ICMAT, Singapore June 25, 2019

SAND2019-12696PE

Crystal Plasticity Predictions of Material Deformation in Body Centered Cubic Tantalum

Jay D. Carroll

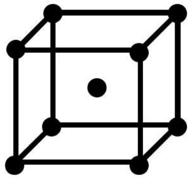
Senior Member of the Technical Staff

Sandia National Laboratories, [2]Clemson University

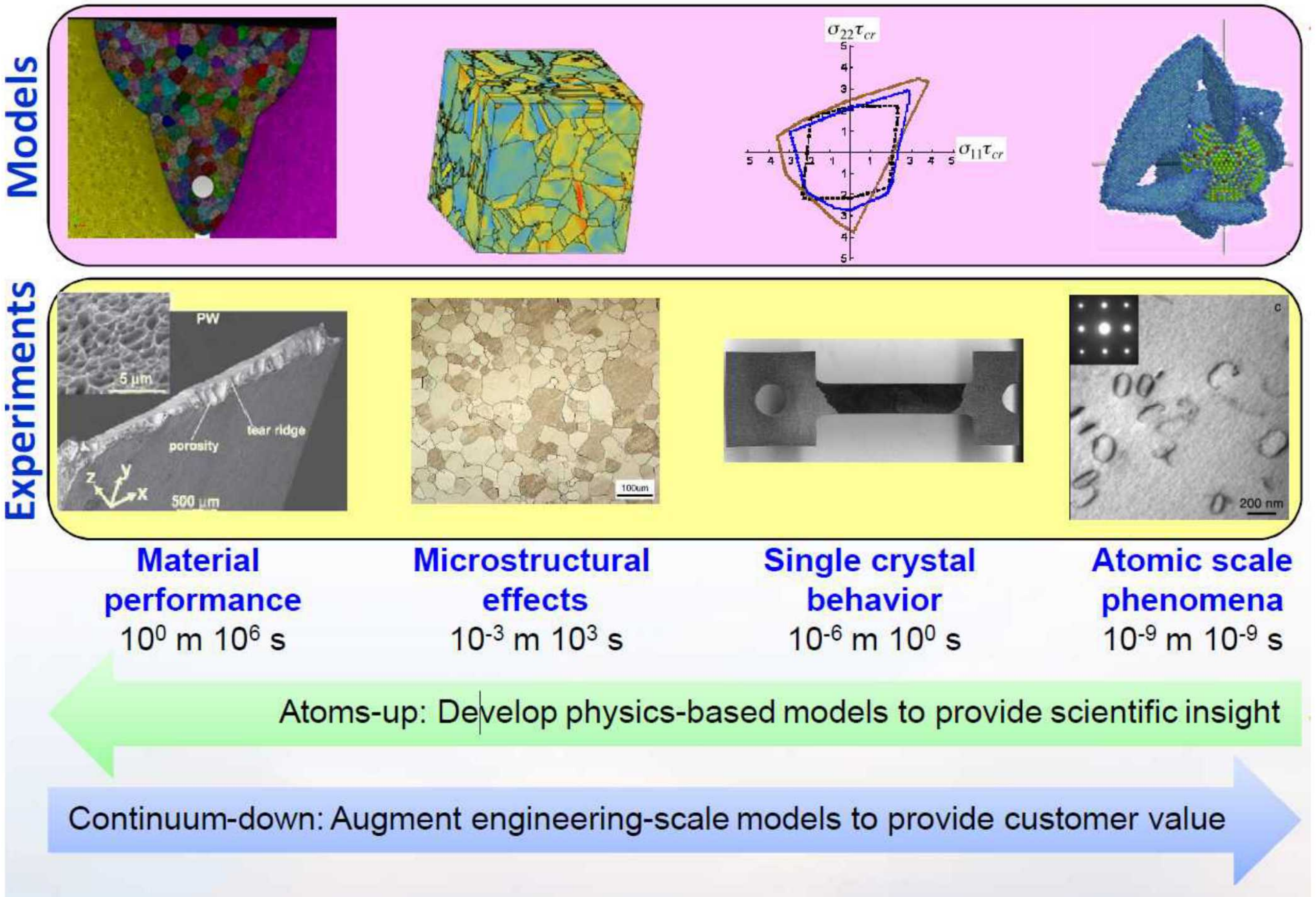
Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND2019-6956 C

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.**



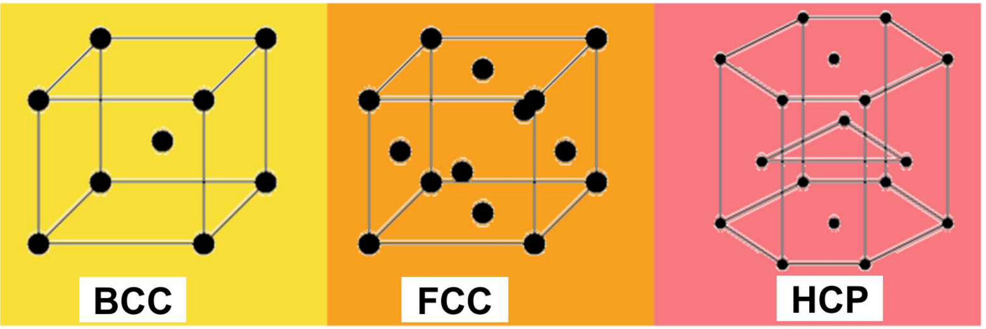
BCC
Ta



Metals are made of atoms in a crystalline arrangement

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	

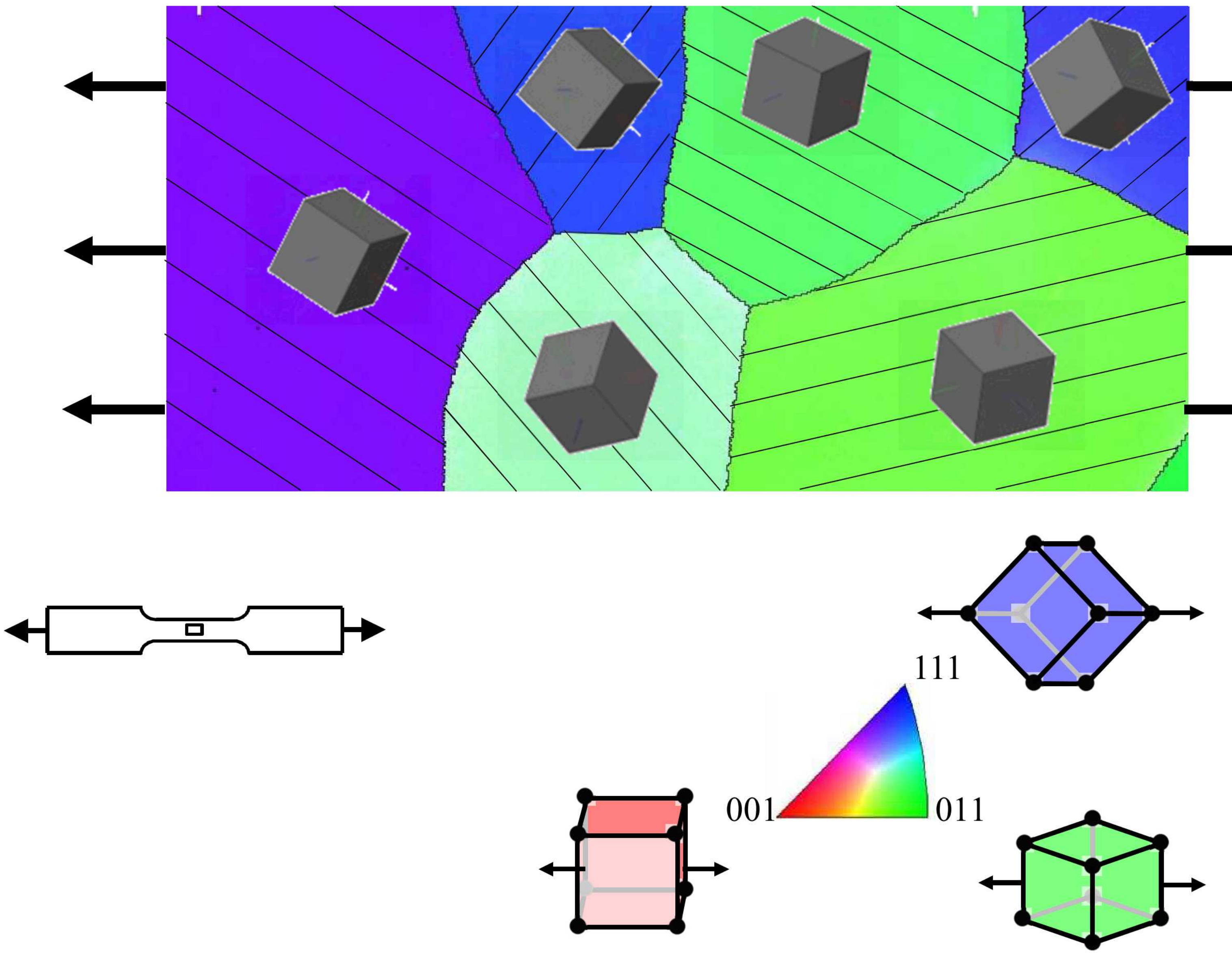


The top number in the cell is the melting point (in K)

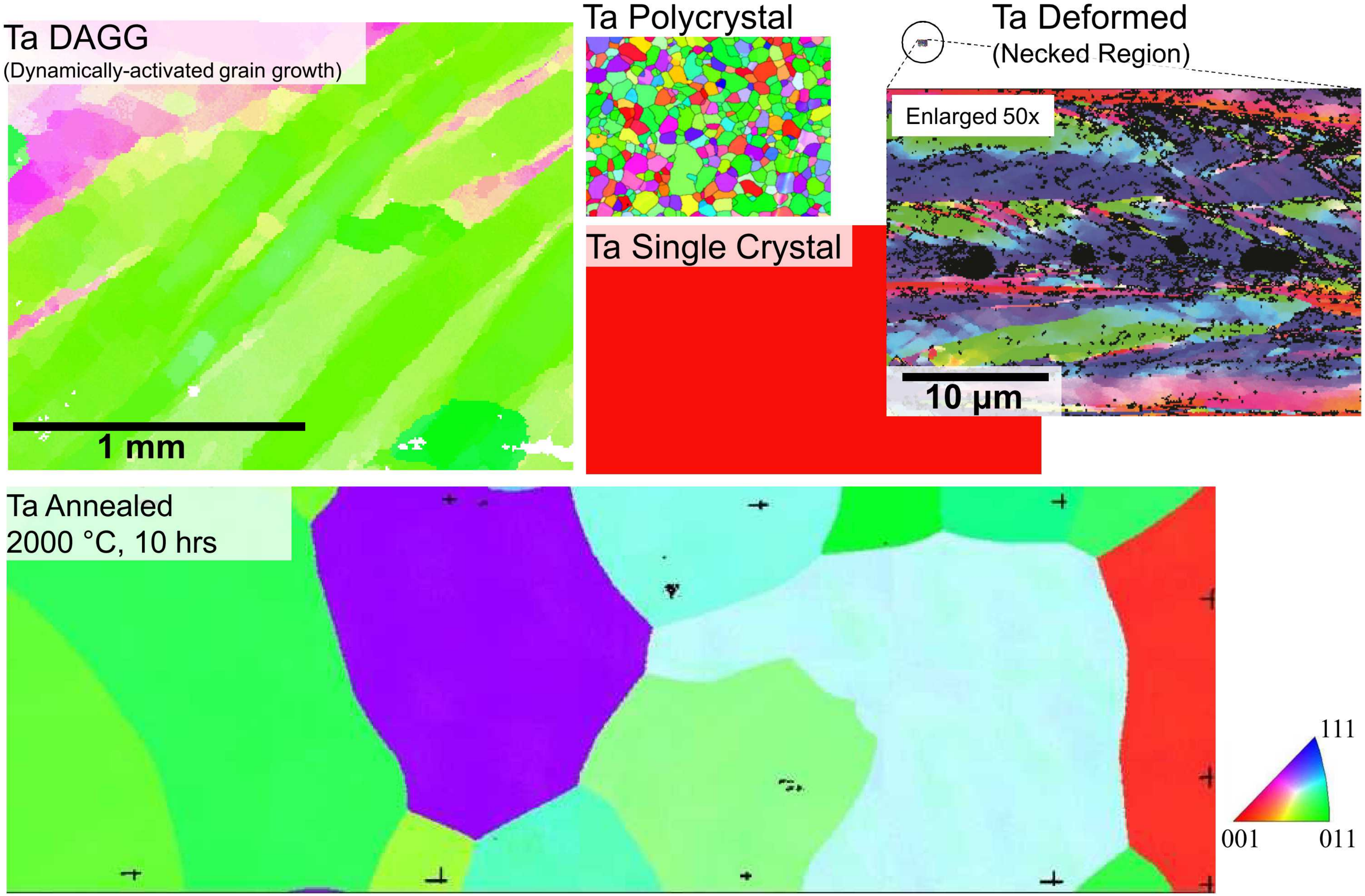
- **dhcp**: double hexagonal close packed
- unusual structure
- nonmetal
- unknown or uncertain

