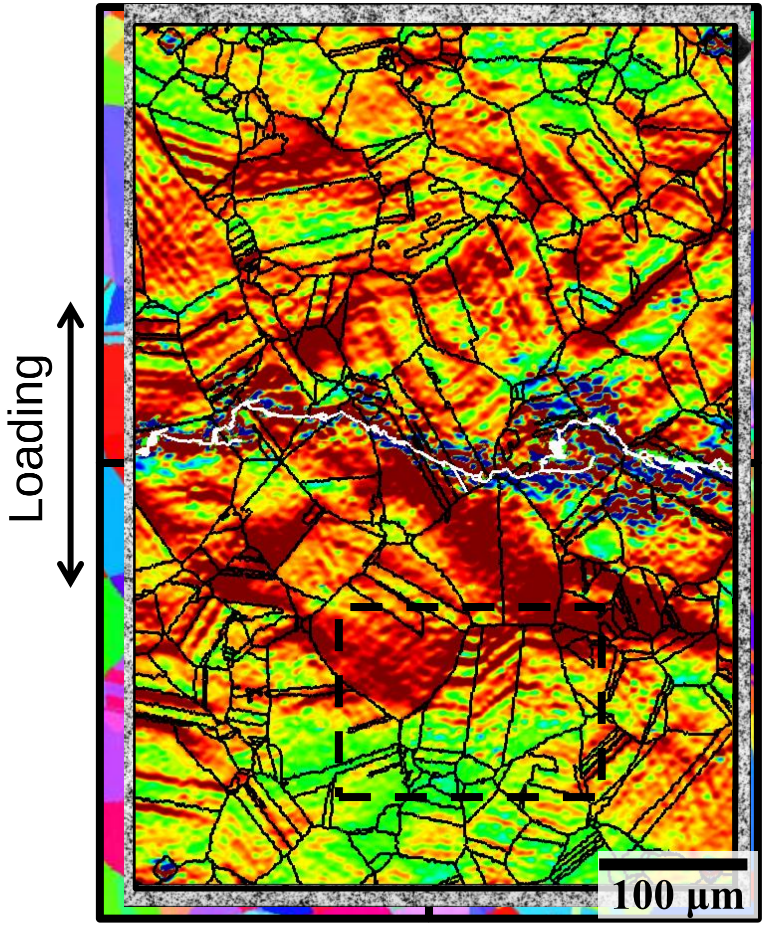
Calculate Strains

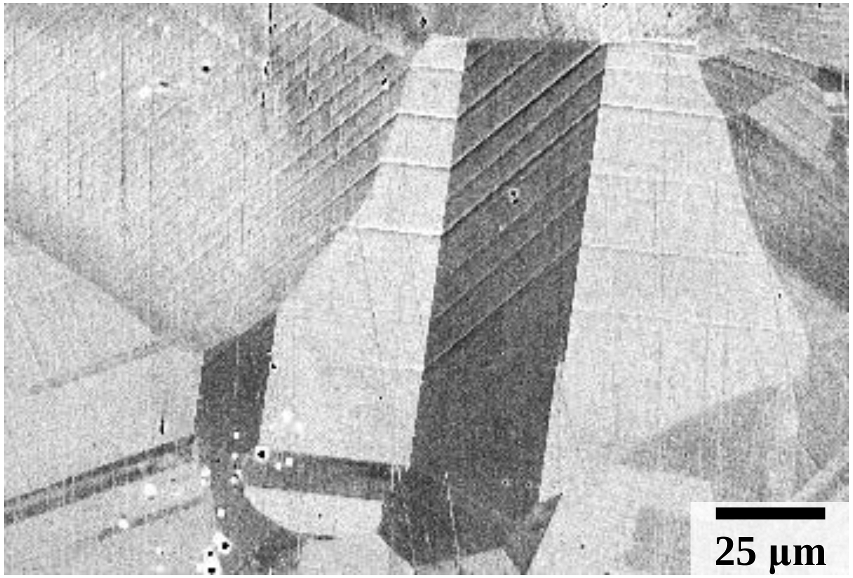


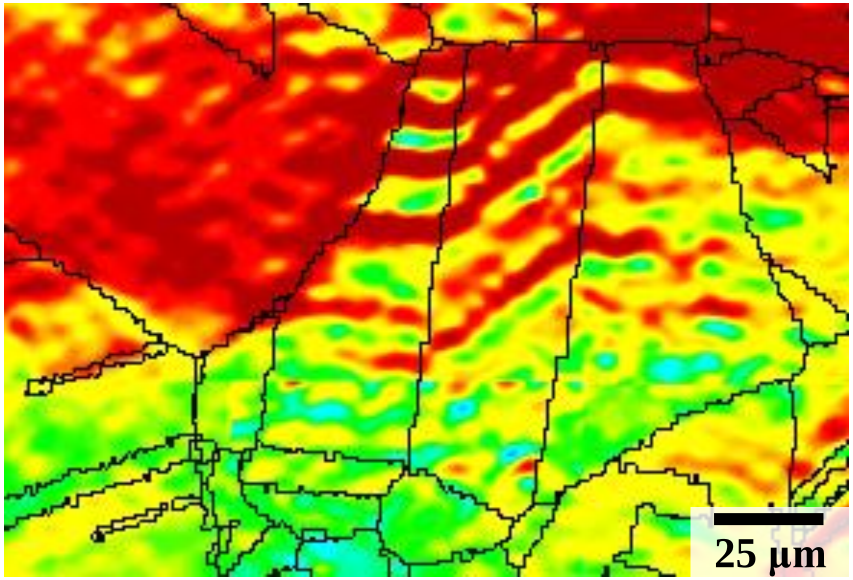
Speckle

$$\varepsilon_{yy} = \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)$$

Our high resolution experimental technique relates subgrain level strains to microstructure.

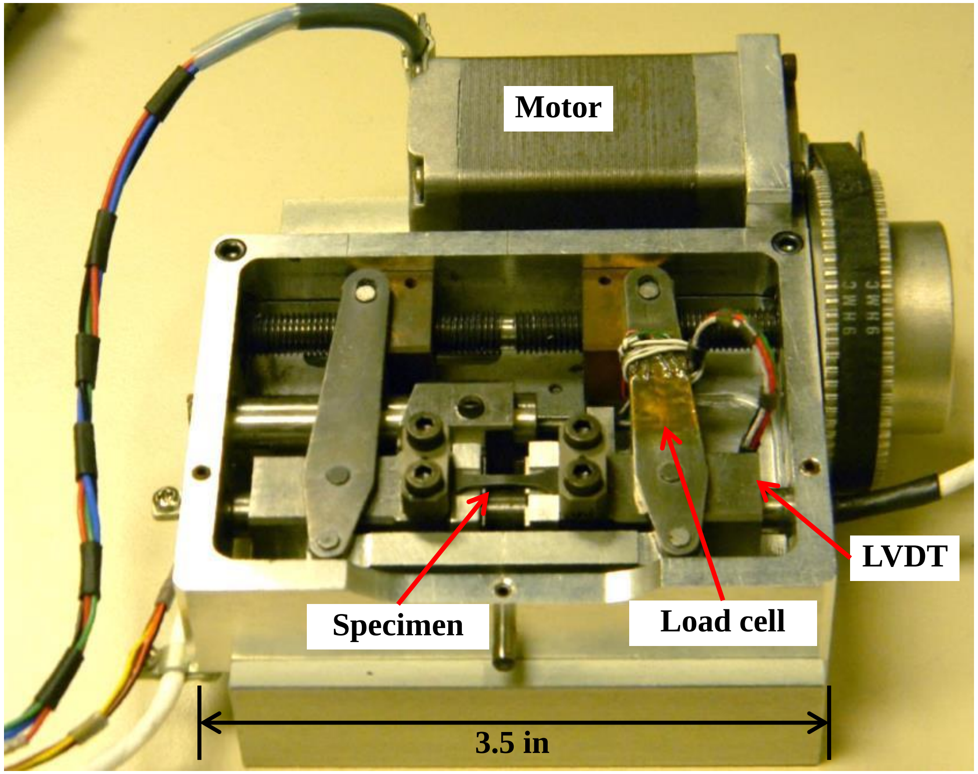




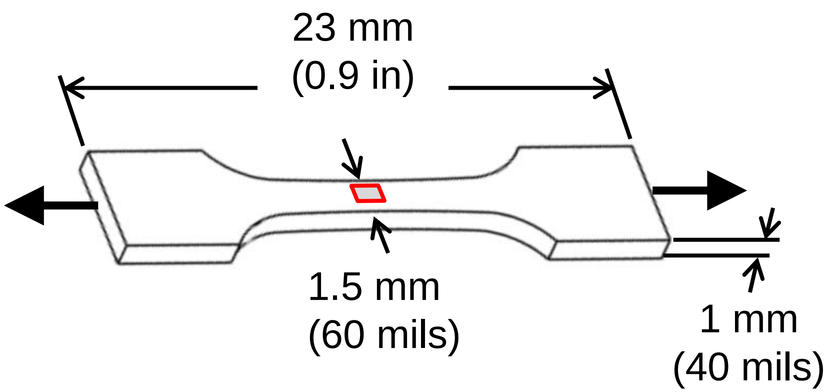


- **Carroll et al., *Rev. Sci Inst.*, v. 81 (2010).**
- Carroll et al., *Int J. Fracture*, v. 180 (2012).
- Carroll et al., *Int. J. Fatigue*, (in press, 2013).

An in situ load frame developed at Sandia allows loading inside the SEM.



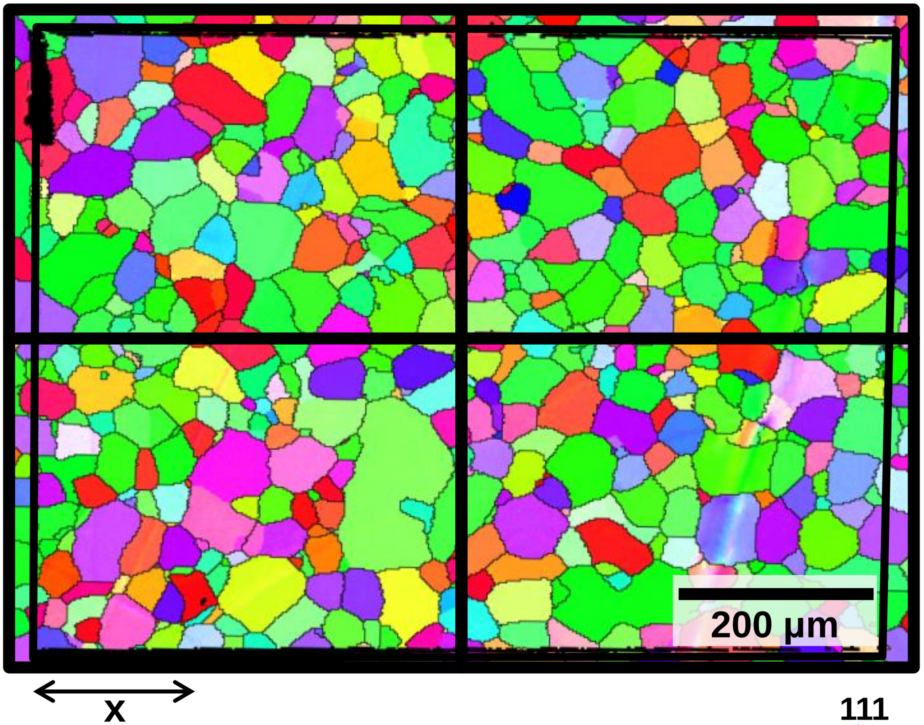
- **Can make DIC and EBSD measurements at load.**

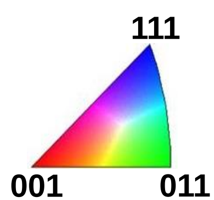


Tapered gage section is narrower at center.

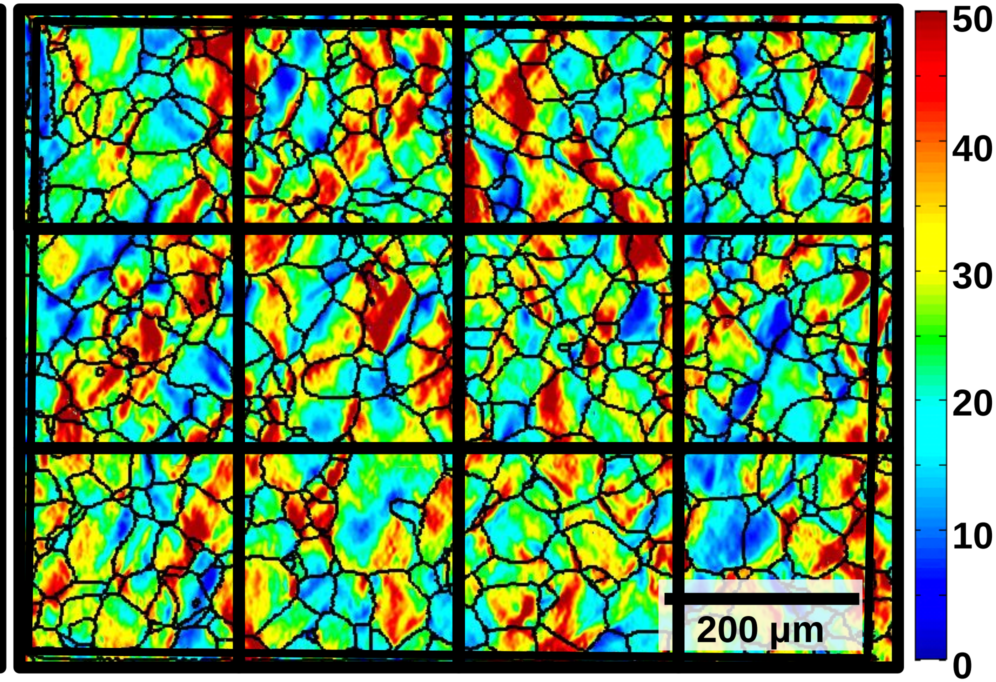
Compare grain structure to local strain measurements in polycrystal Ta (BCC metal).