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

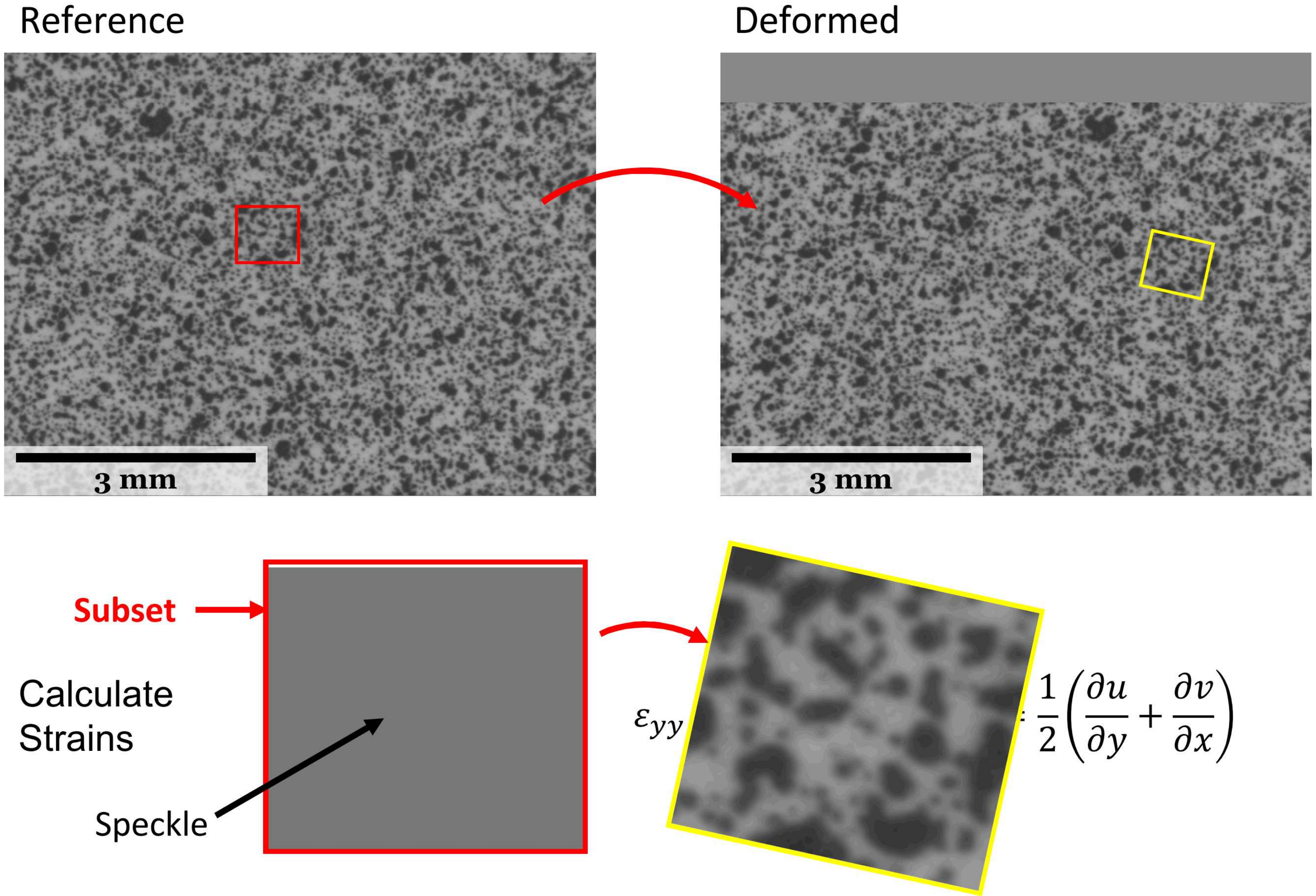
Grains are regions with uniform orientation of the atomic unit cell.



Grain structure strongly depends on the material's history.



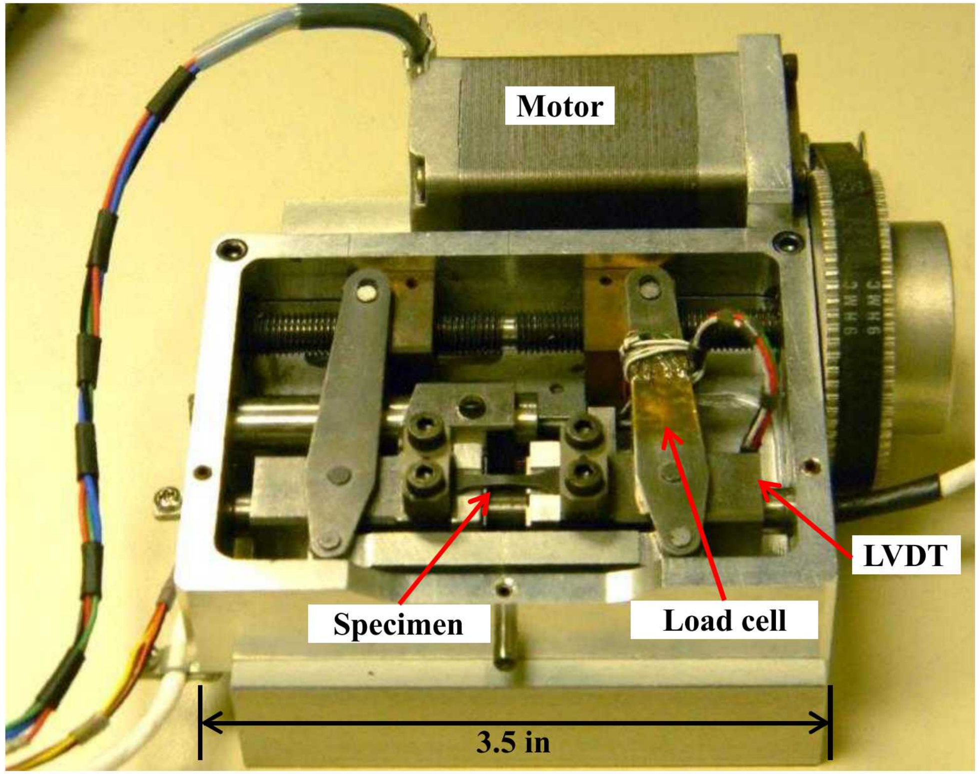
Digital image correlation (DIC) measures full field displacements and strains by tracking speckles.



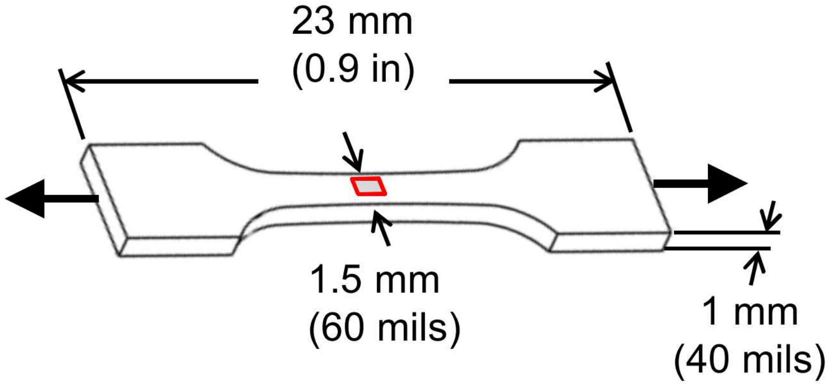
$$\varepsilon_{yy} = \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)$$

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

Sandia National Laboratories



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

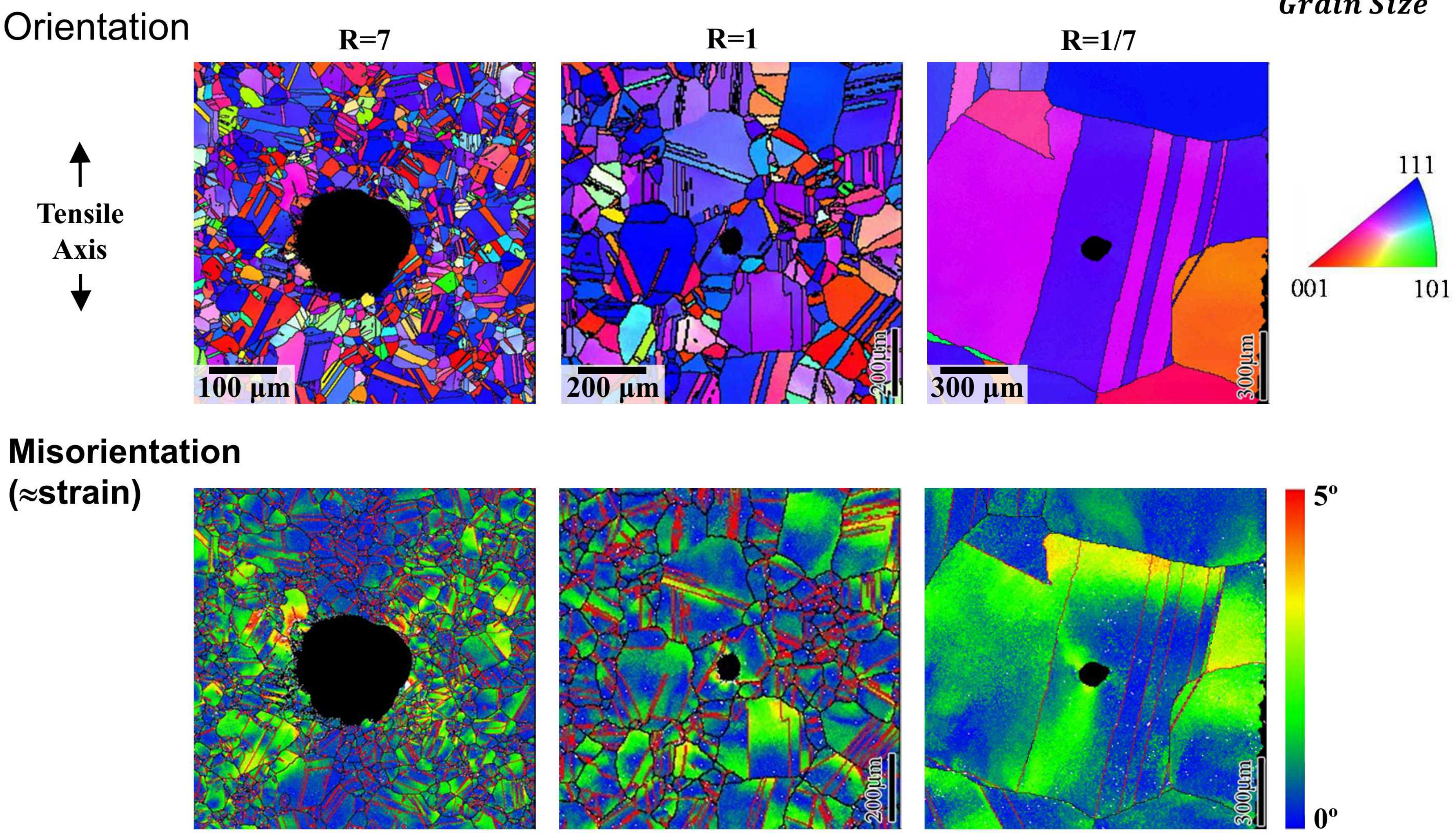


Tapered gage section is narrower at center.

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

- **Experimental measurements**

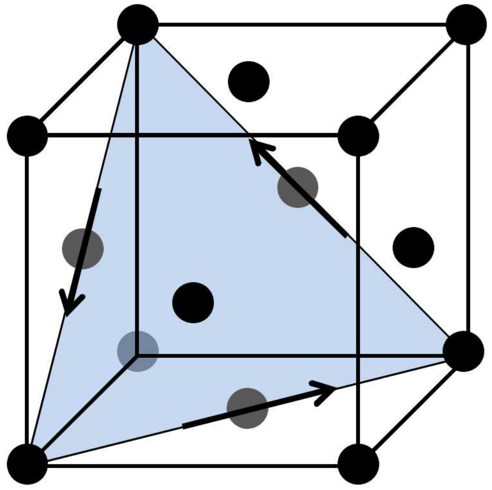
$$R = \frac{Hole\ Size}{Grain\ Size}$$



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

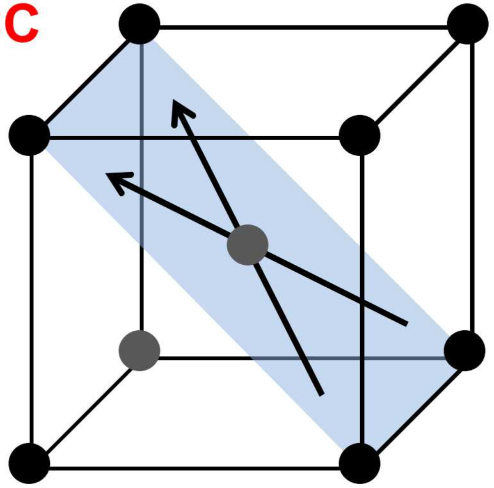
Plastic slip in FCC is much more straightforward than in BCC metals

FCC

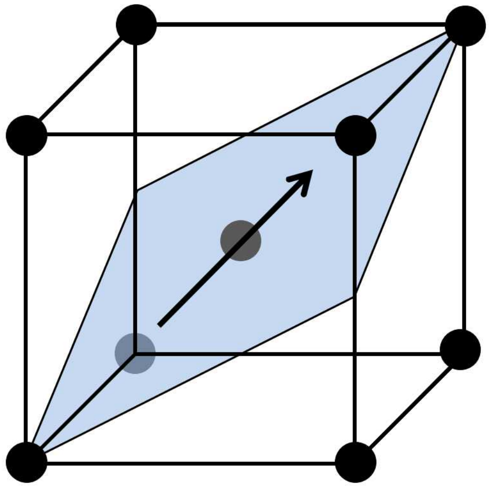


12 Slip systems:
Four {111} Planes each with
three <110> Slip directions

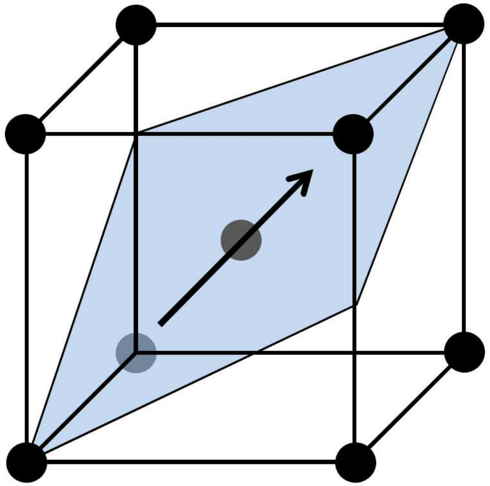
BCC



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



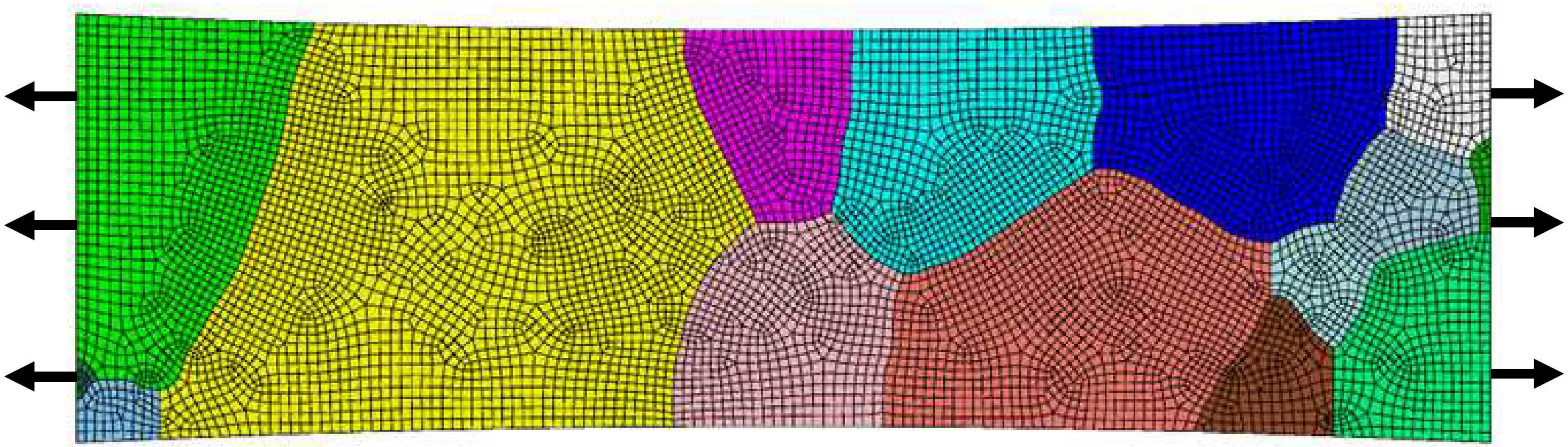
12 {112} slip systems
12 Planes each with
one <111> Direction



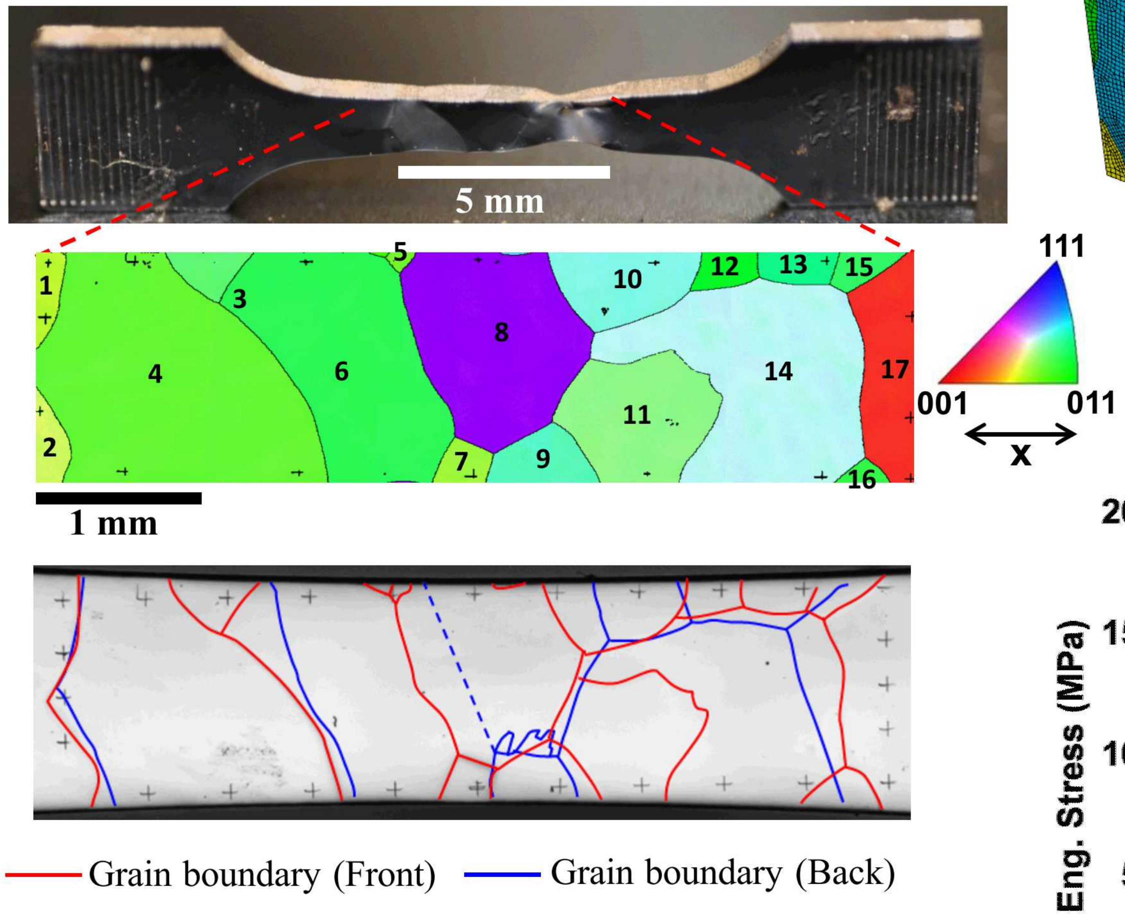
24 {123} slip systems
24 Planes each with
one <111> Direction

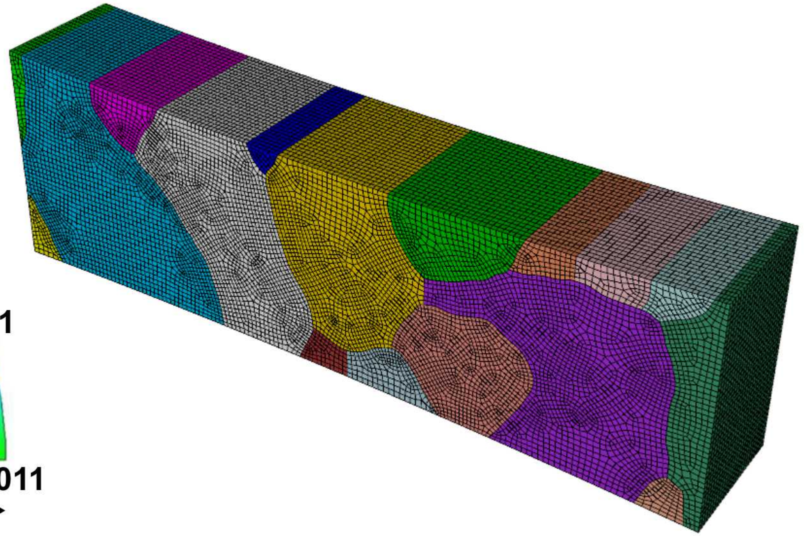
Crystal plasticity finite element models.

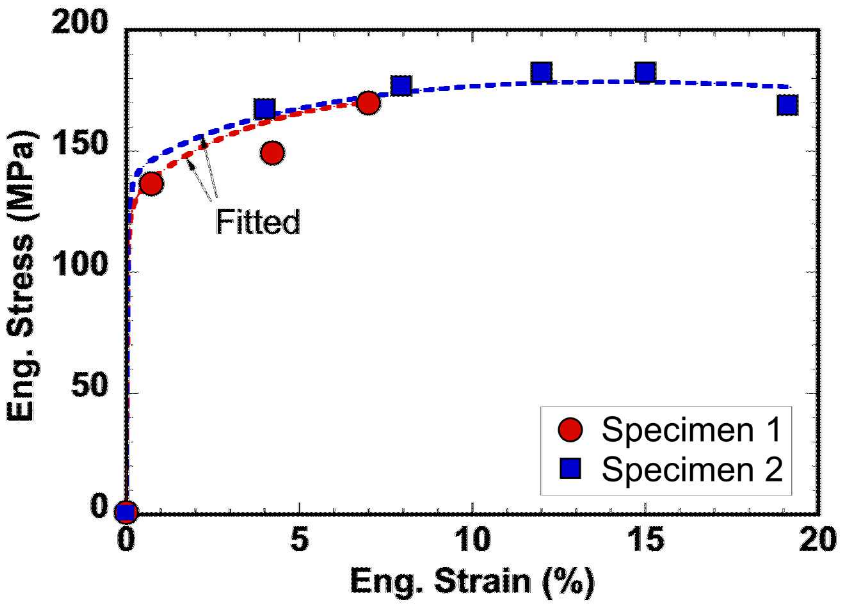
- **Different material properties for the elements within each grain.**
- **Consider the local stress on slip systems within each grain.**
- **Captures neighbor effects.**
- **Assume columnar grains.**



Crystal plasticity finite element models.