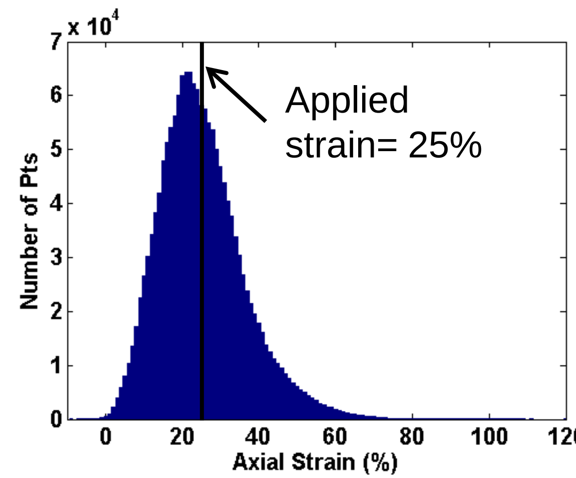
Microstructure (EBSD)





Effective Strain (%) (DIC)





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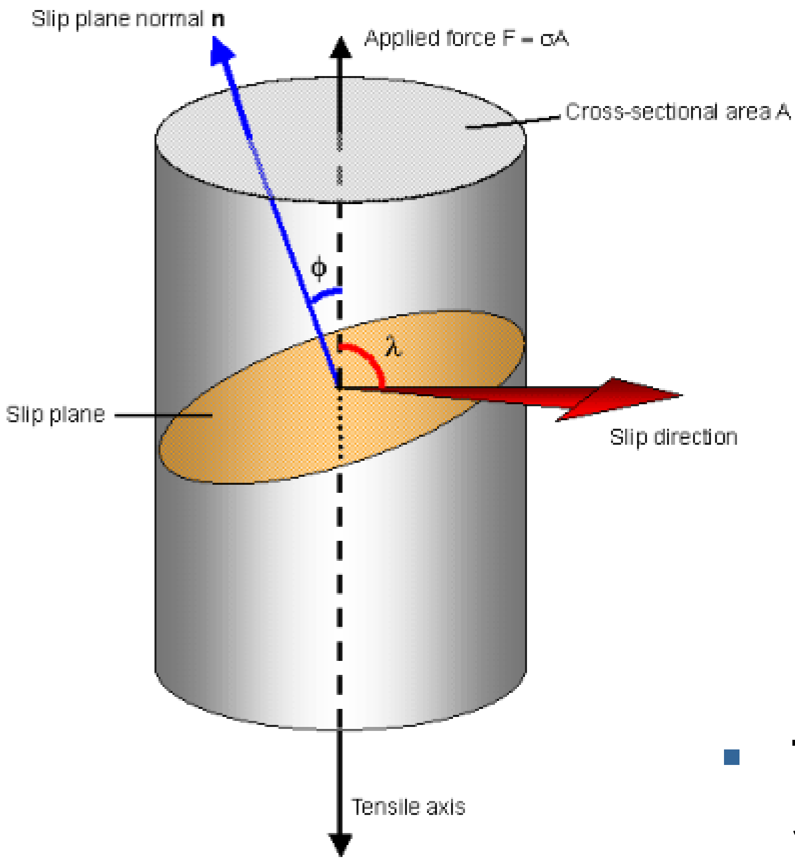
The Schmid Factor is measures how prone each plane is to crystallographic slip.



http://www.doitpoms.ac.uk/tlplib/slip/slip_geometry.php

Shear stress on system

Applied stress

Schmid factor

$$\tau = \frac{F}{A} \cos\phi \cos\lambda$$

0 < Schmid < 0.5

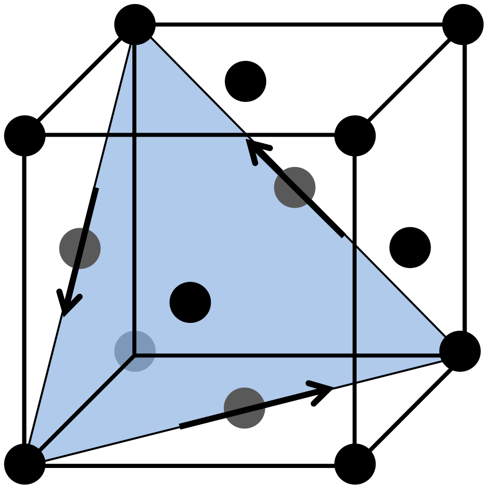
Hard. Slip will not happen on this system.

Soft. Slip will probably happen on this system.

- **The Schmid factor of a grain is the max Schmid factor of all slip systems considered.**

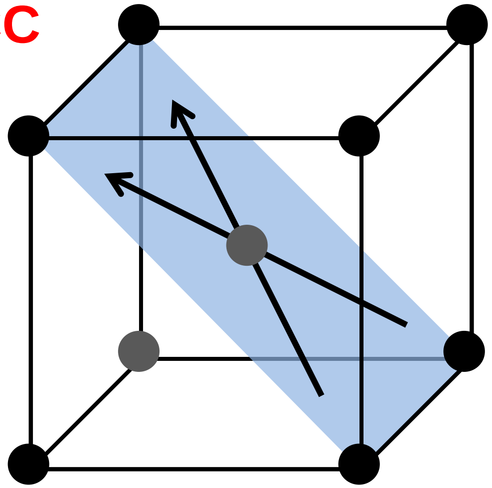
Images showing slip planes and directions in FCC and BCC unit cells.

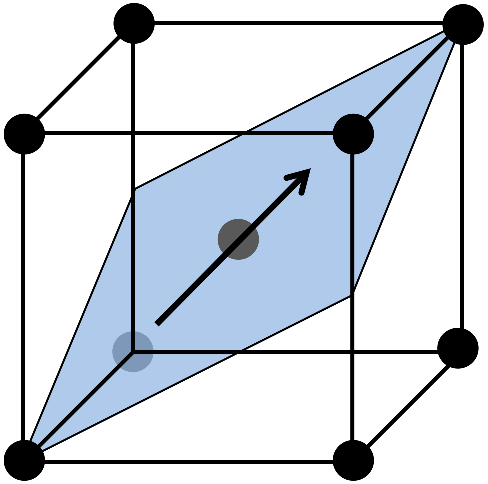
FCC

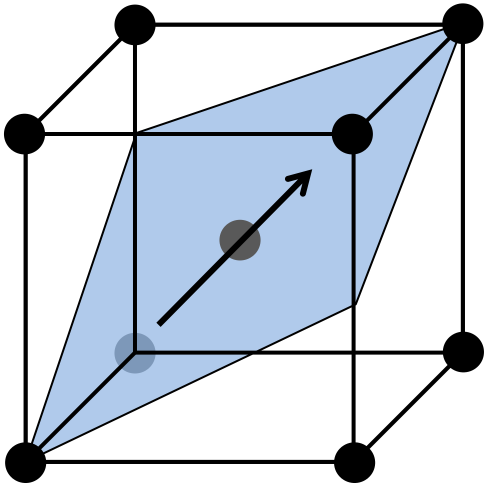


12 Slip systems:
Four {111} Planes each with three <110> Slip directions

BCC





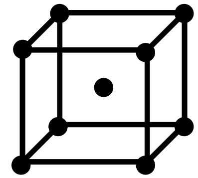


12 {110} slip systems
6 Planes each with two <111> Directions

12 {112} slip systems
12 Planes each with one <111> Direction

24 {123} slip systems
24 Planes each with one <111> Direction

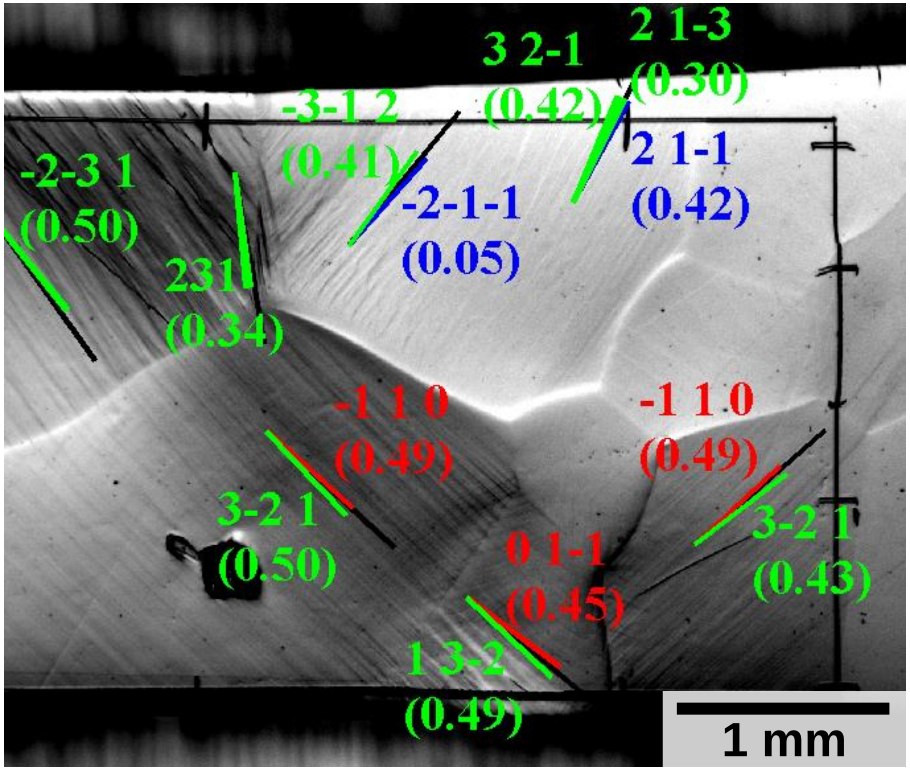
Special challenge with BCC materials: Identifying active slip systems.



- **Slip is in the <111> direction, but on which plane?**
- **At the atomic level, {110} is the most likely slip plane, but no consensus.**
- **Microscopically, slip can be on {110}, {112} or the maximum resolved shear stress plane containing a <111> direction.**

Material	Slip plane	. . .	References
Tungsten	{110}		118
Tungsten	{112}		118
α-iron	{110}		118
α-iron	{112}		118
Chromium	{112}		118
Vanadium	{112}		118
Tantalum	{112}		133
Tantalum	{112}		134
Tungsten	{110}		130
Molybdenum	{110}		130
Molybdenum	{110}		130
Molybdenum	{110}		130
Molybdenum	{110}		130
Niobium	{110}		130
Niobium	{112}		130
Niobium	{110}		130
α-iron	{110}		130
α-iron	{112}		130
α-iron	{112}		130
Vanadium	{110}/{112}		130
Vanadium	{110}/{112}		130
Vanadium	{112}		130

Weinberger C.R., et al., International Materials Reviews (2013)

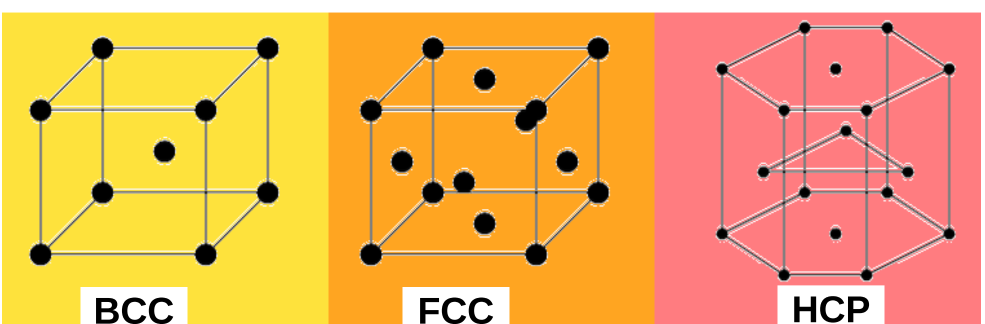


Carroll J.D., Clark B.G., Buchheit T.E., Michael J.R., Boyce B.L., *Materials Science and Engineering A*, v. 581 (2013).

Crystal structure of metals in the periodic table.

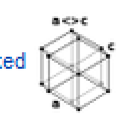
HCP BCC FCC

H																	He
453.69 Li bcc	1560 Be hcp											B	C	N	O	F	Ne
370.87 Na bcc	923 Mg hcp											933.47 Al fcc	Si	P	S	Cl	Ar
336.53 K bcc	1115 Ca fcc	1814 Sc hcp	1941 Ti hcp	2183 V bcc	2180 Cr bcc	1519 Mn	1811 Fe bcc	1768 Co hcp	1728 Ni fcc	1357.8 Cu fcc	692.68 Zn hcp	301.91 Ga	Ge	As	Se	Br	Kr
312.46 Rb bcc	1050 Sr fcc	1799 Y hcp	2128 Zr hcp	2750 Nb bcc	2896 Mo bcc	2430 Tc hcp	2607 Ru hcp	2237 Rh fcc	1828 Pd fcc	1235 Ag fcc	594 Cd	430 In	505 Sn	904 Sb	Te	I	Xe
301.59 Cs bcc	1000 Ba bcc	*	2506 Hf hcp	3290 Ta bcc	3422 W bcc	3186 Re hcp	3306 Os hcp	2446 Ir fcc	1768 Pt fcc	1337.33 Au fcc	234.32 Hg	577 Tl hcp	600.61 Pb fcc	544.7 Bi	527 Po	At	Rn
Fr	973 Ra bcc	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo
		*	1193 La dhcp	1068 Ce fcc	1208 Pr dhcp	1297 Nd dhcp	1315 Pm dhcp	1345 Sm	1099 Eu bcc	1585 Gd hcp	1629 Tb hcp	1680 Dy hcp	1734 Ho hcp	1802 Er hcp	1818 Tm hcp	1097 Yb fcc	1925 Lu hcp
		**	1323 Ac fcc	2115 Th fcc	1841 Pa	1405.3 U	917 Np	912.5 Pu	1449 Am dhcp	1613 Cm dhcp	1323 Bk dhcp	1173 Cf dhcp	1133 Es fcc	Fm	Md	No	Lr



The top number in the cell is the melting point (in K)

dhcp: double hexagonal close packed



unusual structure

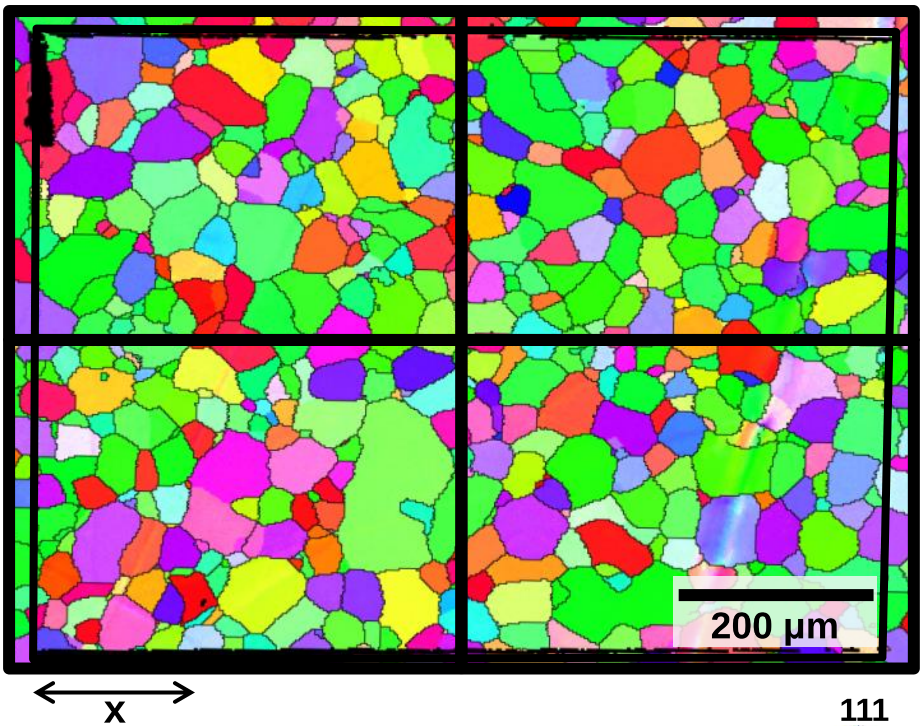
nonmetal

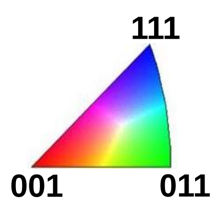
unknown or uncertain

http://en.wikipedia.org/wiki/Periodic_table_(crystal_structure)

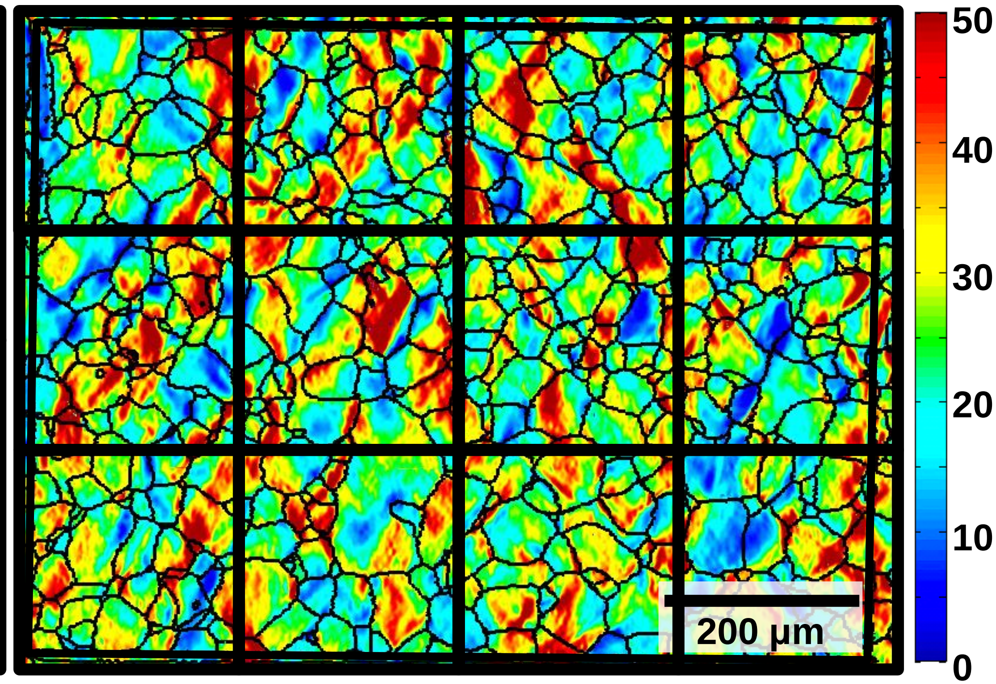
Compare grain structure to local strain measurements in polycrystal Ta (BCC metal).