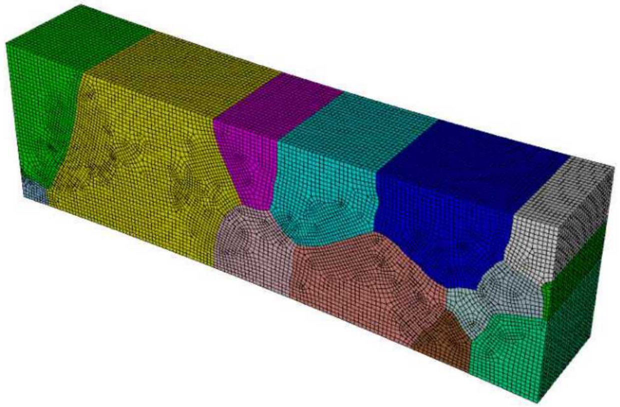


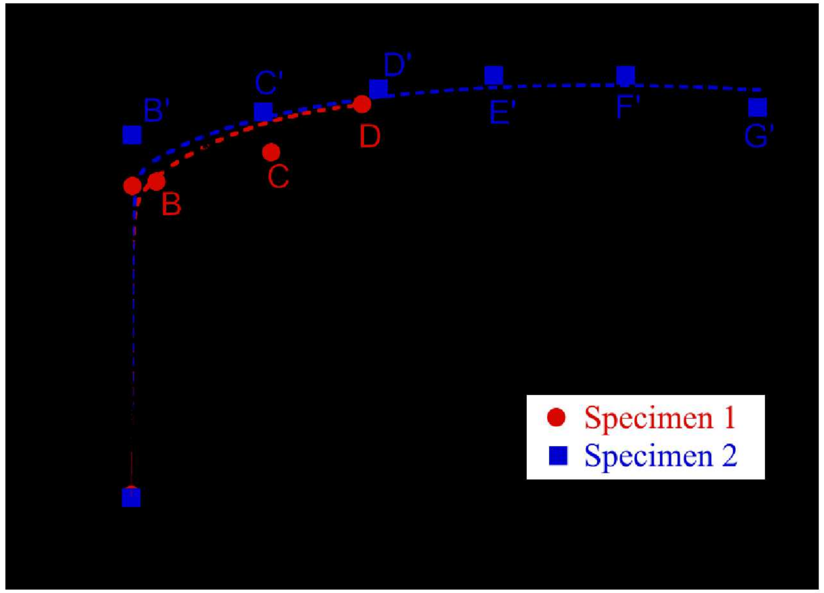


- **Different material properties for the elements within each grain.**
- **Captures neighbor effects.**
- **Assume columnar grains.**

Crystal plasticity finite element model.

- **FEM code (JAS-3D) developed at Sandia.**
- **Dislocation density based hardening model.**
- **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**

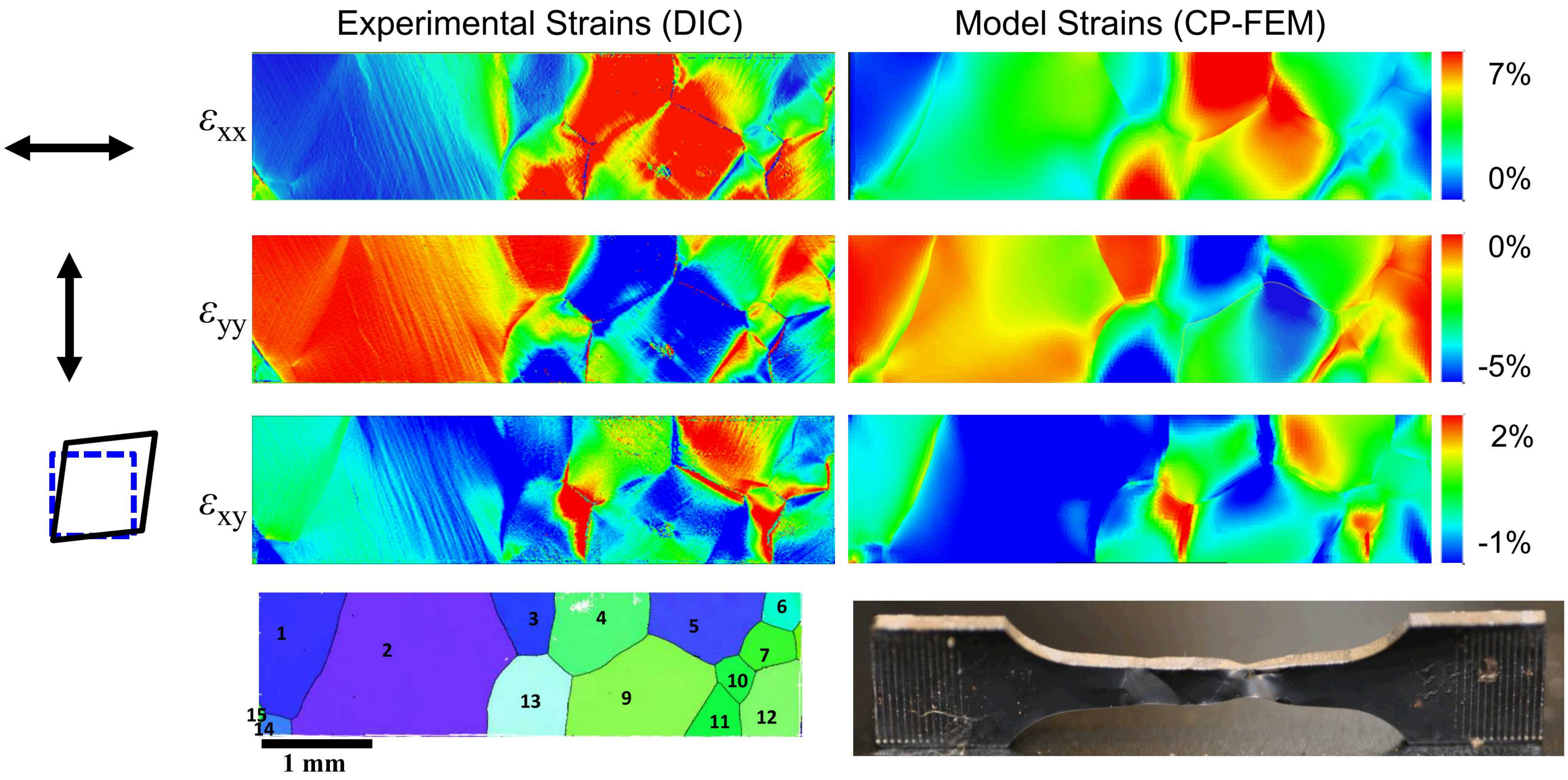




Parameters	Values	Parameters	Values	Parameters	Values
τ_0^{LT}	406 MPa	C_{11}	267 GPa	k_a	$1.4 \times 10^6\ (m^{-1})$
τ_0^{EI}	320 MPa	C_{12}	161 GPa	k_b	14
$2H_k$	0.85 eV	C_{44}	82.5 GPa	$\bar{\tau}_1$	27 MPa
$\dot{\gamma}_0$	$2.99{\times}10^6 s^{-1}$	b	2.87 Å	$\bar{\tau}_2$	37 MPa

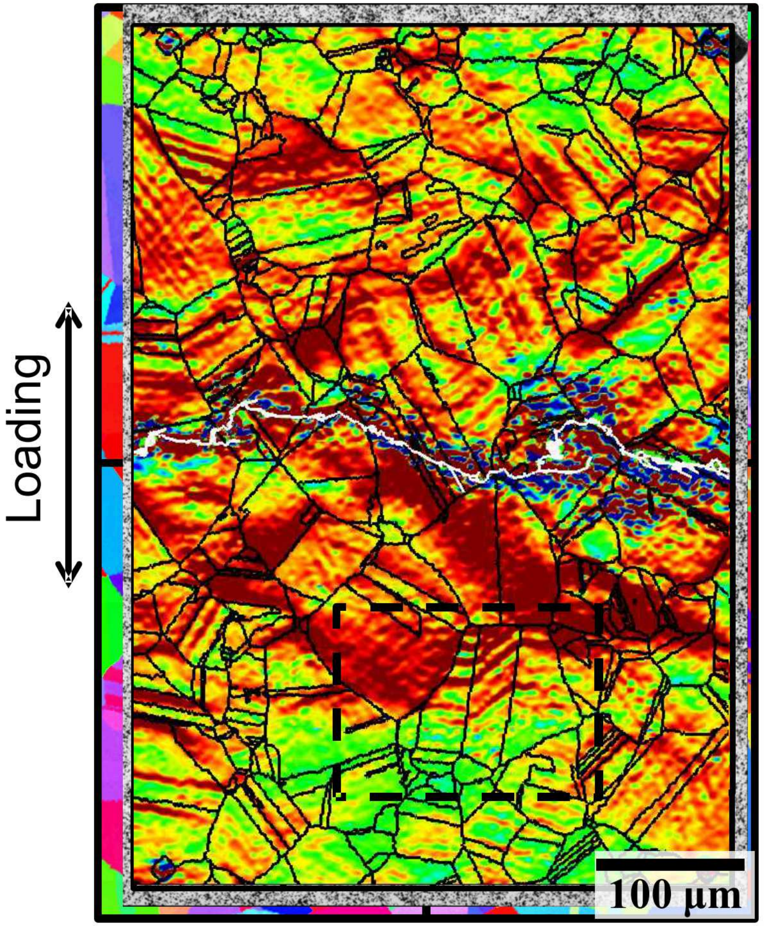
Model predictions of strain agree well with experimental measurements in most places.

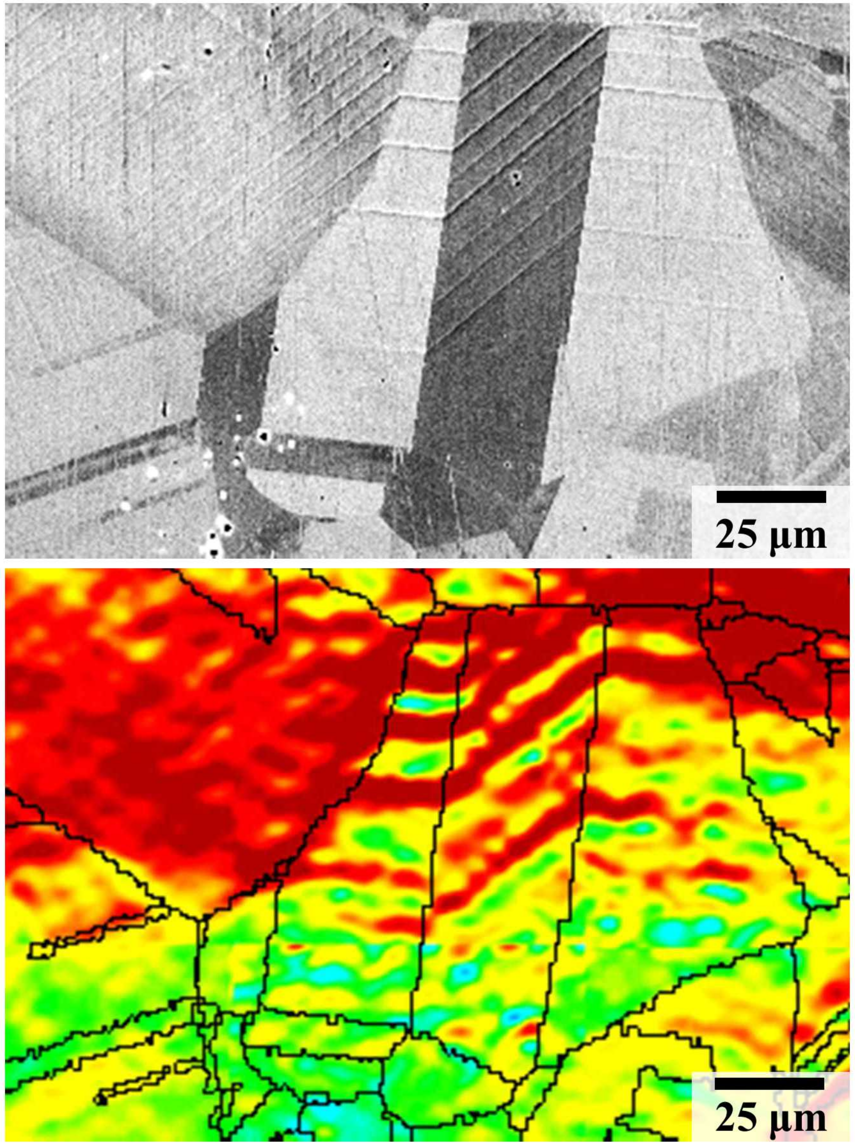
Sandia National Laboratories



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).

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

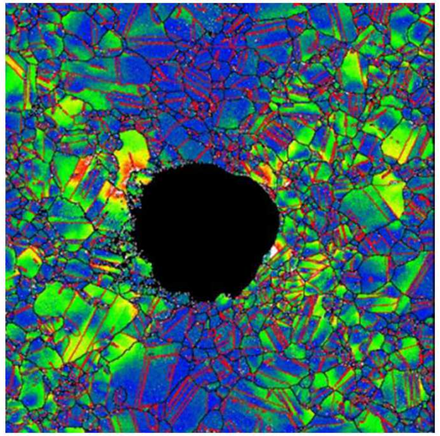


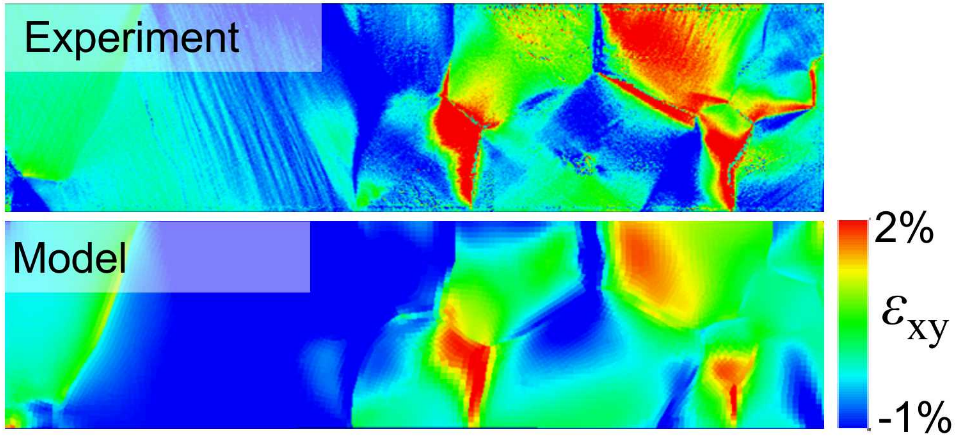


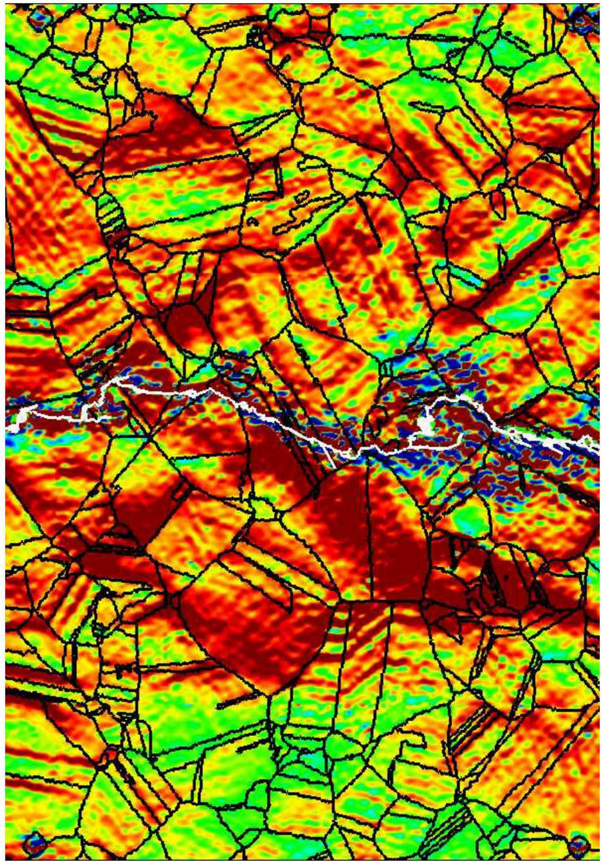
- **Carroll et al., *Rev. Sci Inst.,* v. 81 (2010).**
- Carroll et al., *Int J. Fracture*, v. 180 (2012).
- Carroll et al., *Int. J. Fatigue*, (in press, 2013).

Conclusions

1. **The crystalline structure of metals can affect structural behavior such as strength and deformation.**
2. **Crystal Plasticity Finite Element Models (CP-FEM) can predict the effects of microstructure on deformation.**
3. **We are investigating the effects of microstructure on fatigue crack growth and other phenomena.**







Jay Carroll
Sandia National Laboratories
jcarrol@sandia.gov

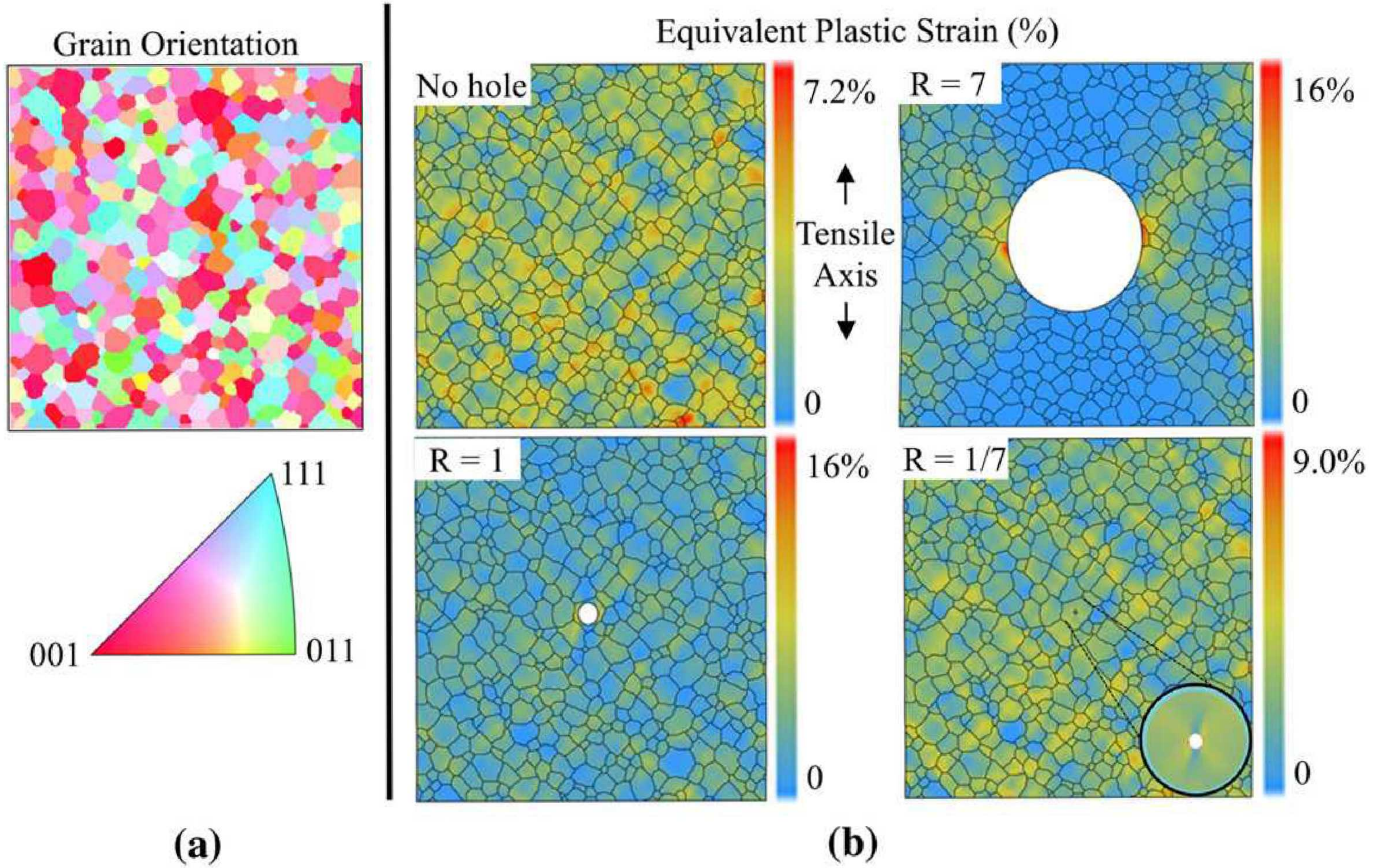
Thank You

Jay Carroll
Sandia National Laboratories
jcarrol@sandia.gov

Extra Slides

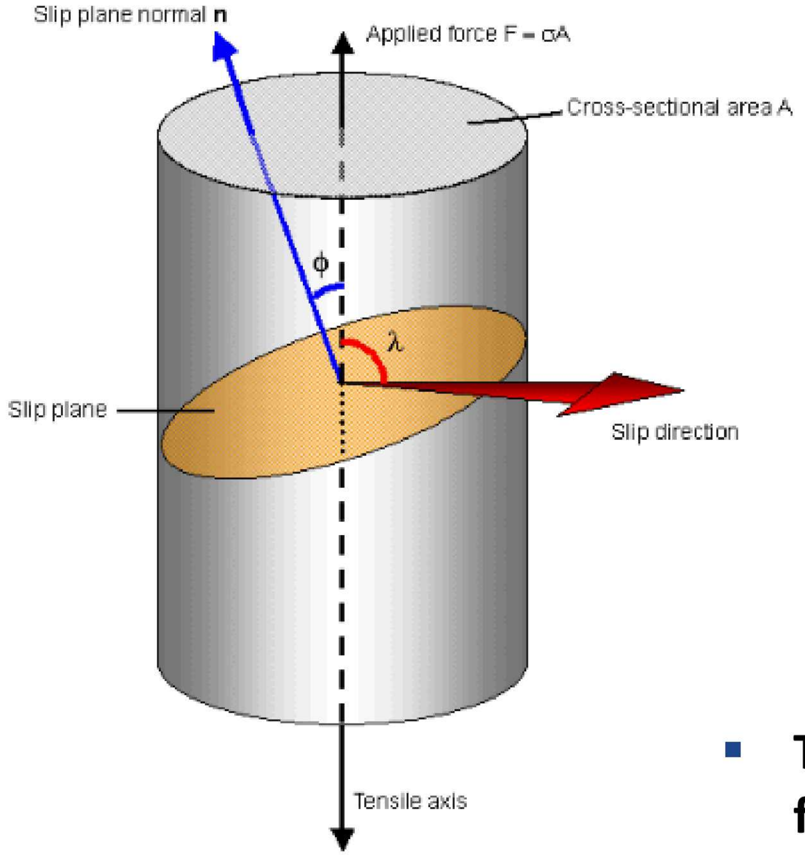
For small features, microstructure can be more important than the stress concentrator.

- **Model predictions**



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

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

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

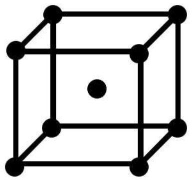
0 < Schmid < 0.5

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.**

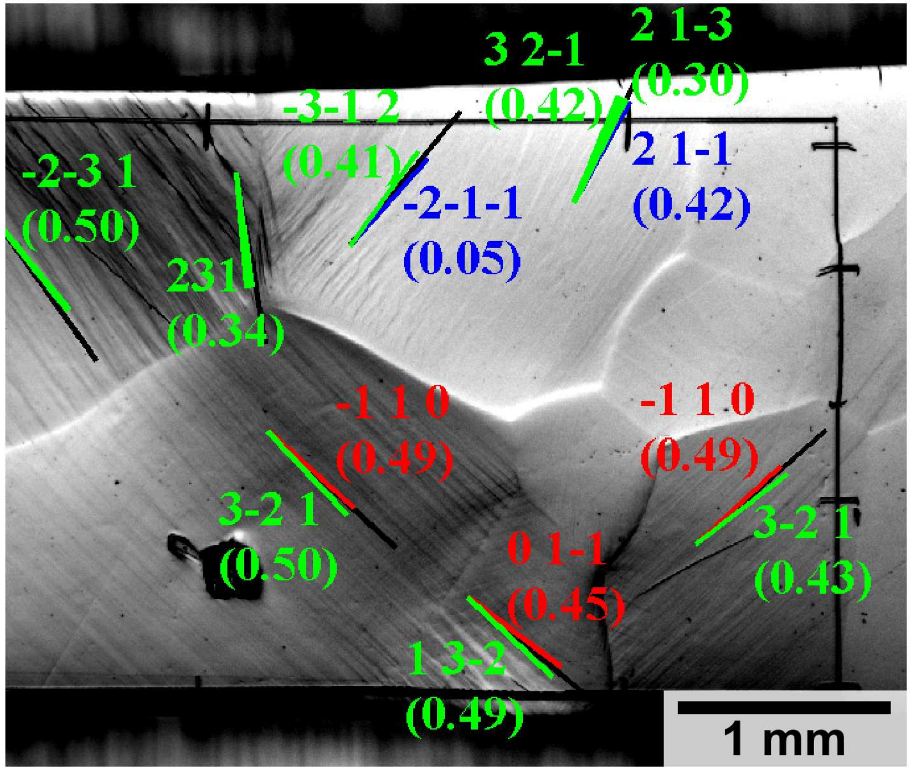
Special challenge with BCC materials: Identifying active slip systems.