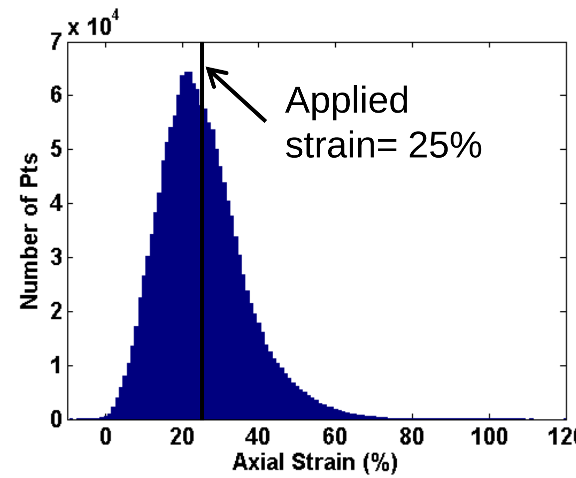
Microstructure (EBSD)



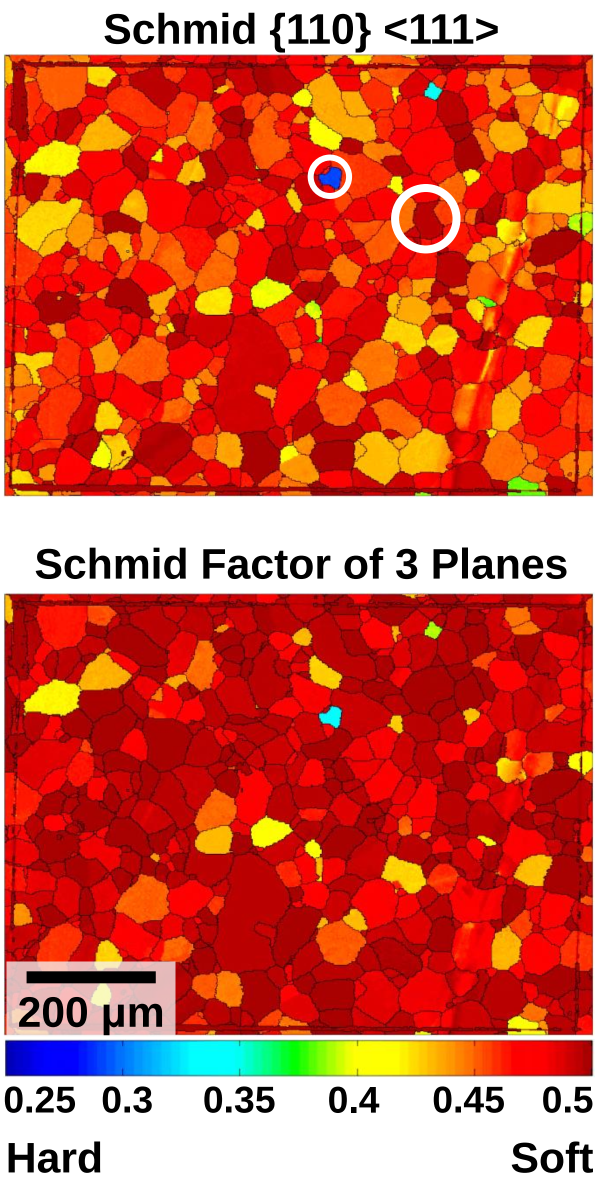


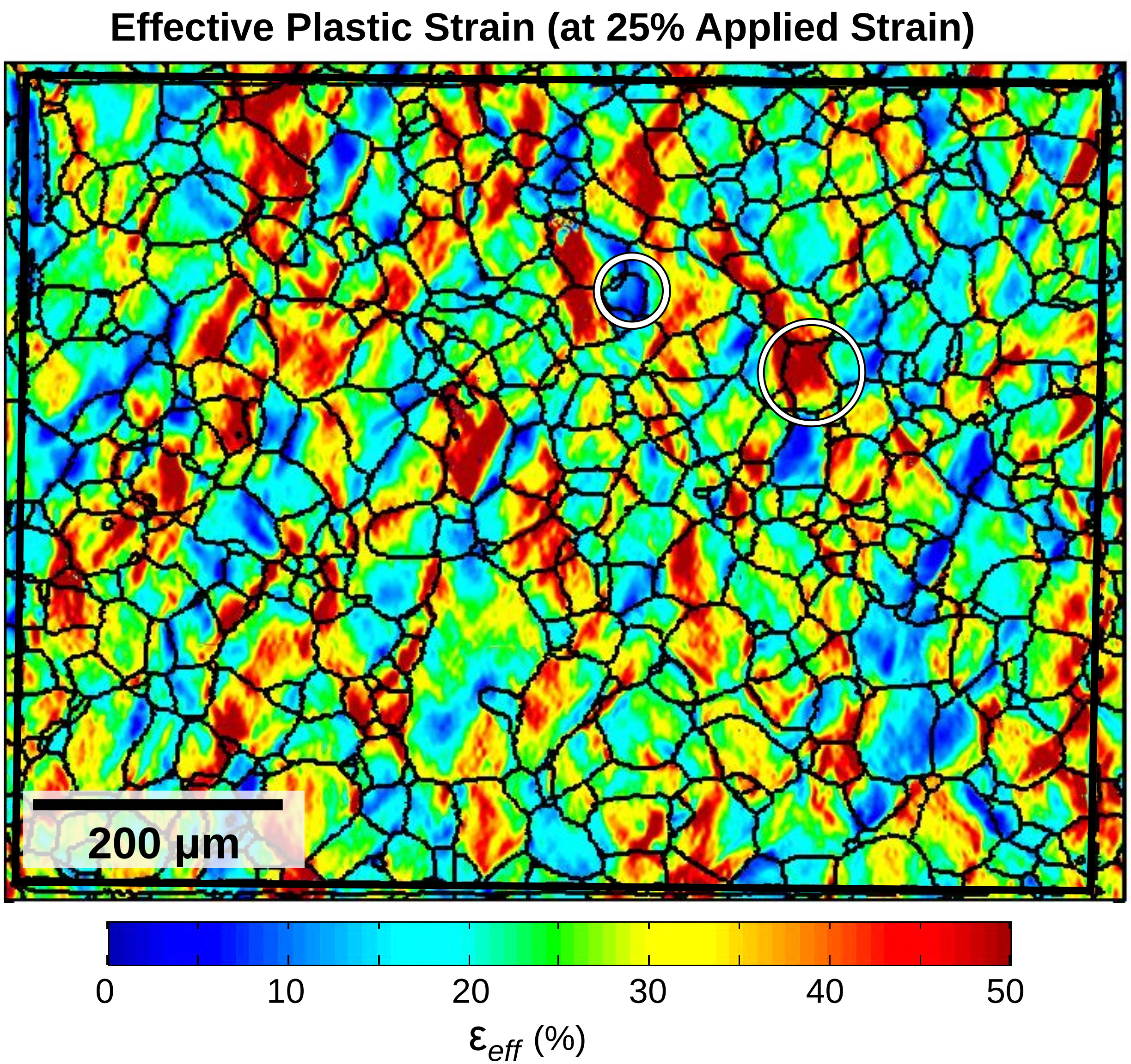
Effective Strain (%) (DIC)



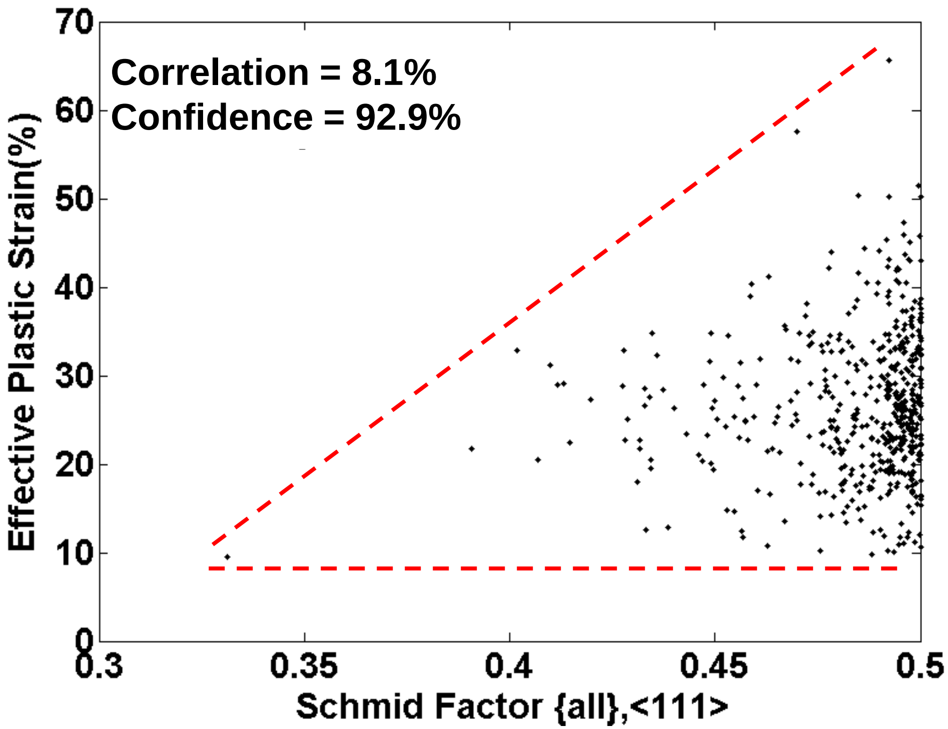


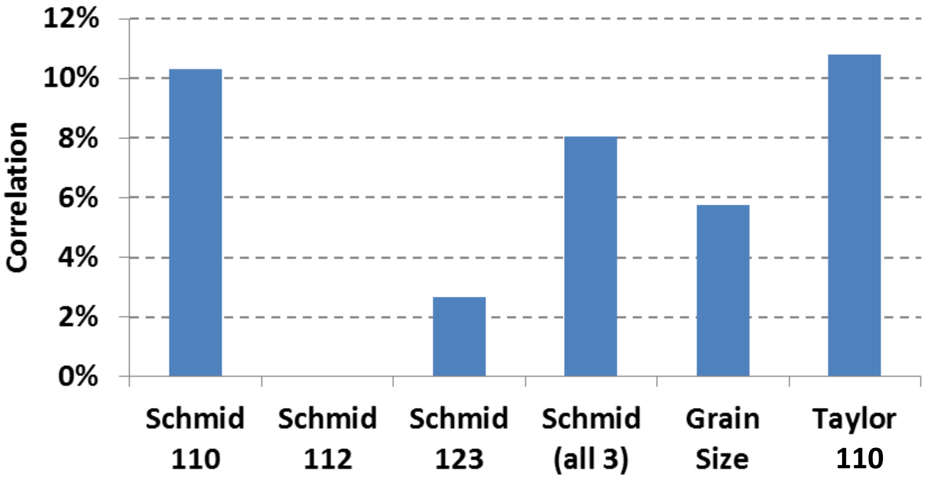
The effects of six microstructural parameters on local strain were considered.





There is some correlation between microstructure and average strain within each grain.

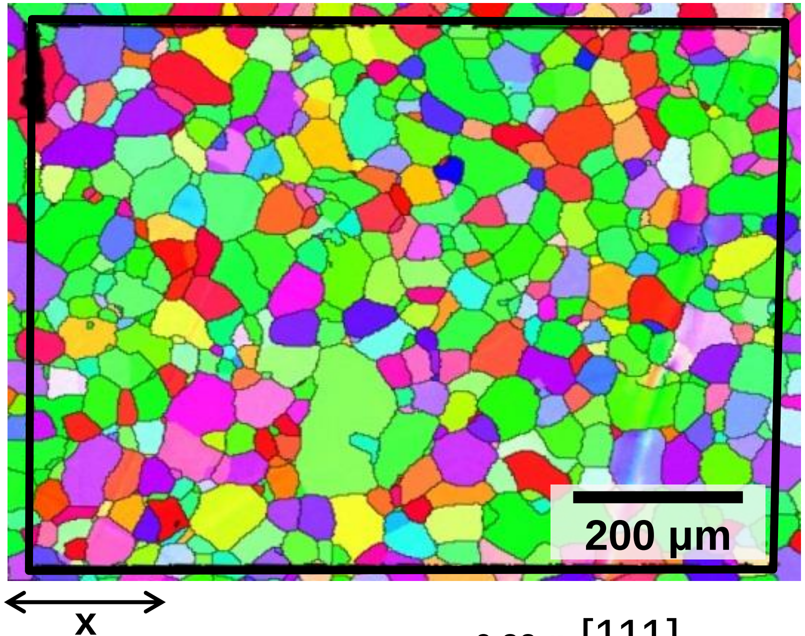




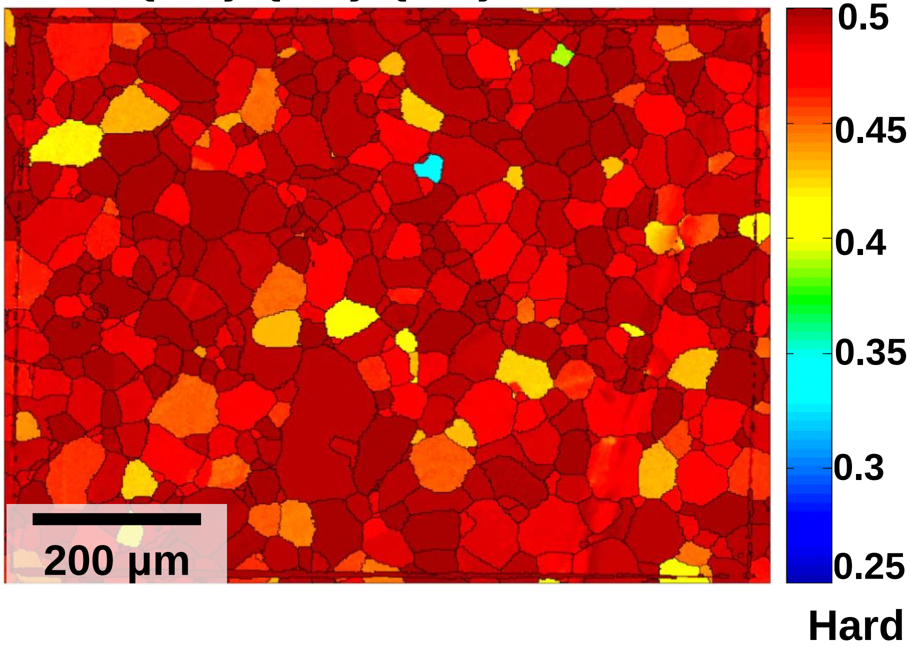
Parameter	Correlation	Confidence
Schmid 110	10%	98%
Schmid 112	-0.4%	6%
Schmid 123	2.7%	45.1%
Schmid (all 3)	8.1%	92.9%
Grain Size	5.8%	80%
Taylor 110	11%	99%

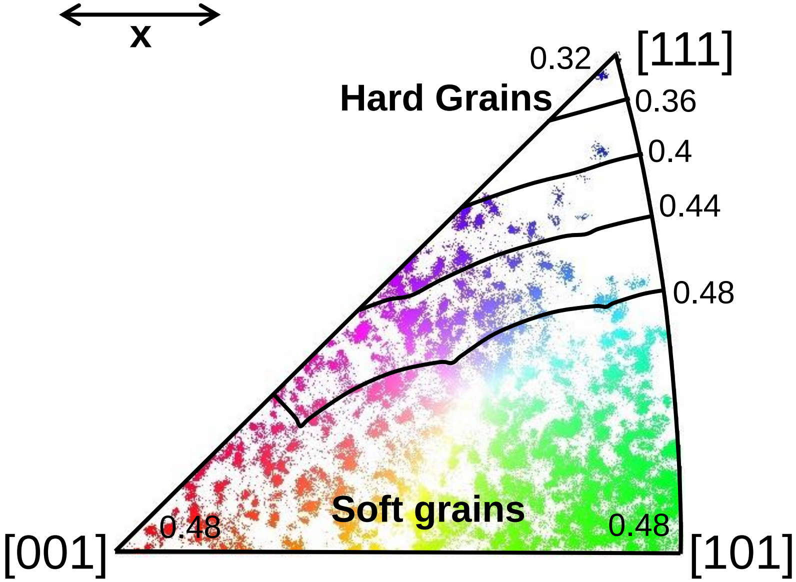
In BCC metals, only the <111> grains are hard (low Schmid factors).

Grain Orientation



Schmid Factor
{110}, {112}, {123}, <111>

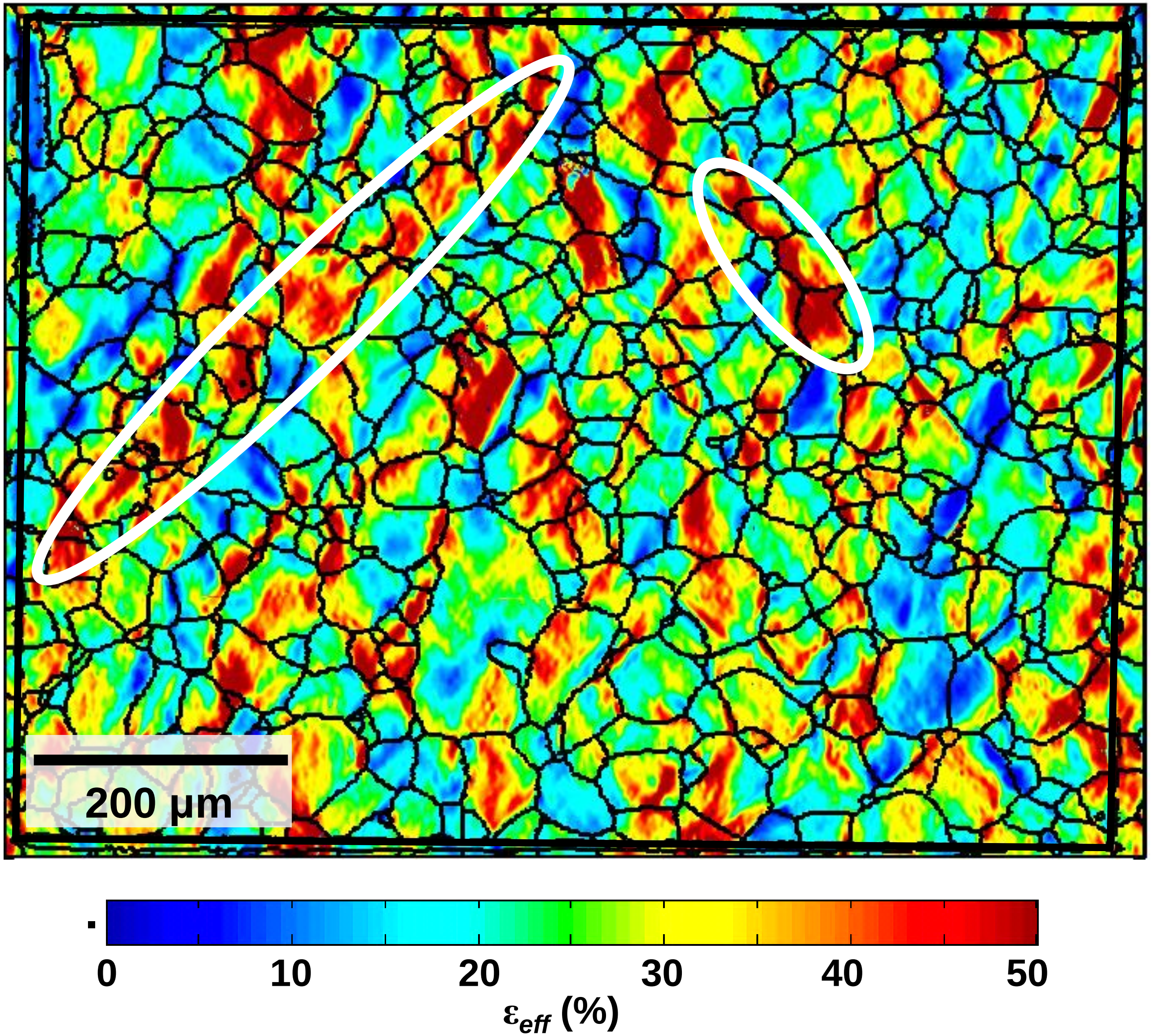




Schmid contours {110},{112},{123} <111>

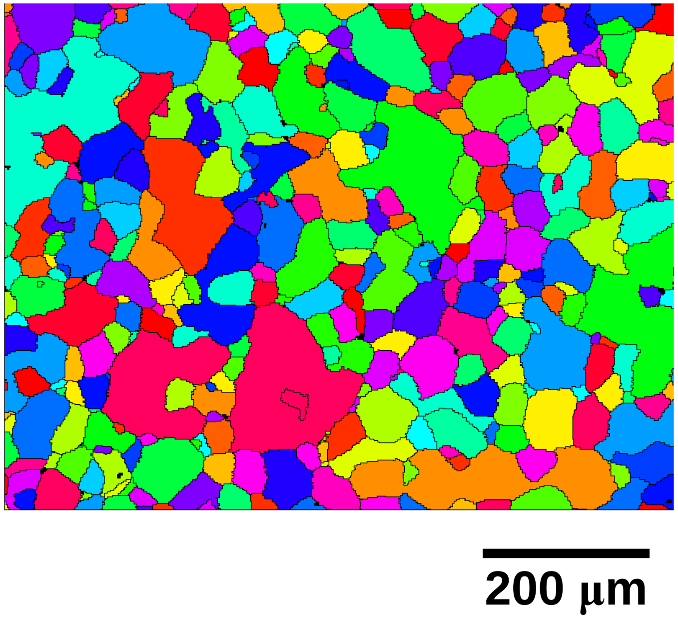
Neighborhood effects are apparent in strain fields.

Local Effective Strain at 25% Applied Strain

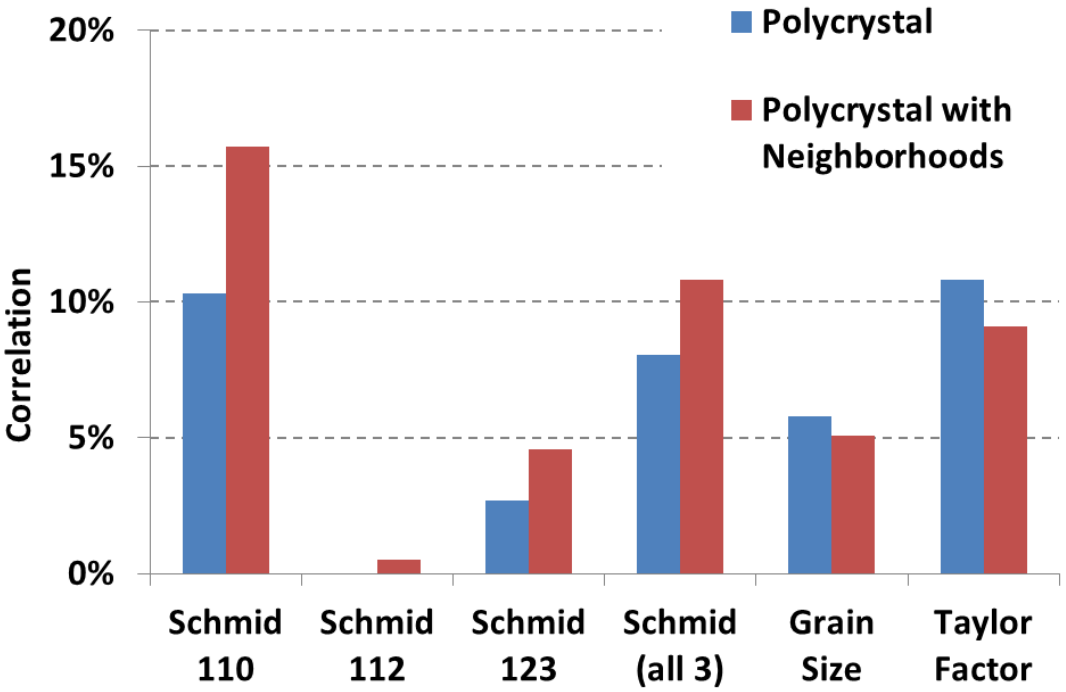


Grain neighborhoods can be identified by grouping grains with similar orientations.

Grain Neighborhoods
(random colors)



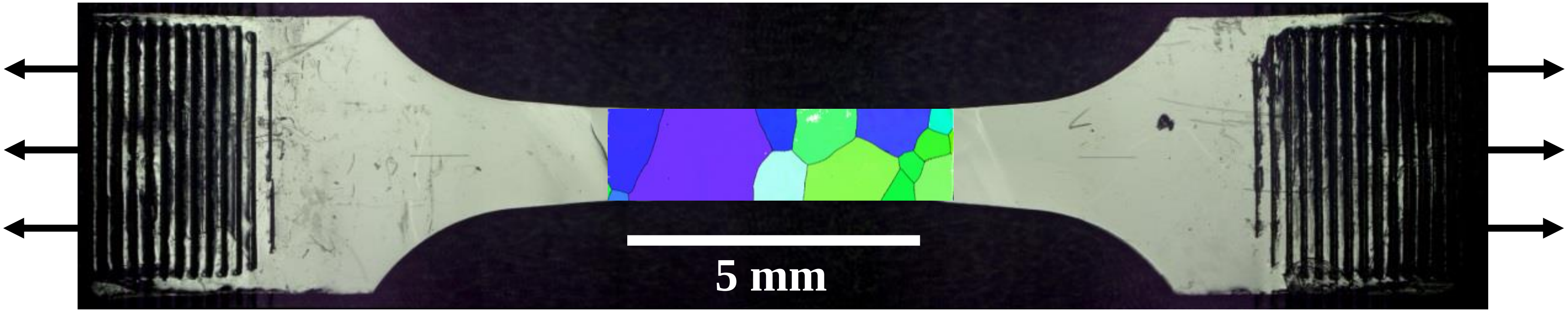
Misorientation angle of 20° defines GBs instead of 5°.



	Polycrystal		Neighborhoods	
Parameter	**Correlation**	**Confidence**	**Correlation**	**Confidence**
Schmid 110	10%	98%	16%	100%
Schmid 112	-0.4%	6%	0.5%	8%
Schmid 123	2.7%	45.1%	4.6%	61%
Schmid (all 3)	8.1%	92.9%	10.8%	96%
Grain Size	5.8%	80%	5.1%	65%
Taylor Factor	11%	99%	9.1%	91%

Oligocrystals

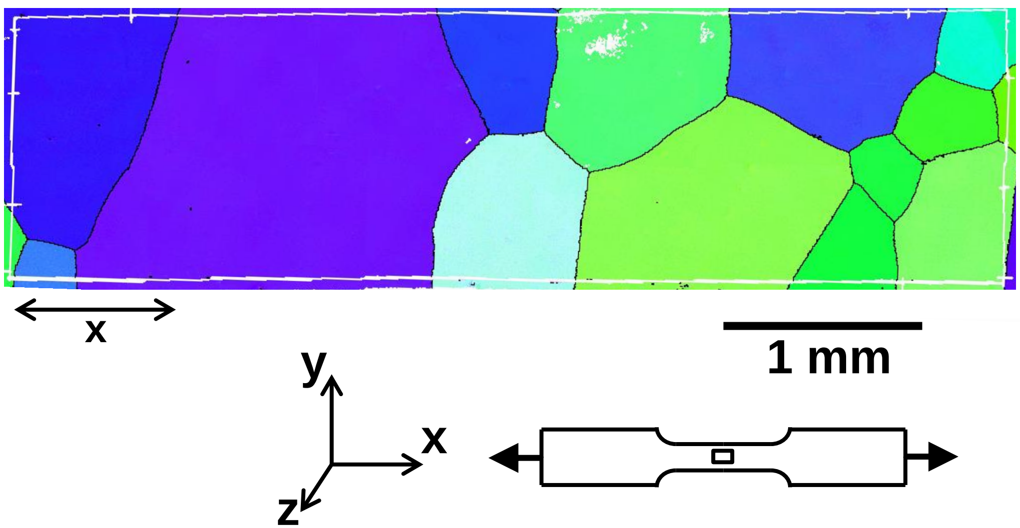
Specimens where deformation is controlled by a few grains (3–20).

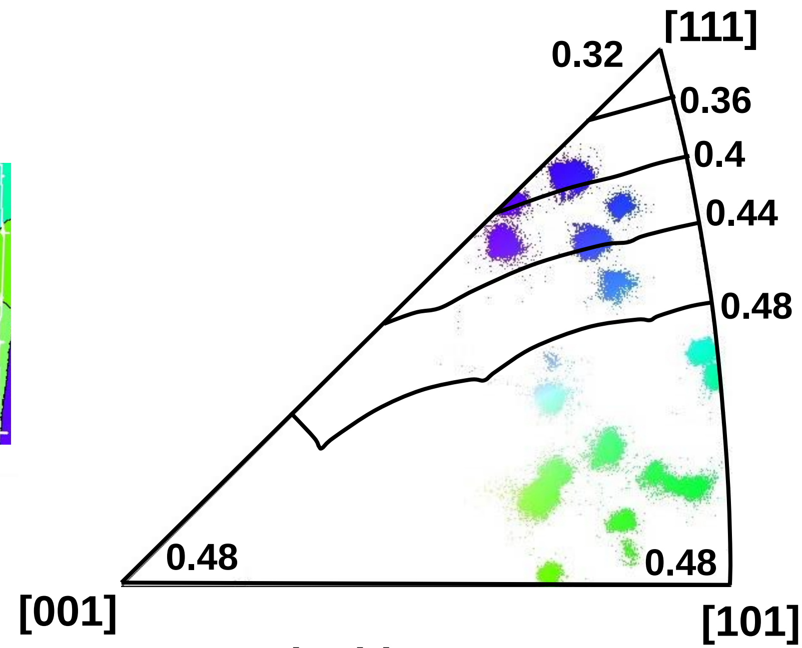


- Ta oligocrystals were made by annealing.
- This has much fewer neighborhood effects.

This oligocrystal also has more hard grains.