- **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.**

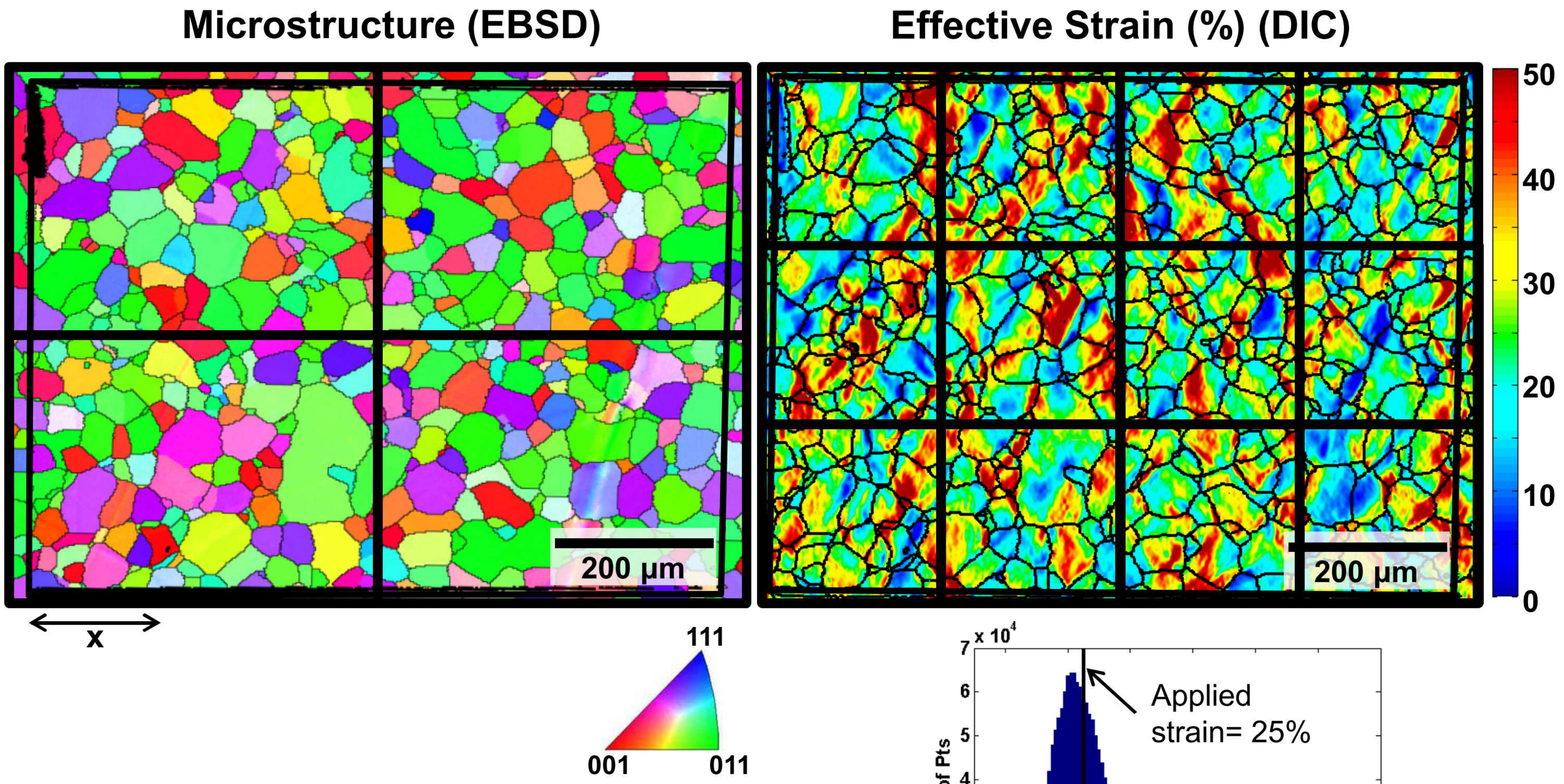
Material	Slip plane	…	References
Tungsten	{110}		118
Tungsten	{112}		118
α-iron	{110}		118
α-iron	{112}		118
Chromium	{112}		118
Vanadium	{112}		118
Tantalum	{112}		133
Tantalum	{112}		134
Tungsten	{110}		130
Molybdenum	{110}		130
Molybdenum	{110}		130
Molybdenum	{110}		130
Molybdenum	{110}		130
Niobium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

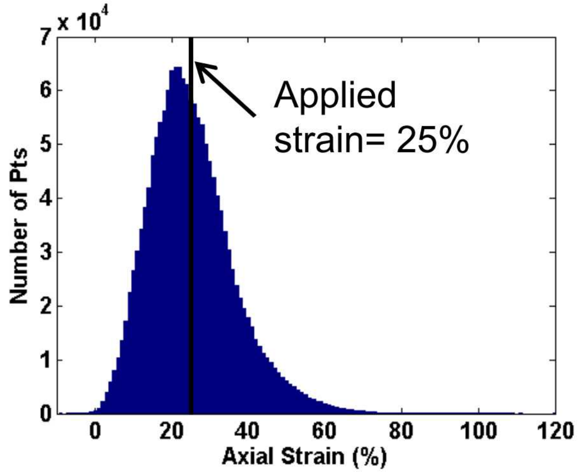
Weinberger C.R., et al.,
International Materials Reviews (2013)



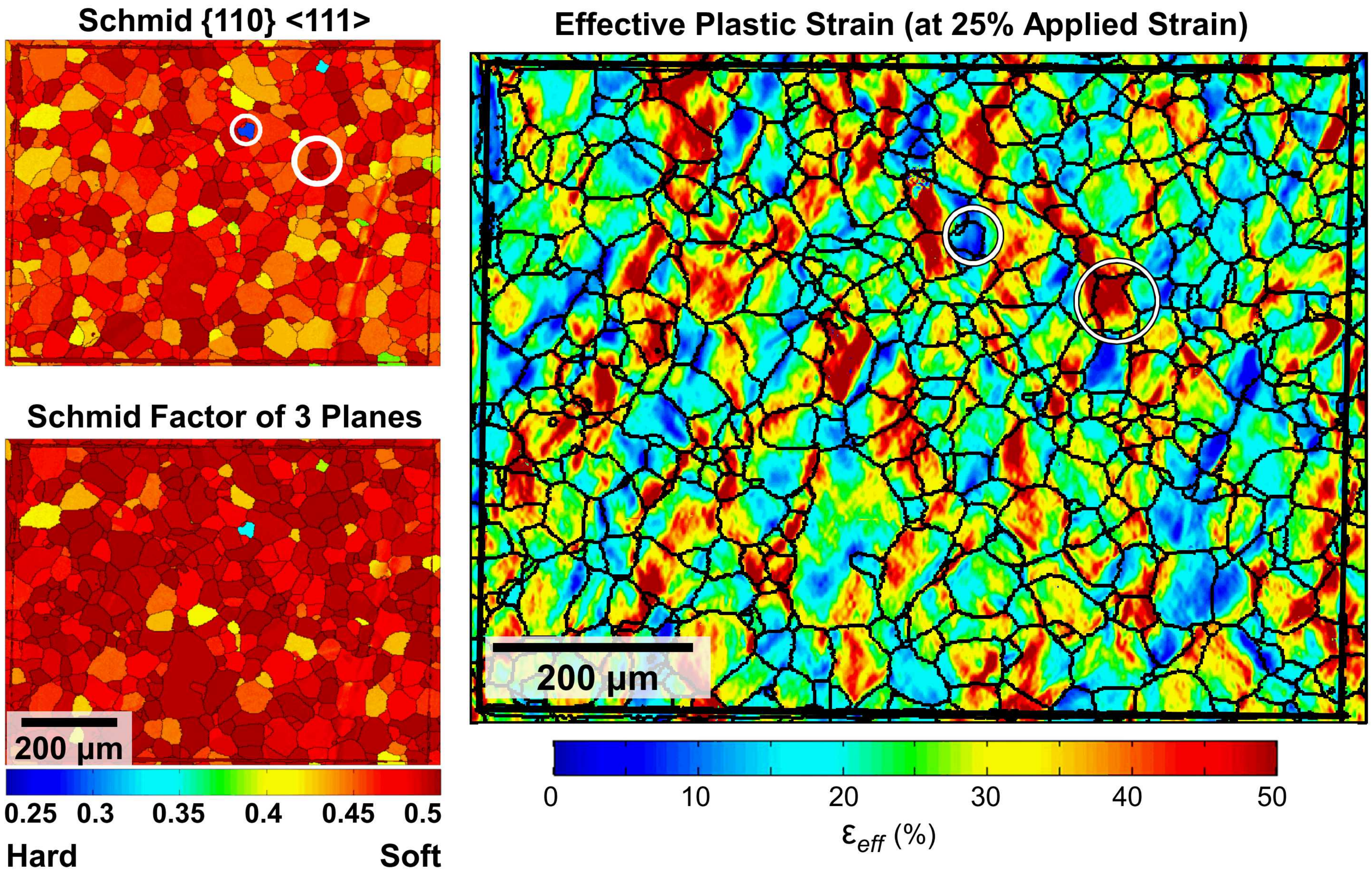
Carroll J.D., Clark B.G., Buchheit T.E., Michael J.R., Boyce B.L., *Materials Science and Engineering A*, v. 581 (2013).

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

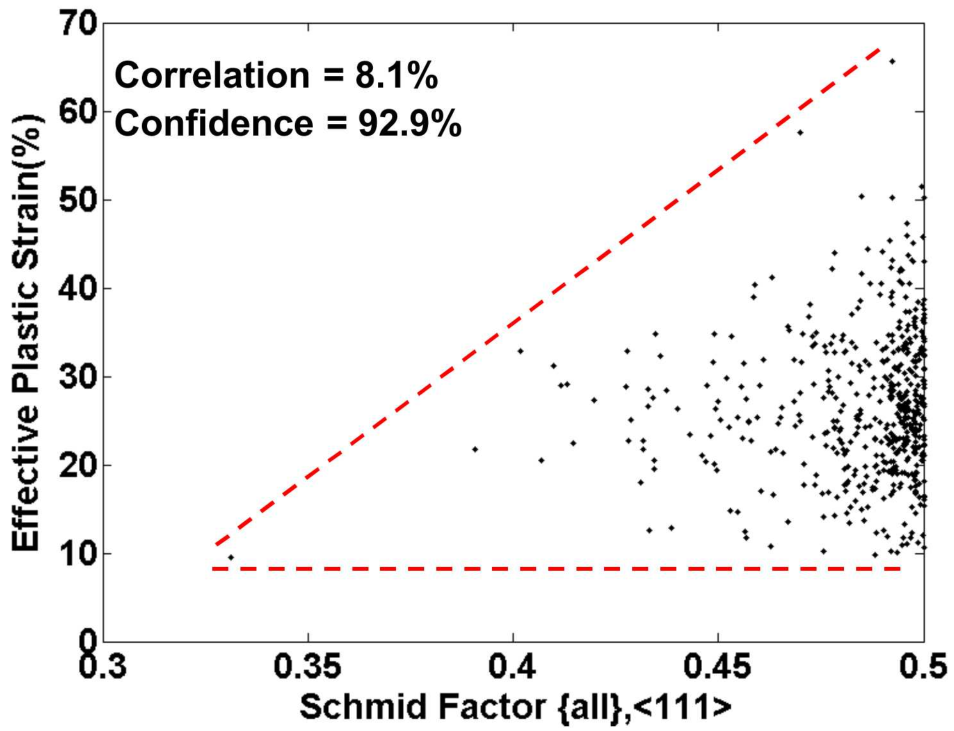


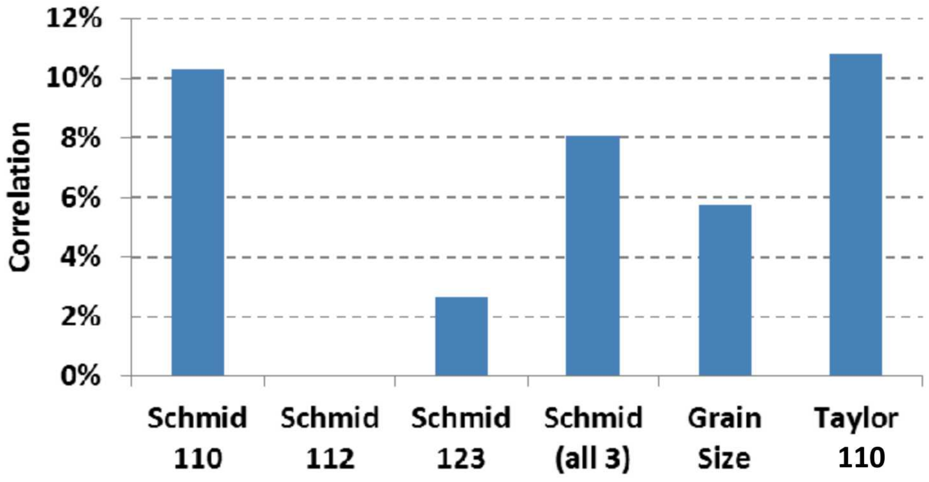


The effects of six microstructural parameters on local strain were considered.