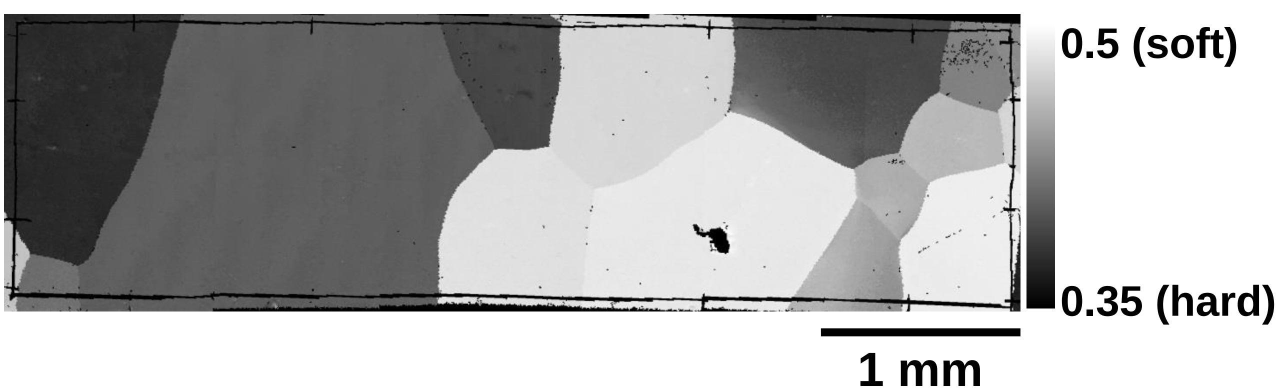
Grain orientation



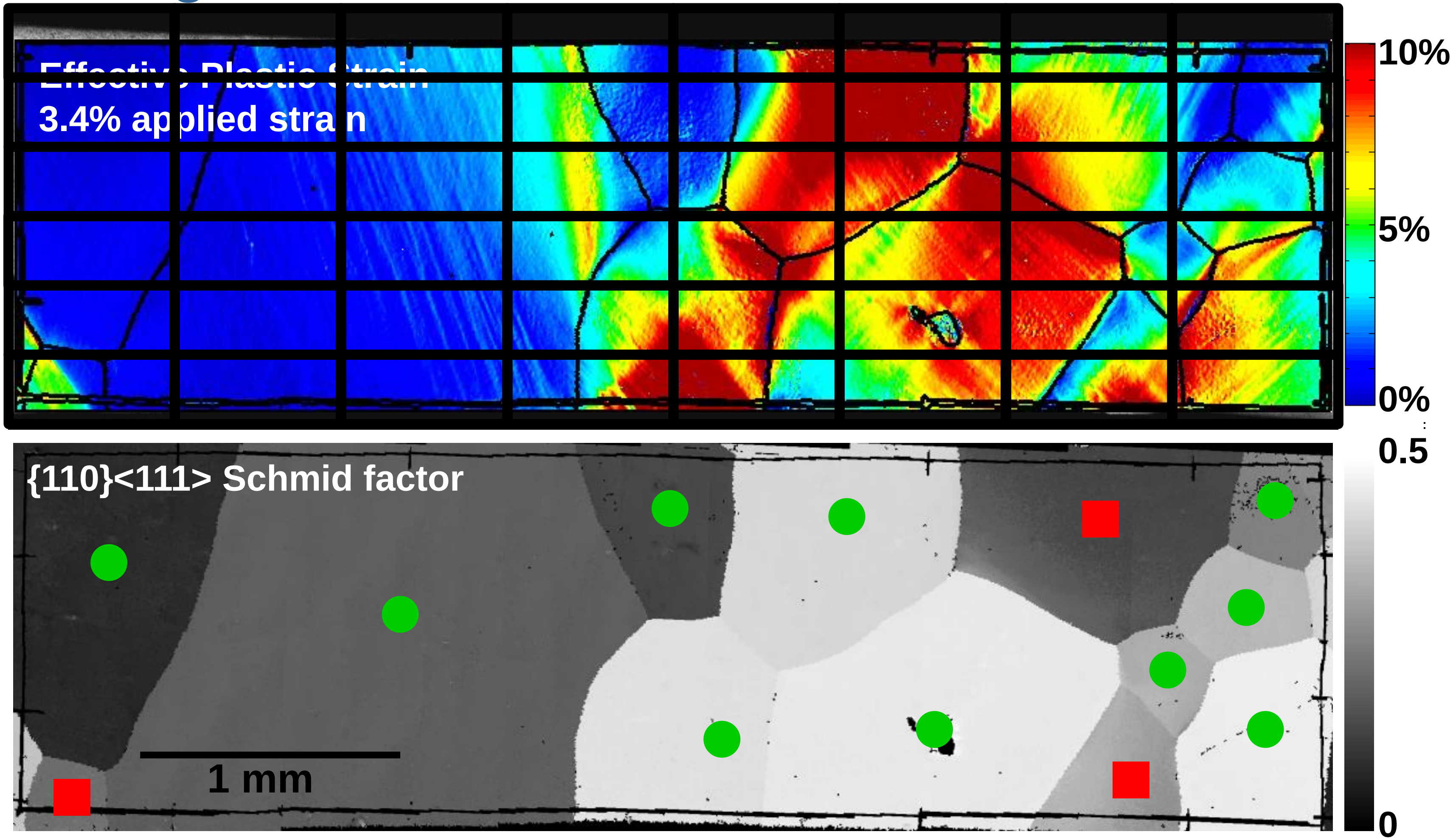


Schmid contours {110},{112},{123} <111>

Schmid {110}<111>

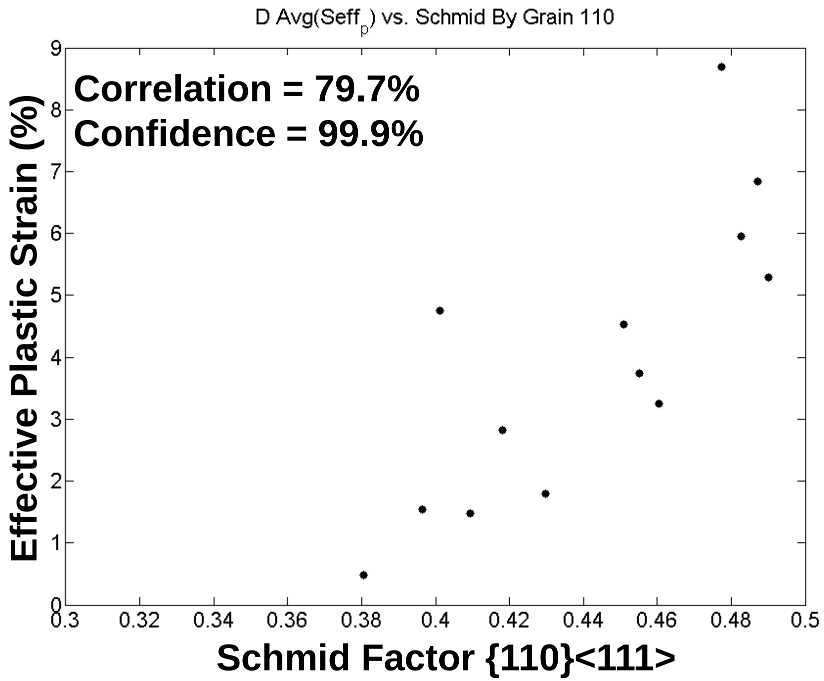


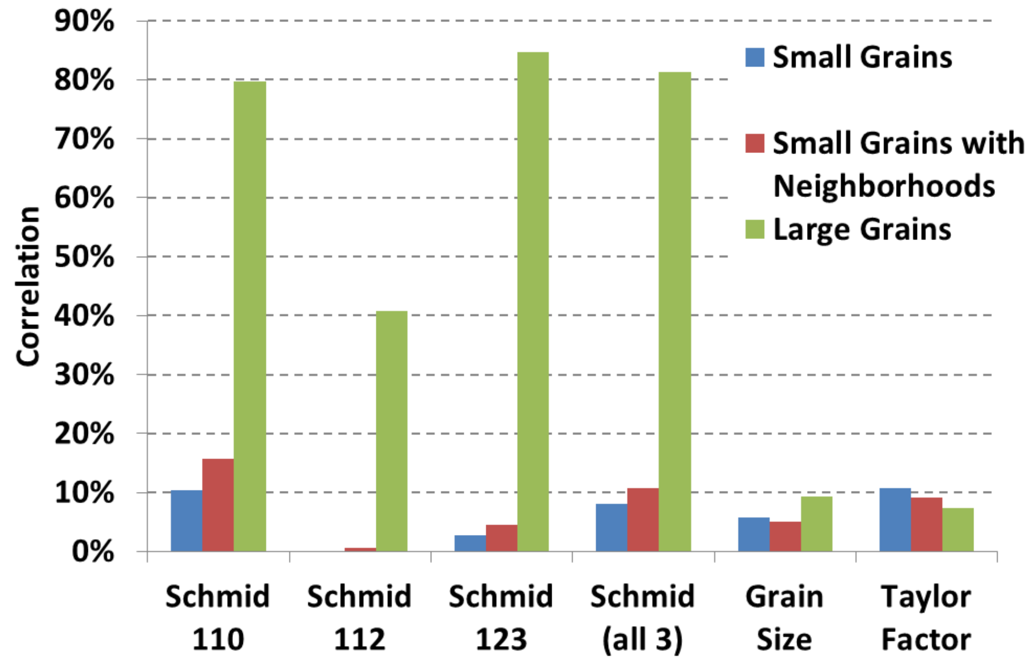
Strain accumulation agrees with Schmid factor for most grains.



- 10 out of 13 grains have strain and Schmid agree (77%).
- Neighbor effects may explain the other cases.

Oligocrystal shows strong correlations between Schmid factor and strain.



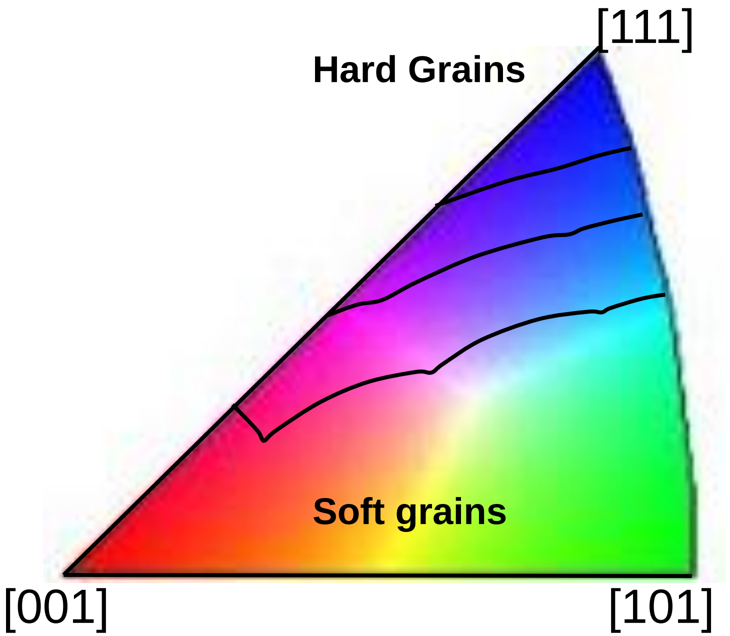


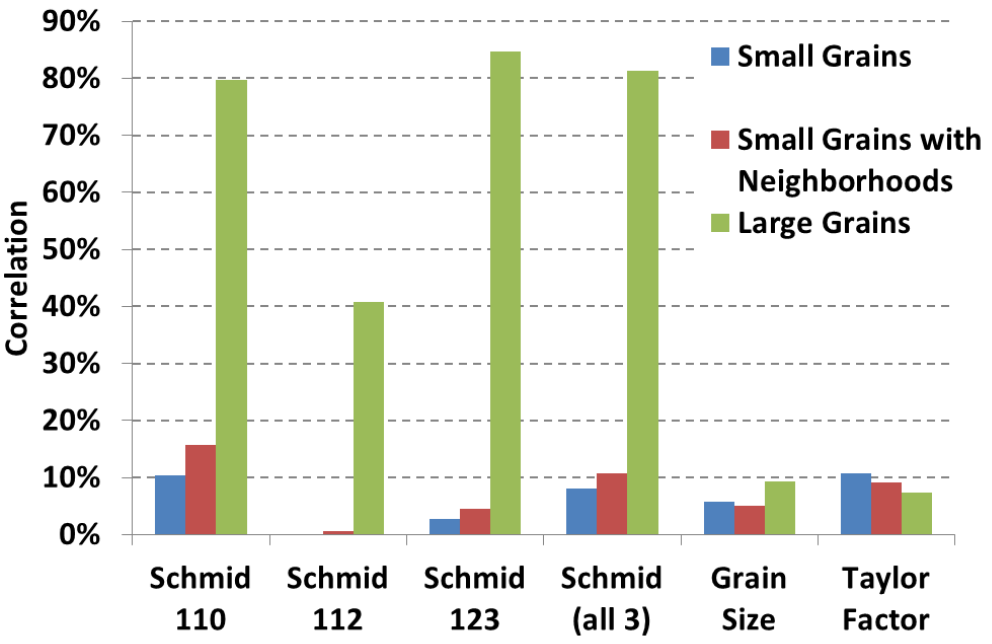
	Polycrystal		Neighborhoods		Oligocrystal	
Parameter	**Correlation**	**Confidence**	**Correlation**	**Confidence**	**Correlation**	**Confidence**
Schmid 110	10%	98%	16%	100%	80%	98%
Schmid 112	-0.4%	6%	0.5%	8%	41%	83%
Schmid 123	2.7%	45%	4.6%	61%	85%	100%
Schmid (all 3)	8.1%	93%	10.8%	96%	81%	100%
Grain Size	5.8%	80%	5.1%	65%	9.3%	24%
Taylor Factor	11%	99%	9.1%	91%	7.3%	19%

Carroll J.D., Clark B.G., Buchheit T.E., Michael J.R., Boyce B.L., *Materials Science and Engineering A*, v. 581 (2013).

Summary on relating microstructure to deformation.

- In BCC metals, the only hard grains are those with the <111> direction aligned near the tensile axis.
- {110} are the most likely slip planes in Ta.
- Strain accumulation is related to Schmid factor.
- Grain neighbors are important!

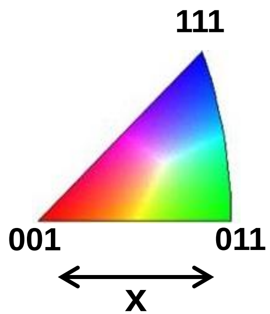


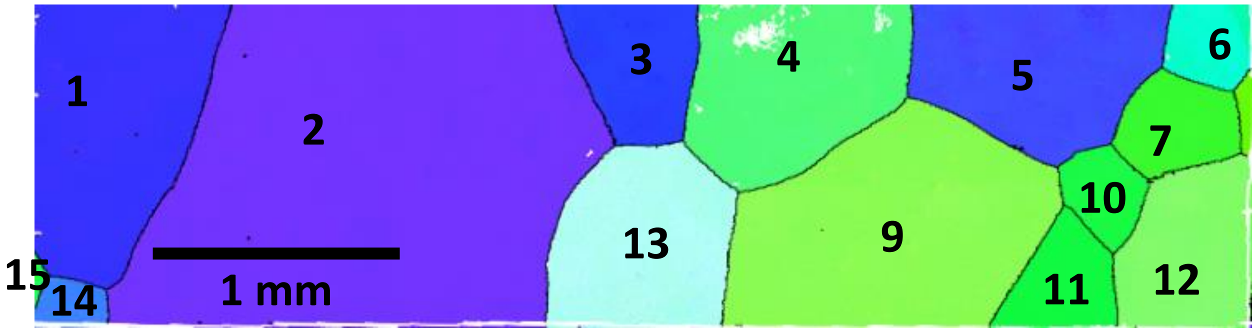


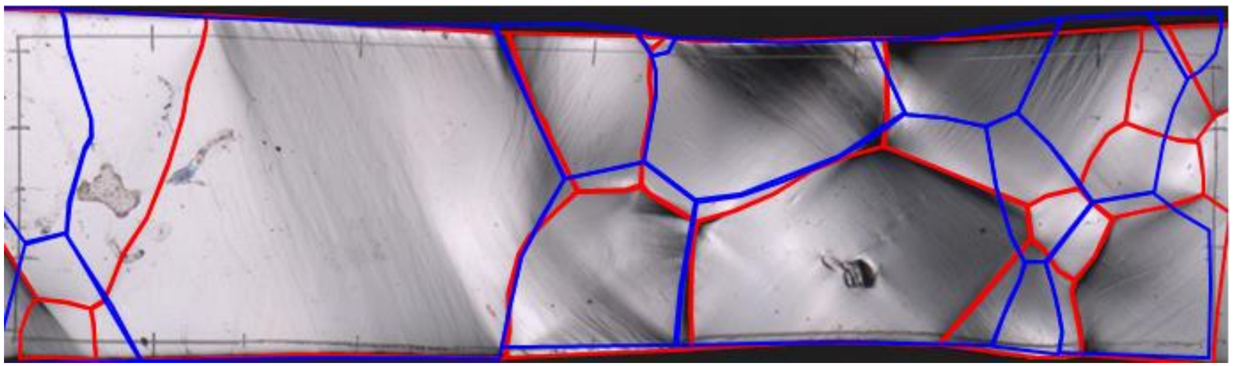
Outline

1. **Motivation**
   - Why do we need to understand grain scale deformation?
2. **Background**
   - Slip in FCC and BCC metals
3. **Relating microstructure to deformation**
   - Schmid factors, etc.
4. **Predicting deformation behavior at the grain scale**
   - Crystal plasticity models
5. **Conclusions**

Oligocrystals with pseudo-2D grains provide more accurate comparisons between models and experiments.

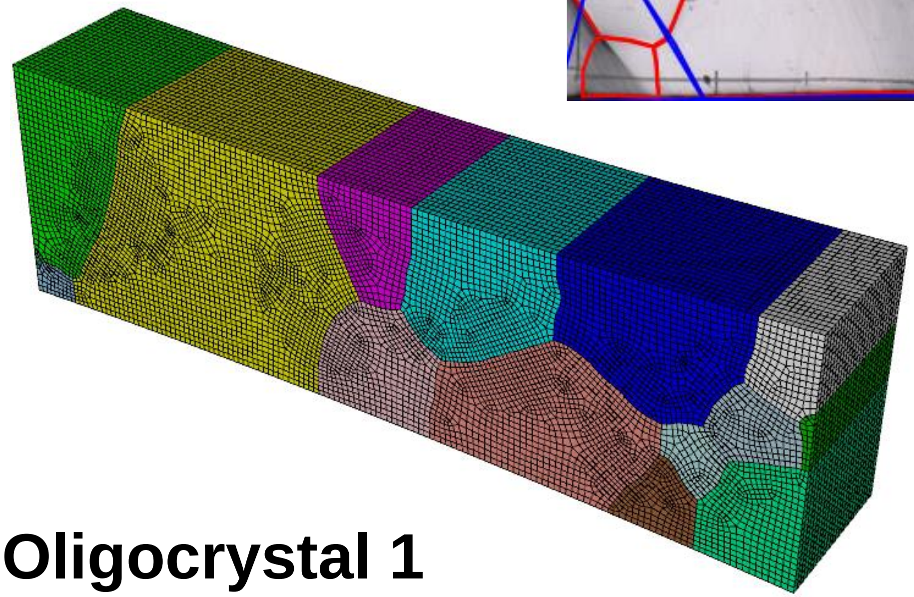






Front grain boundary

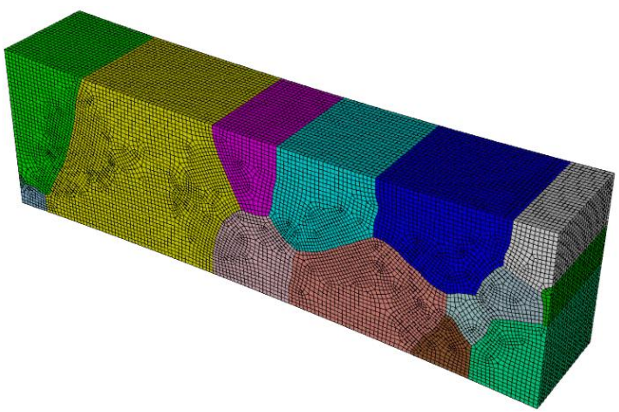
Back grain boundary



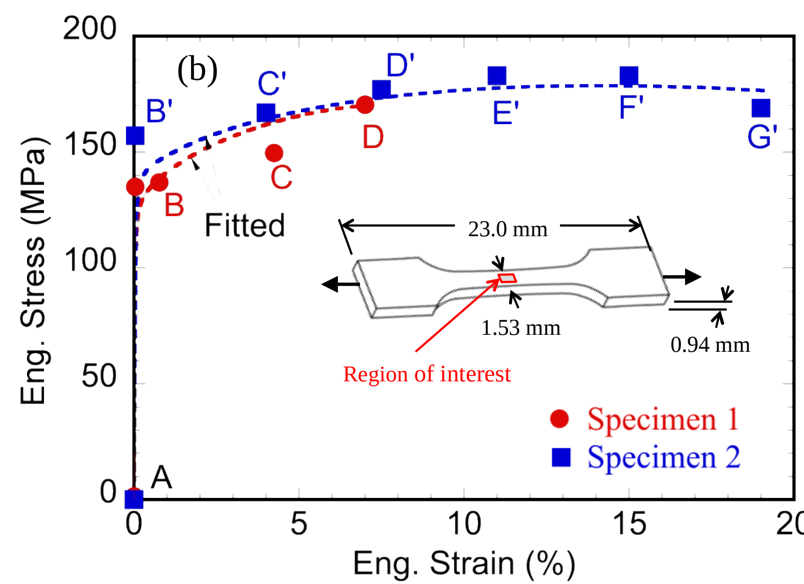
Oligocrystal 1

Crystal plasticity finite element model.

- **FEM code (JAS-3D) developed at Sandia.**
- **Dislocation density based hardening.**
- **Temperature and rate dependent, based on kink pair theory.**
- **Hexahedral elements (8 nodes).**
- **50 elements through specimen thickness.**
  - **~1.5 million total elements**
  - **~30,000 surface elements**

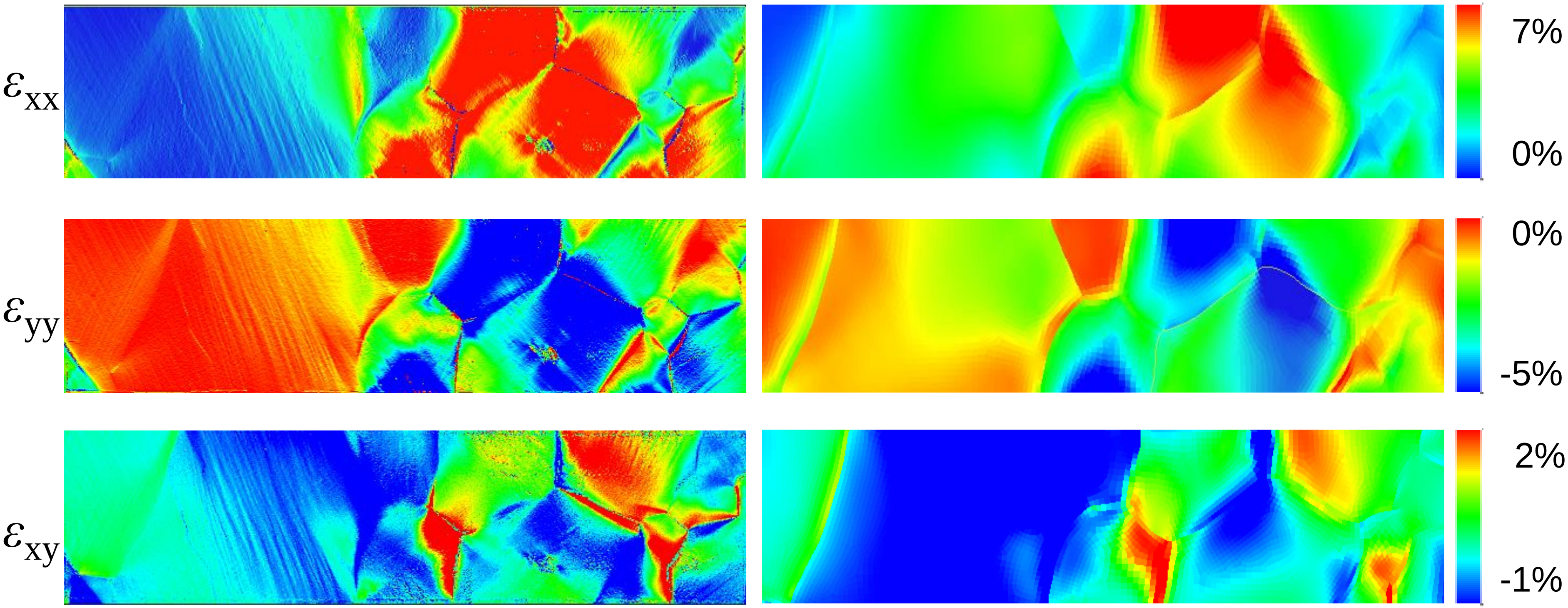


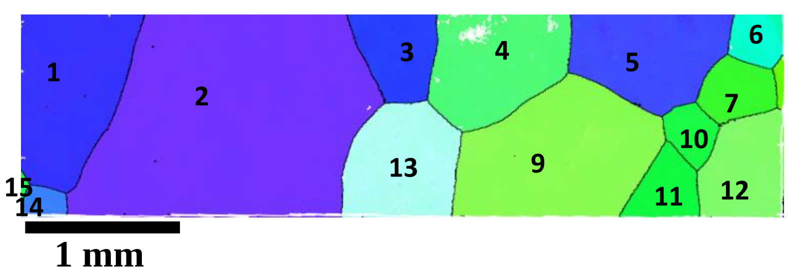
Parameters	Values	Parameters	Values	Parameters	Values
τ_0^{LT}	406 MPa	C_{11}	267 GPa	k_a	$1.4 \times 10^6\ (m^{-1})$
τ_0^{EI}	320 MPa	C_{12}	161 GPa	k_b	14
$2H_k$	0.85 eV	C_{44}	82.5 GPa	$\bar{\tau}_1$	27 MPa
$\dot{\gamma}_0$	$2.99 \times 10^6 s^{-1}$	b	2.87 Å	$\bar{\tau}_2$	37 MPa



Model predictions of strain agree well with experimental measurements in most places.

Experimental Strains (DIC) | Model Strains (CP-FEM)





Model predictions only consider slip on {110} planes.

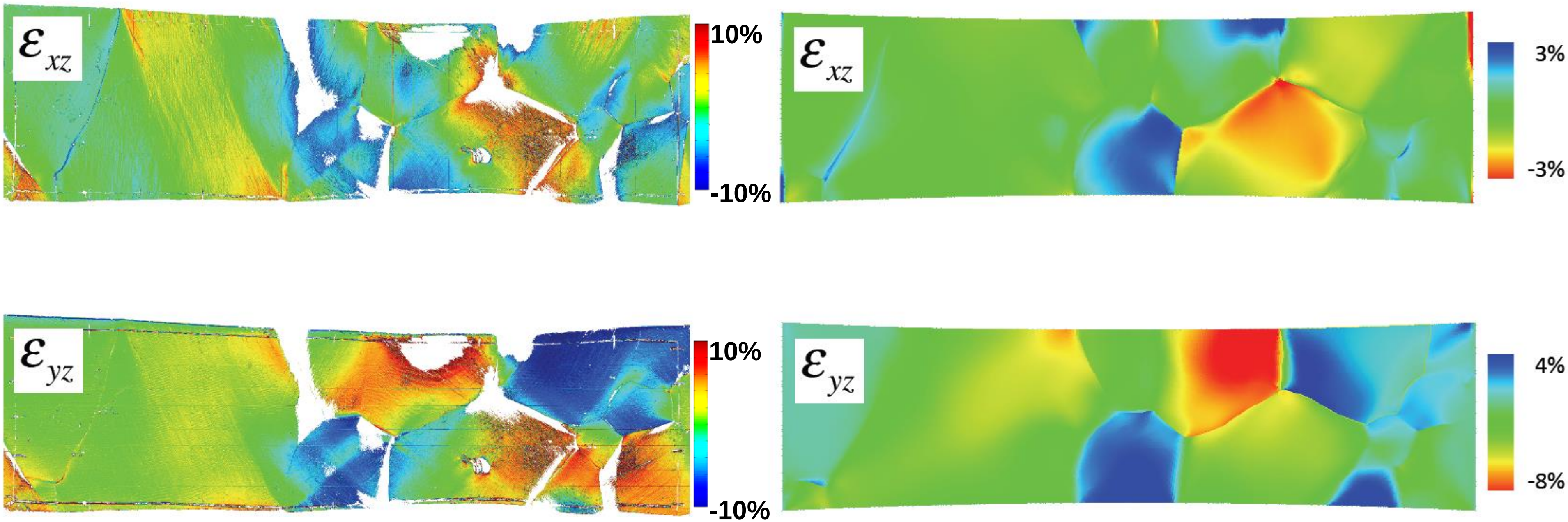
Lim H., Carroll J.D., Battaile C.C., Buchheit T.E., Boyce B.L., Weinberger C.R., “Validation of Crystal Plasticity Simulations of Tantalum Oligocrystals using HR-DIC and EBSD Methods” (in preparation).

Compare out-of-plane strain (profilometry).

Oligocrystal 1 (7% deformation)