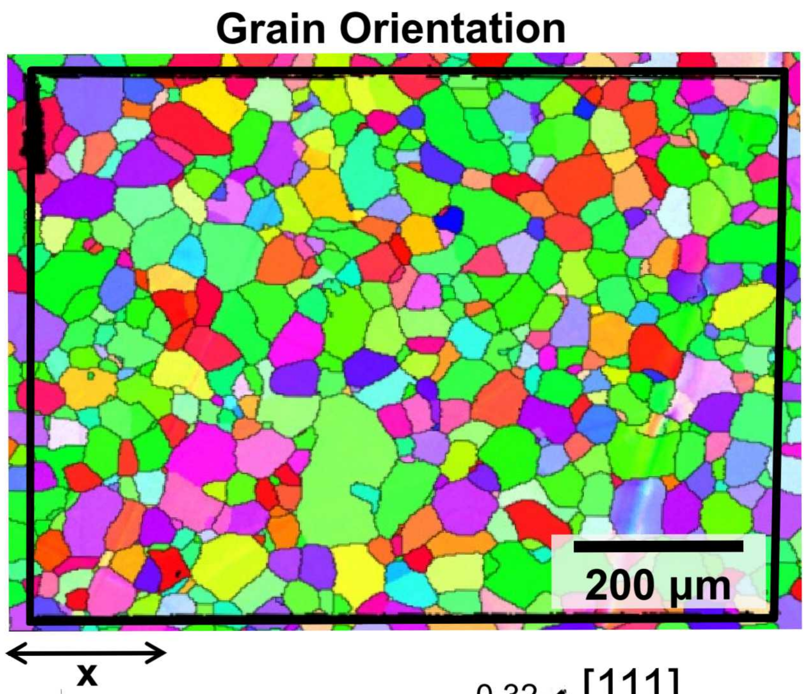
There is some correlation between microstructure and average strain within each grain.

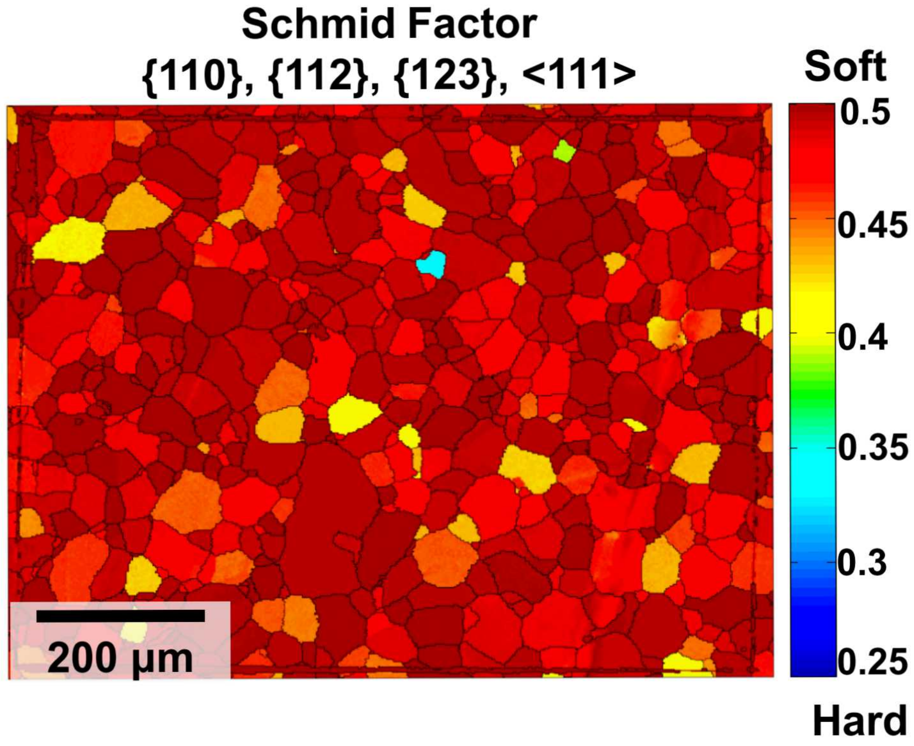


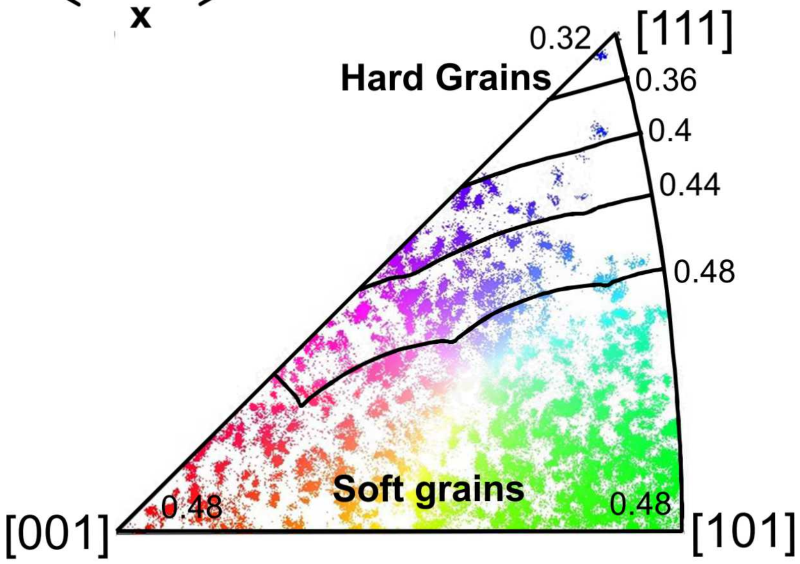


Parameter	Correlation	Confidence
Schmid 110	10%	98%
Schmid 112	-0.4%	6%
Schmid 123	2.7%	45.1%
Schmid (all 3)	8.1%	92.9%
Grain Size	5.8%	80%
Taylor 110	11%	99%

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

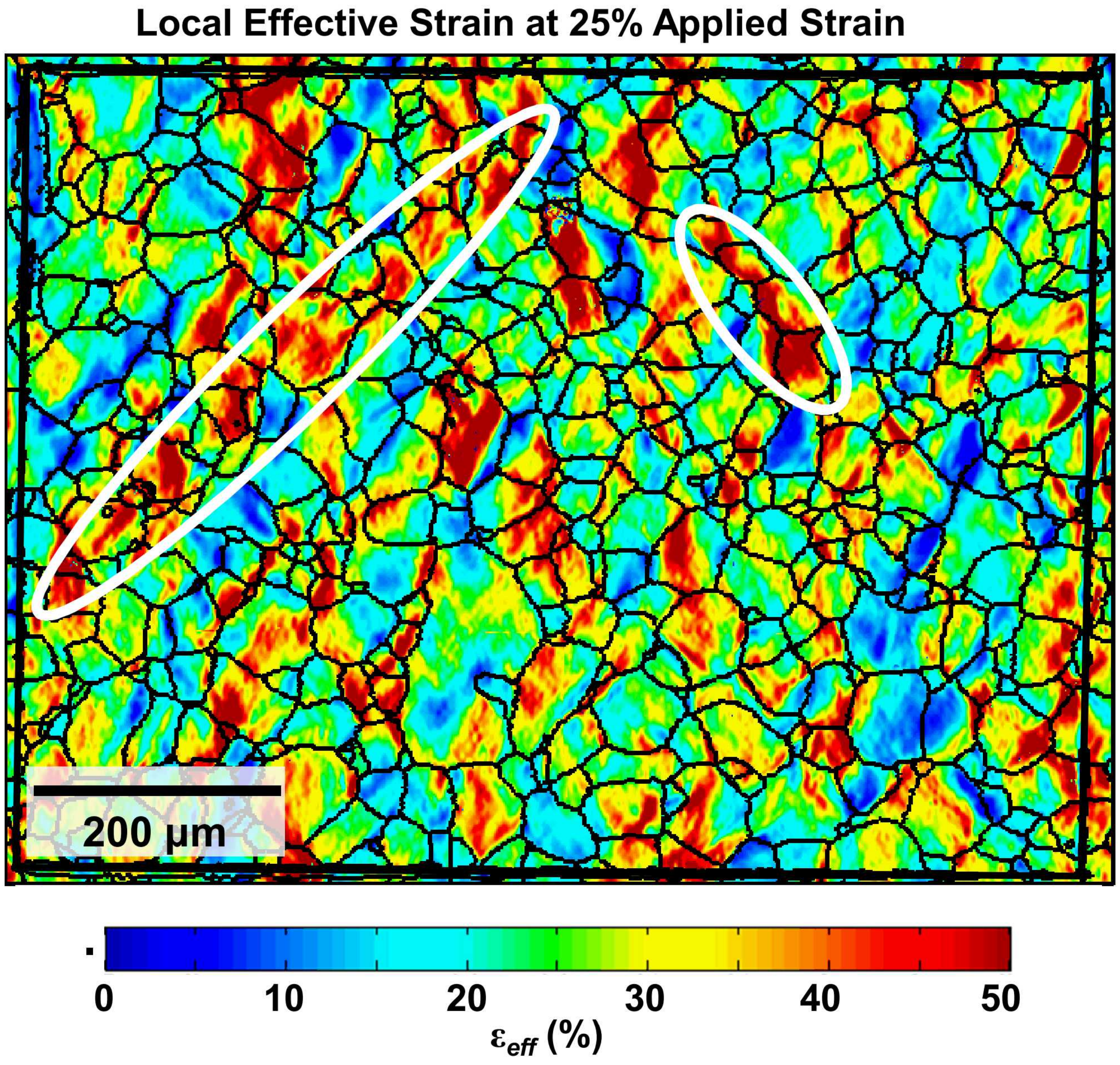






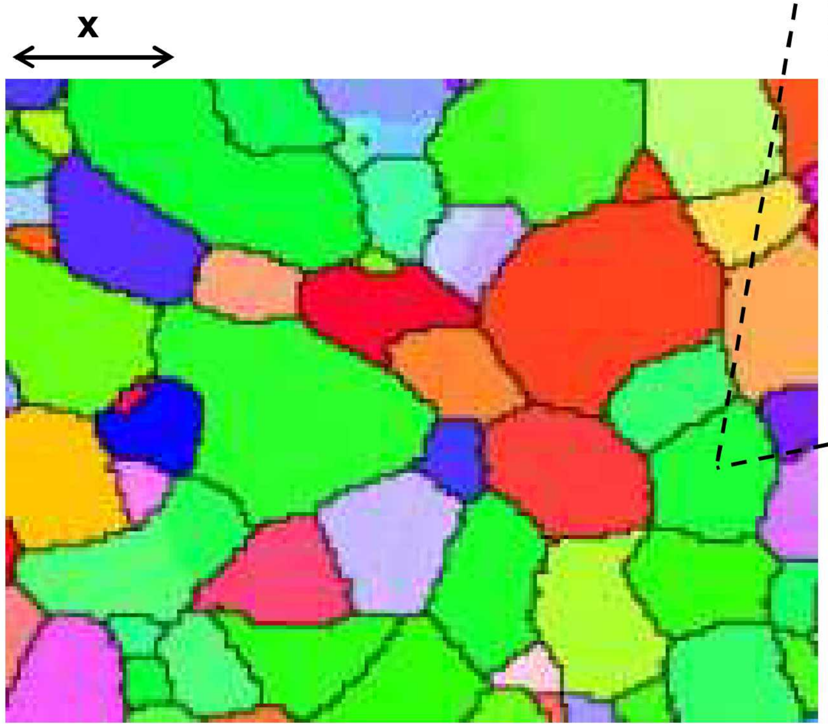
Schmid contours
{110},{112},{123}
<111>

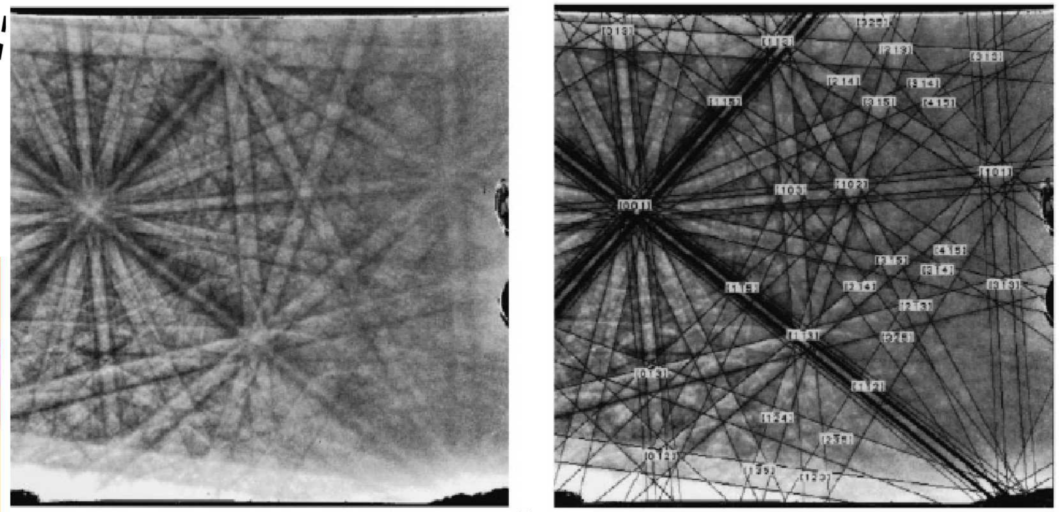
Neighborhood effects are apparent in strain fields.