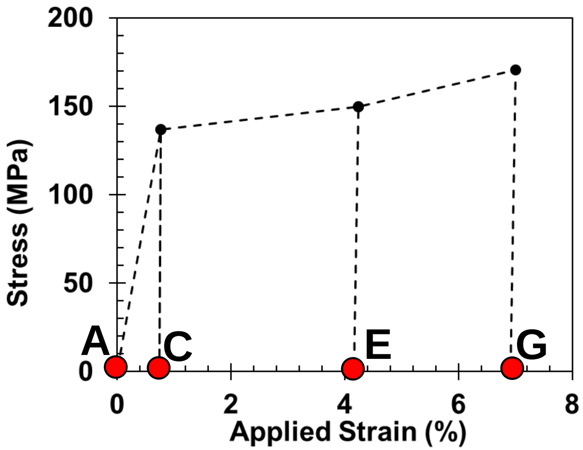
Profilometry Measurements

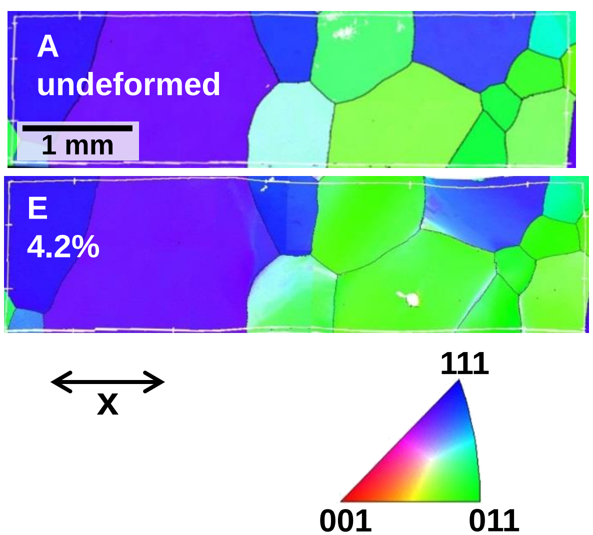
CP-FEM Predictions

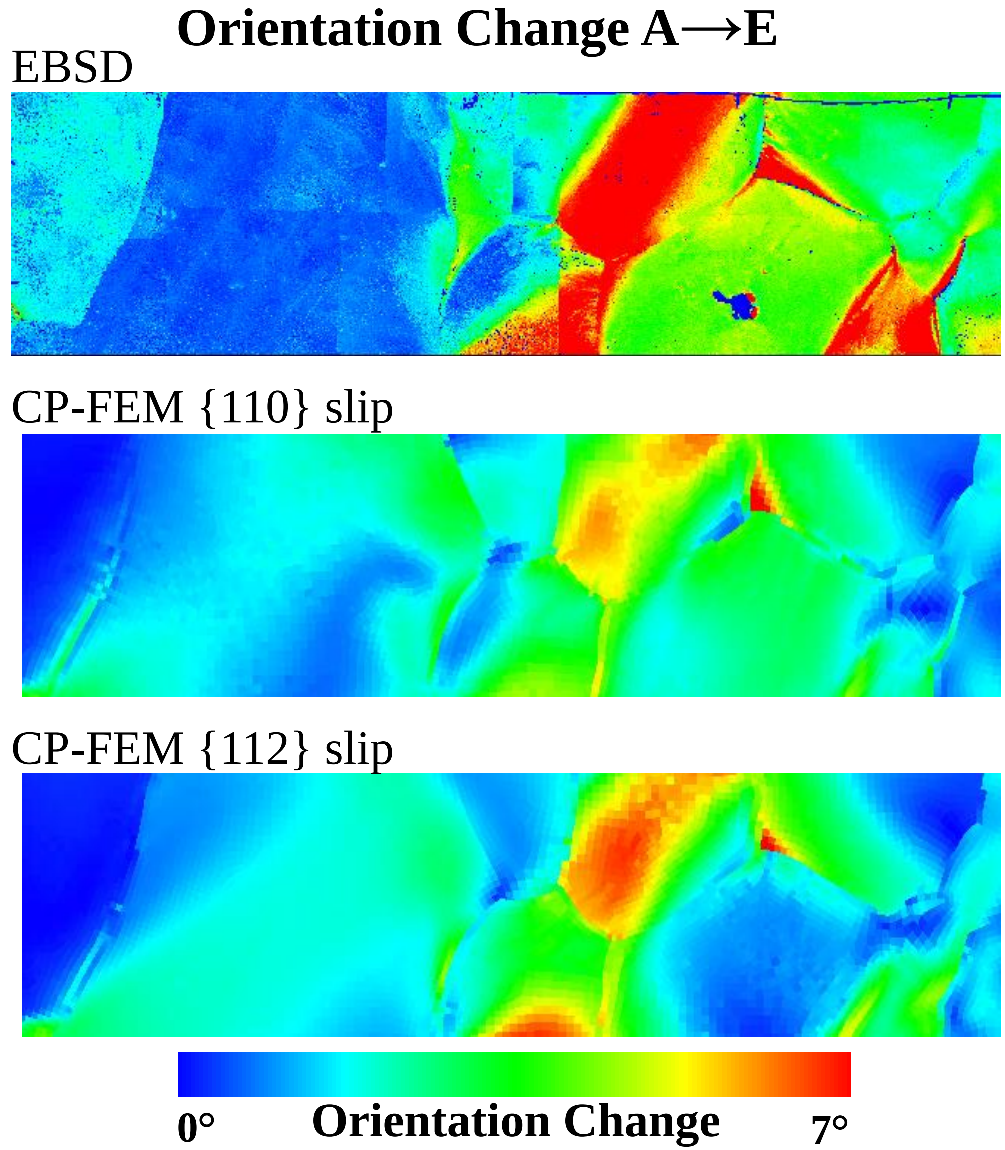


- **Good qualitative agreement within grains.**
- **Grain boundaries have large strains not captured by model.**

Compare orientation changes between model and experiment.

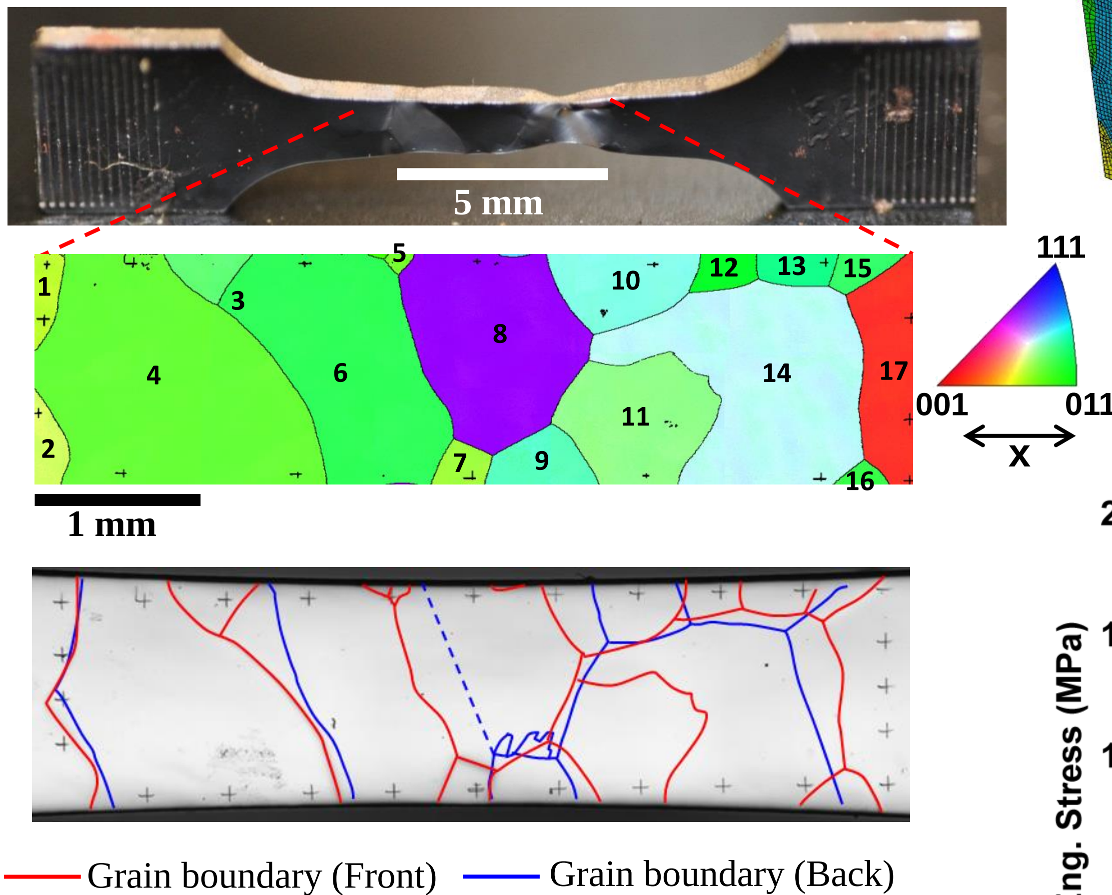


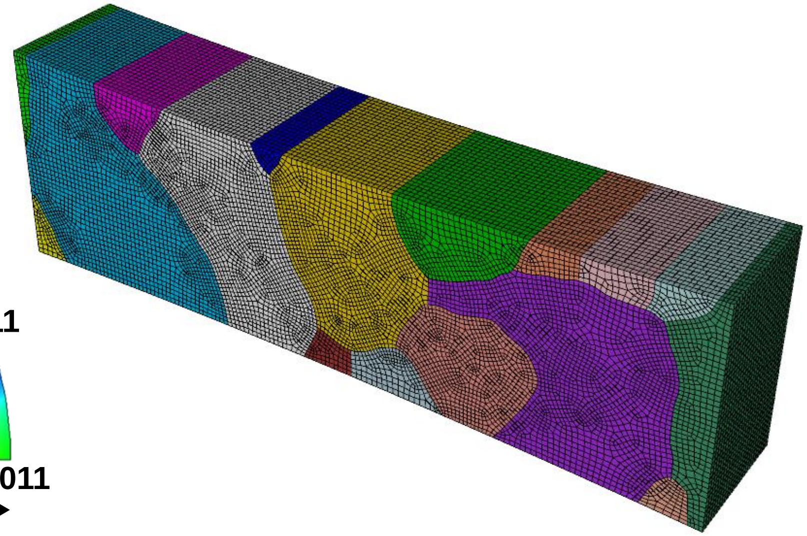


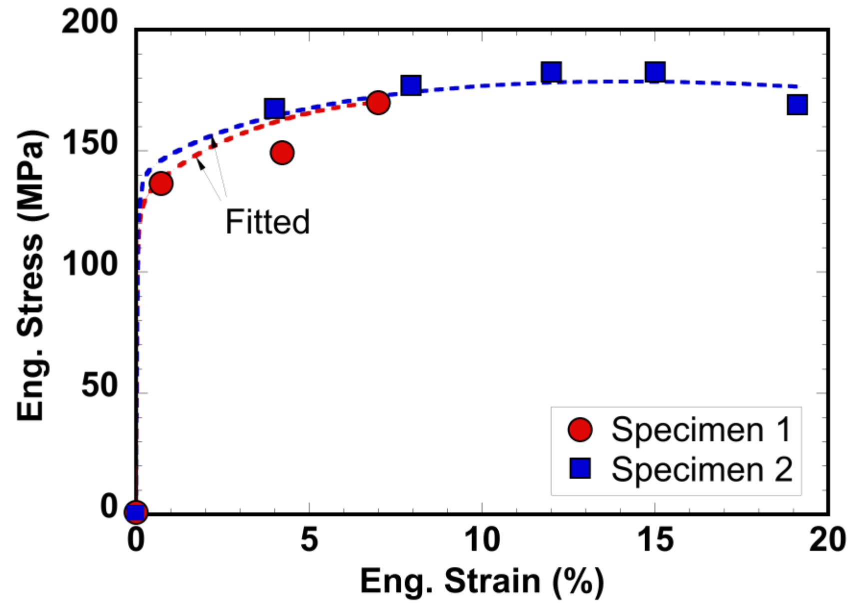


Buchheit T.E., Carroll J.D., Clark B.G., Boyce B.L., "Evaluating Absolute Rotation in a Polycrystal During in-situ Tensile Deformation using EBSD" (in preparation).

Oligocrystal 2. Loading to 19.2% to see failure initiation.







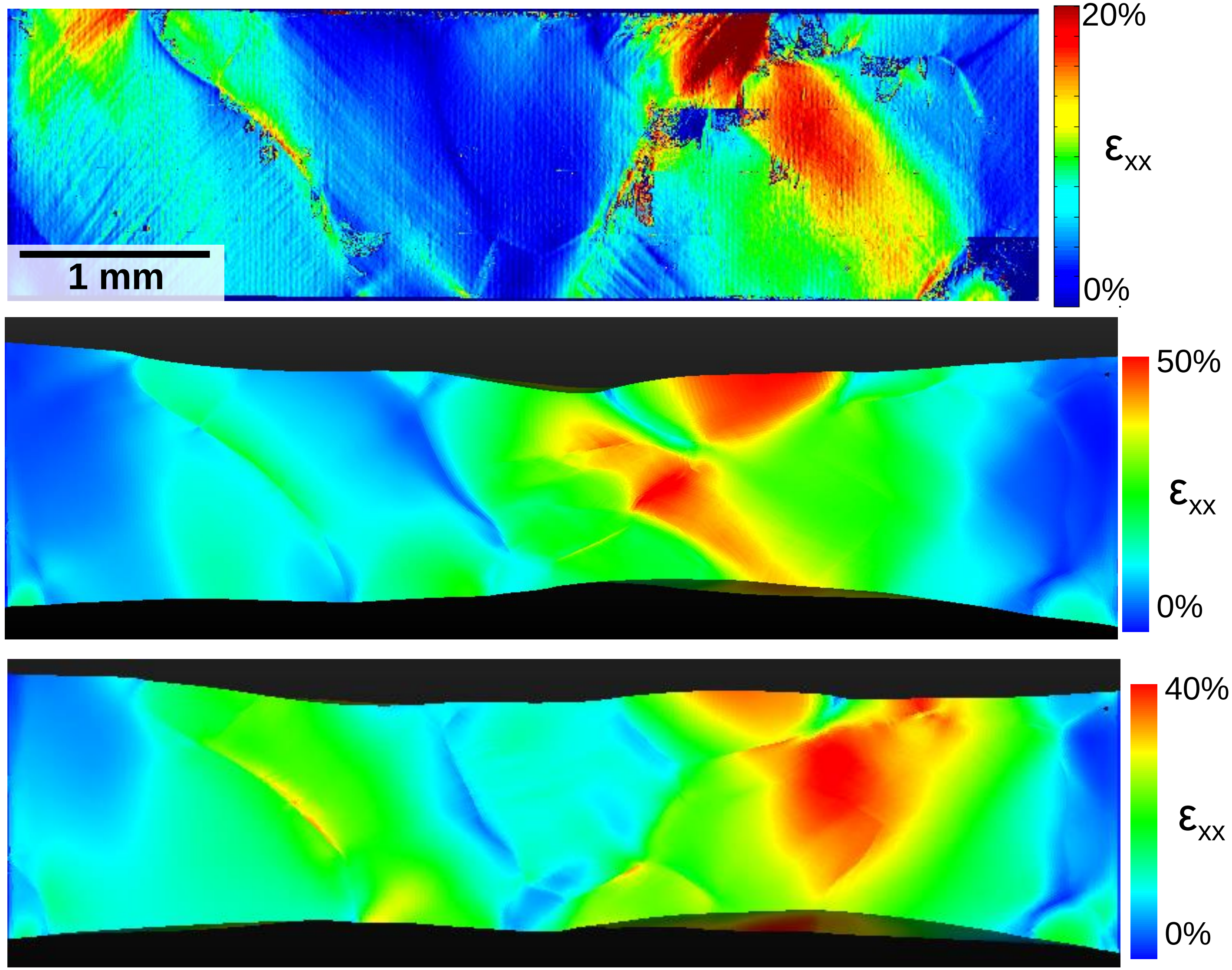
EBSD before and after only.

Each model matches experiment better in some locations.

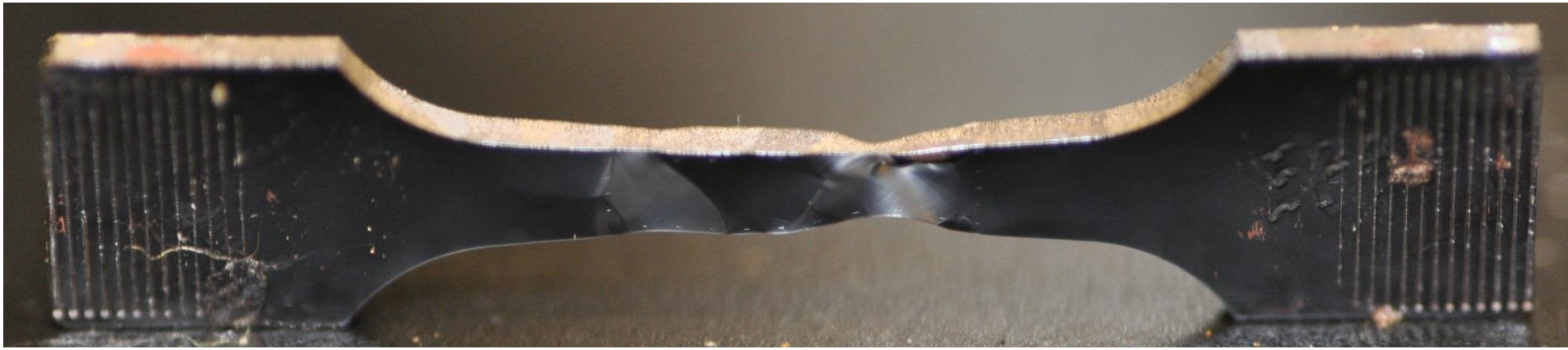
Experiment
DIC
~10% strain

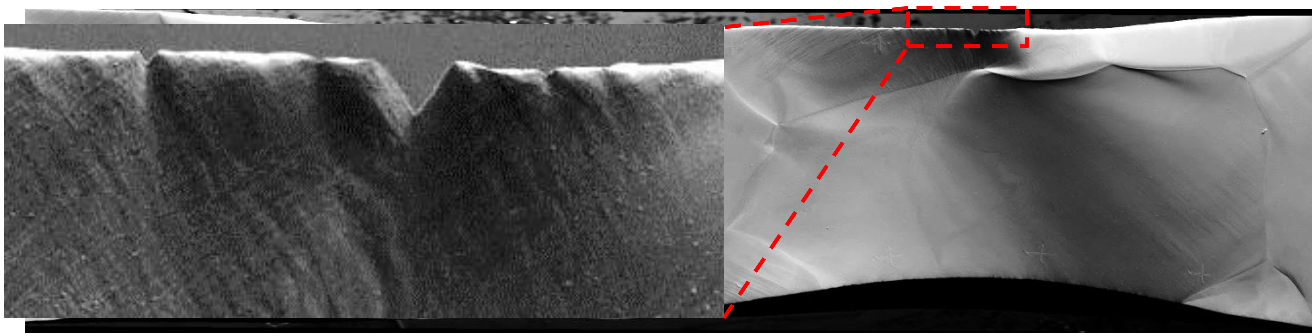
Model
{110} slip
19% strain

Model
{112} slip
19% strain

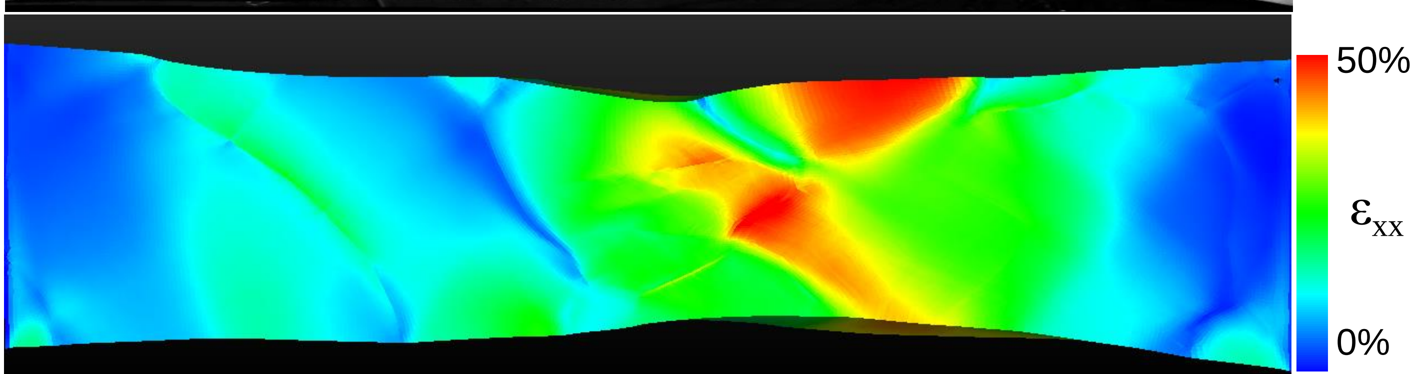


Model predicts high strain at location of observed crack initiation.

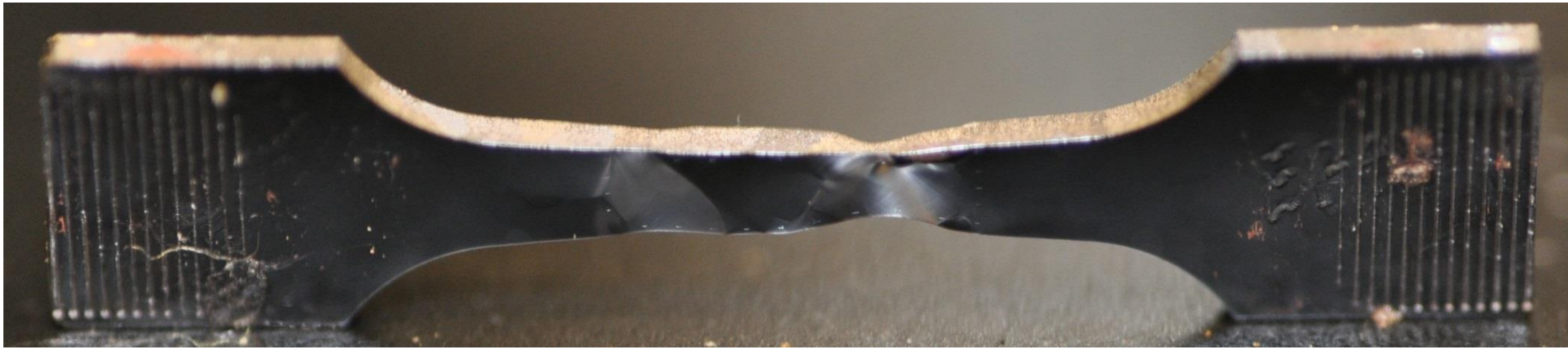


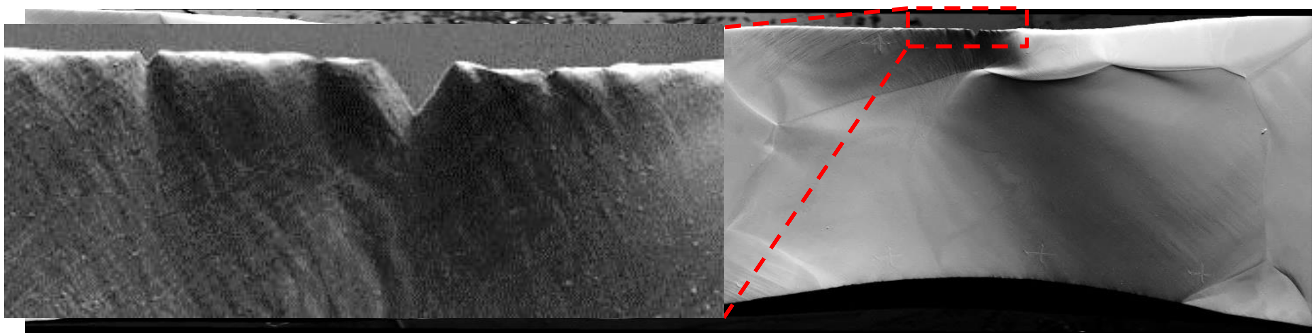


{110} slip

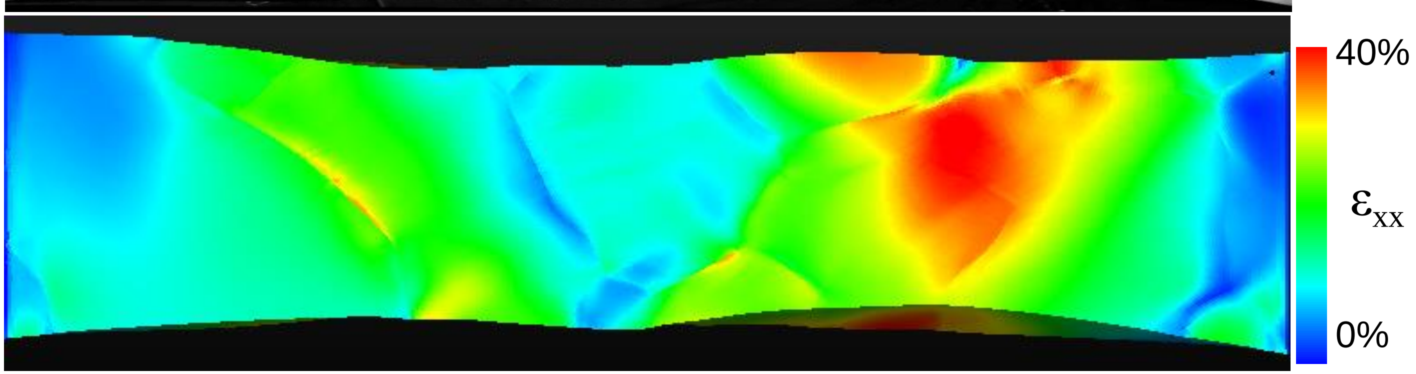


Model predicts high strain at location of observed crack initiation.

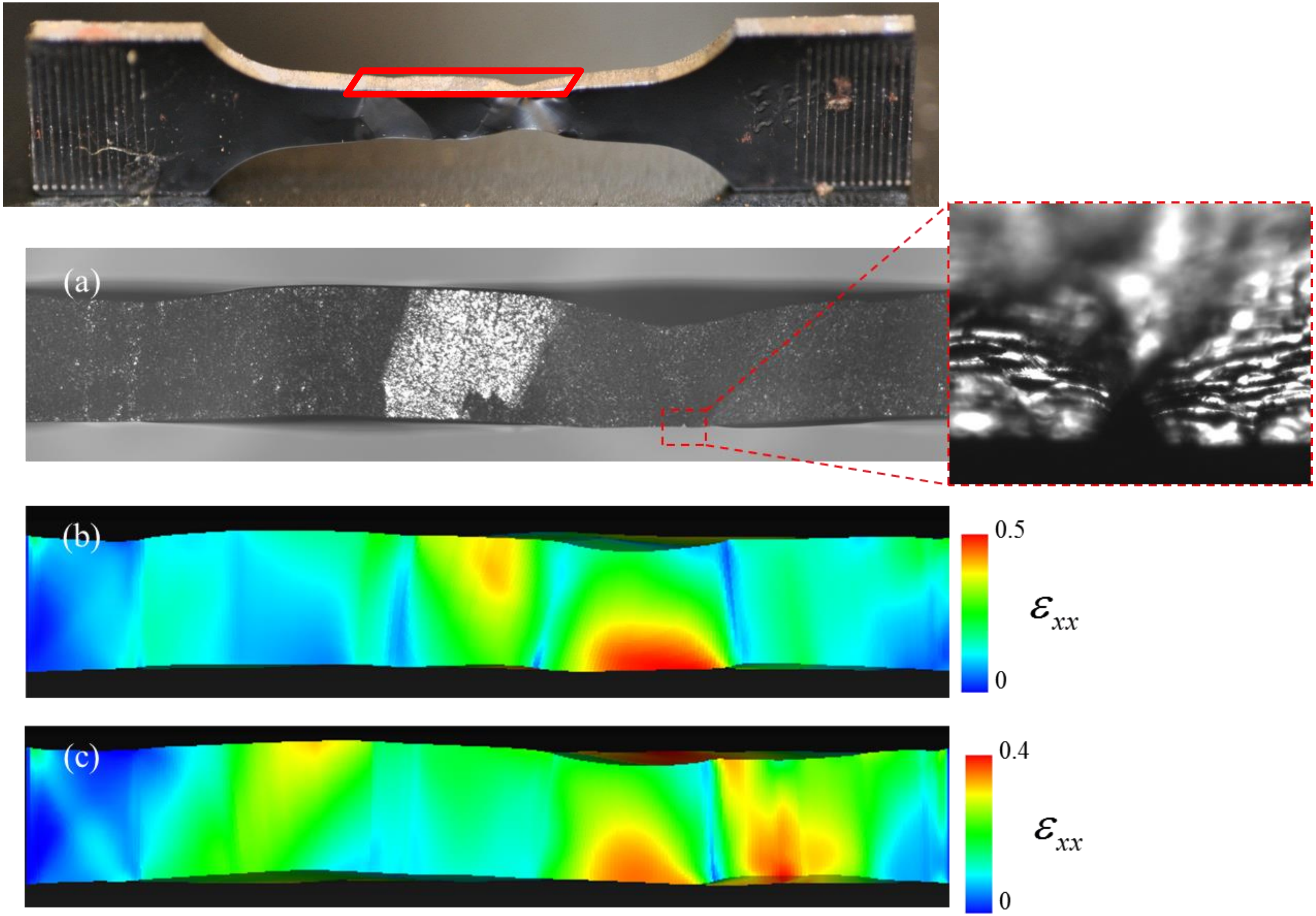




{112} slip



The pseudo-2D model predicts failure in 3D (on front surface).



{110} slip

{112} slip

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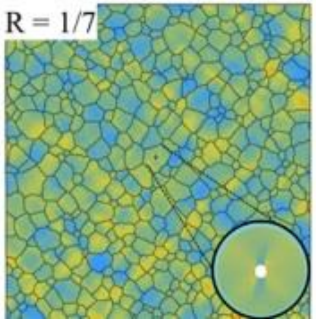
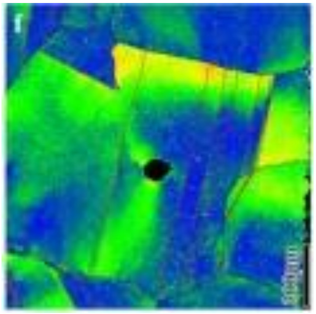
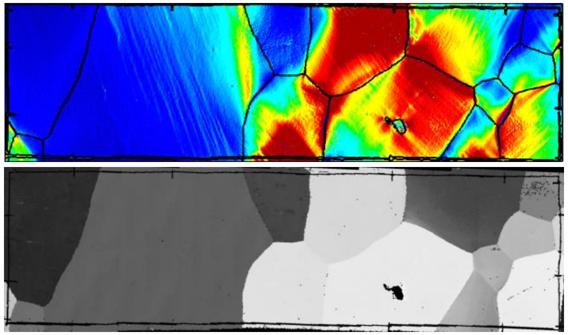
   – **Schmid factors, etc.**
4. **Predicting deformation behavior at the grain scale**
   – **Crystal plasticity models. Conclusions**
   – **Time to wake up.**

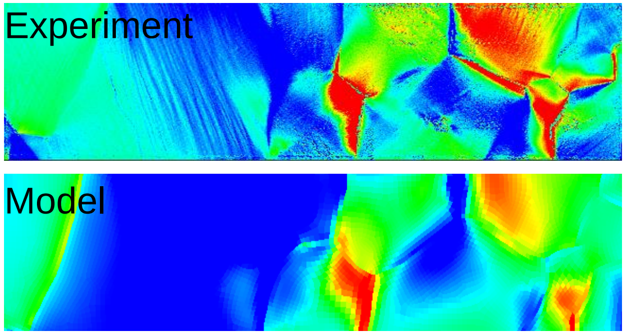
Conclusions

1. **Need to consider microstructural effects when specimen dimensions are comparable to grains size.**
2. **Local microstructure can be more important than small geometrical stress concentrators.**
3. **Schmid factor is predictive of deformation.**
4. **Grain neighbor effects are important!**
5. **Our crystal plasticity model agrees with experiments!**







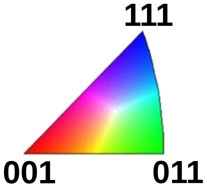


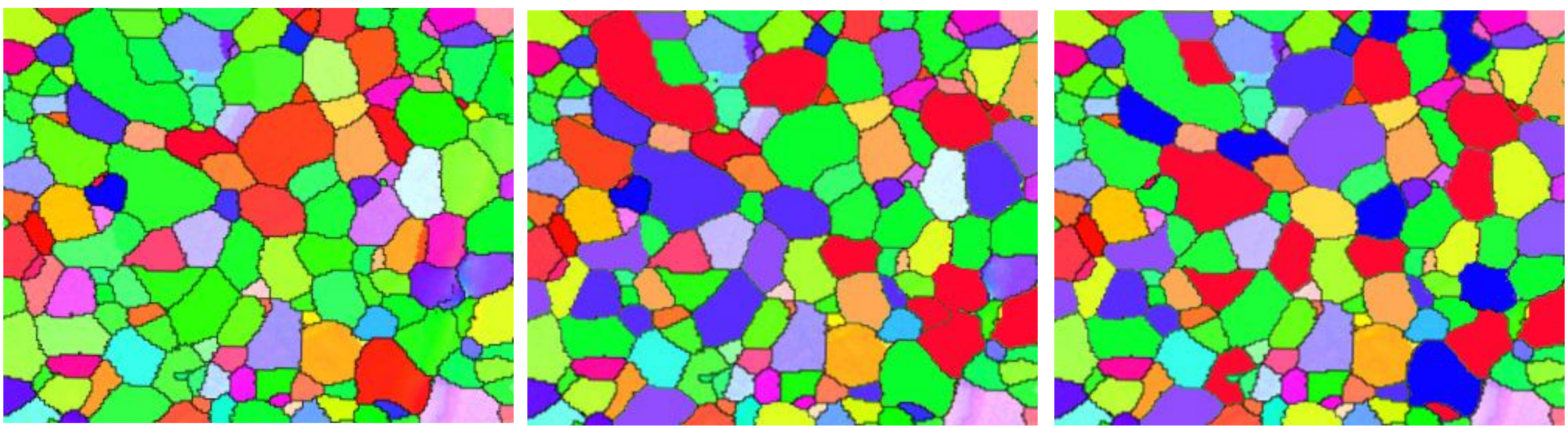
Next steps in modeling

1. **Refine and verify model further.**
   - **Apply to polycrystals**
   - **Other materials**
   - **3D**

2. **Run the model on similar, different microstructures.**

3. **Calculate variability in material properties from statistical microstructural variability.**





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