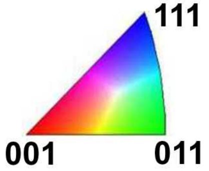


Electron Backscatter Diffraction (EBSD) measures local grain orientation.

- Put specimen in scanning electron microscope.
- Capture an image of diffraction bands.
- Determine orientation based on band angles.
- Repeat for all pixels in the map.



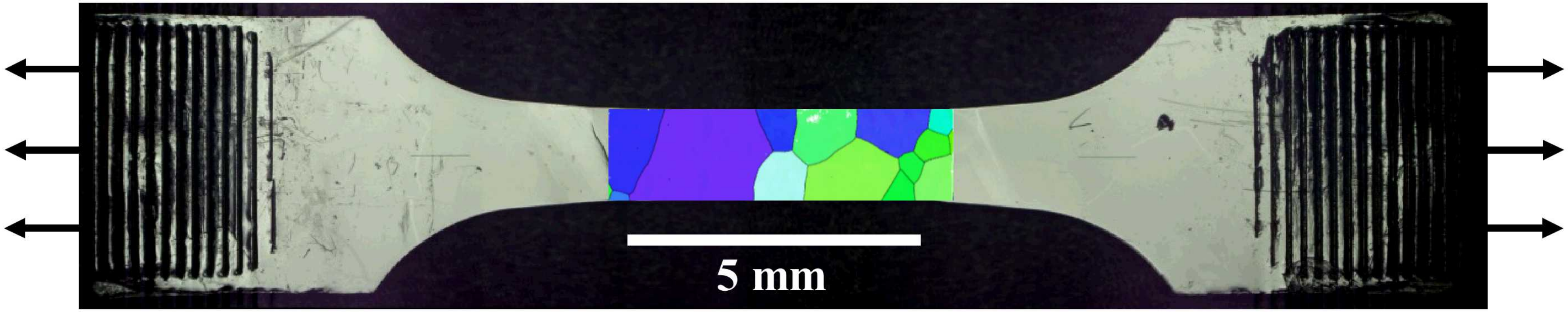




- J.A. Small, J.R. Michael, Journal of Microscopy-Oxford, v. 201 (2001).

Oligocrystals

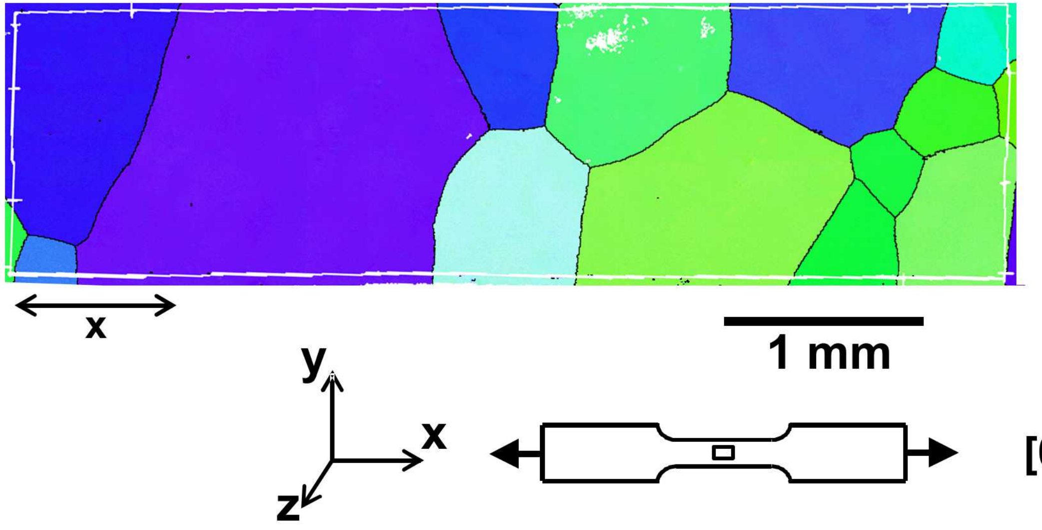
Specimens where deformation is controlled by a few grains (3–20).

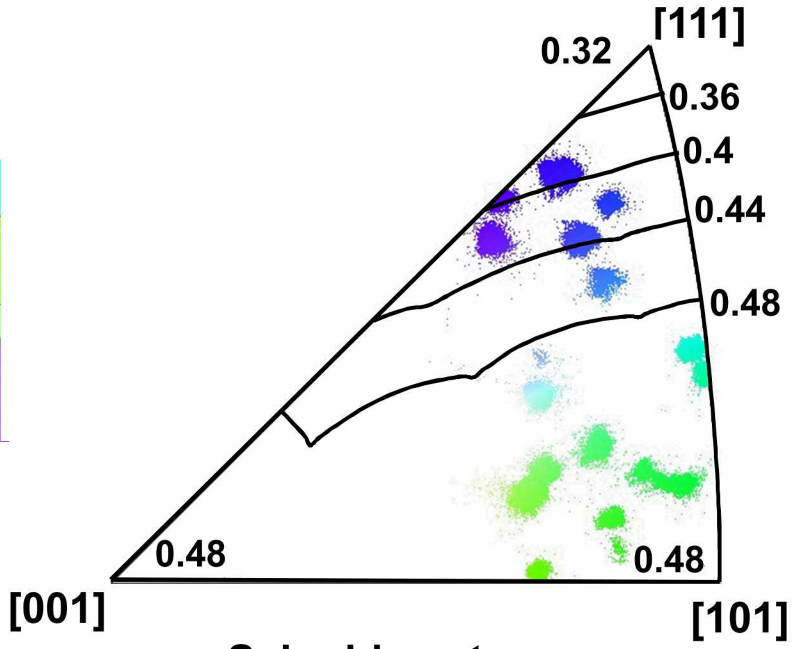


- Ta oligocrystals were made by annealing.
- This has much fewer neighborhood effects.

This oligocrystal also has more hard grains.

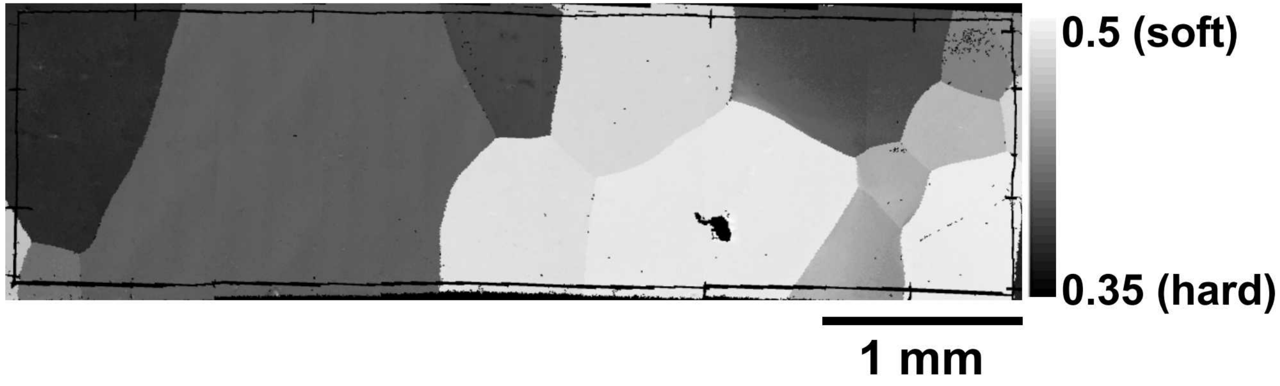
Grain orientation



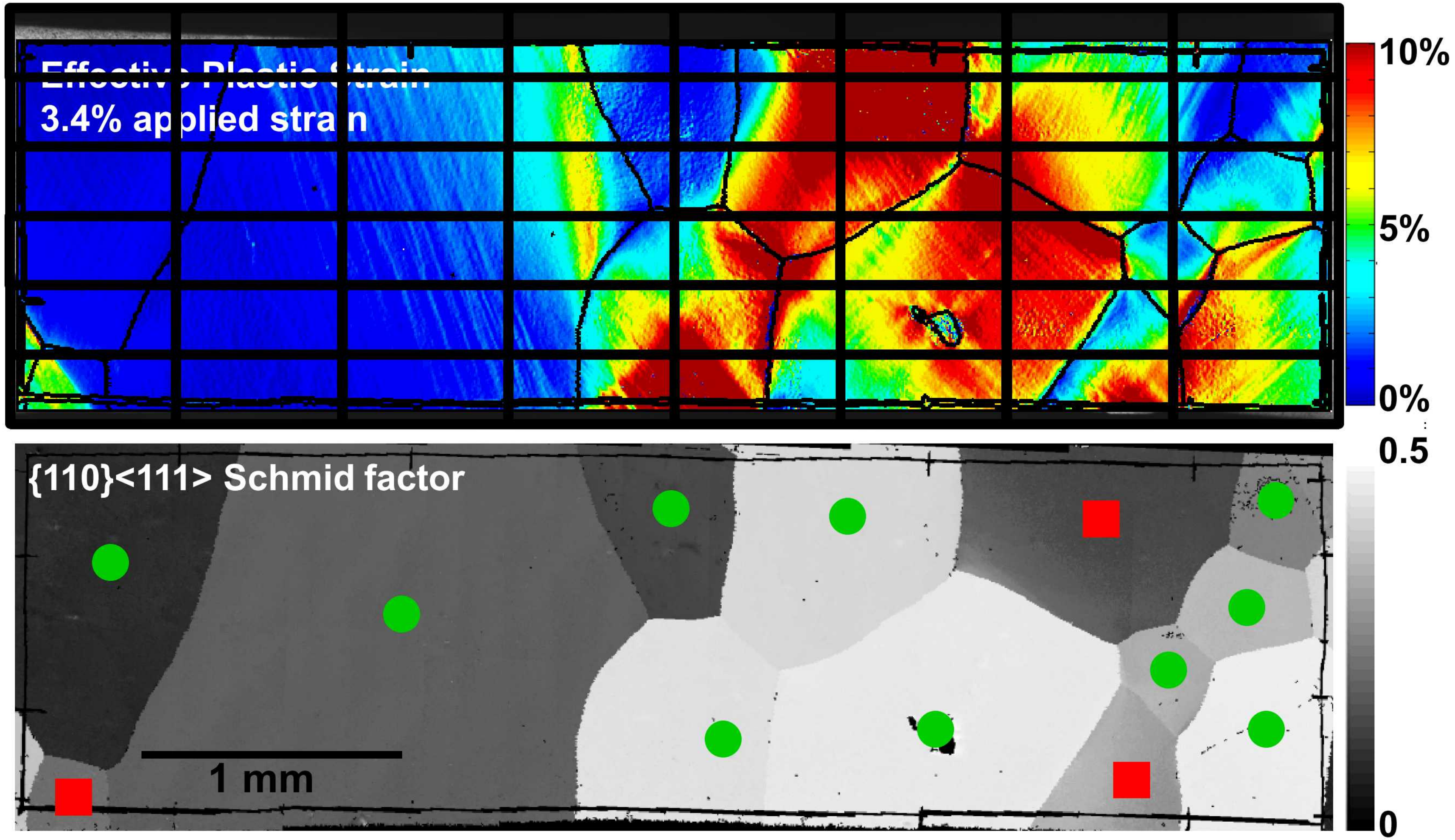


Schmid contours
{110},{112},{123}
<111>

Schmid {110}<111>

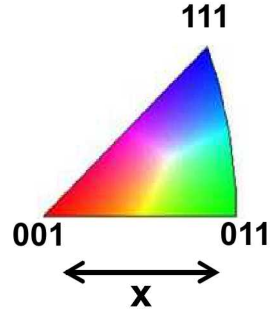


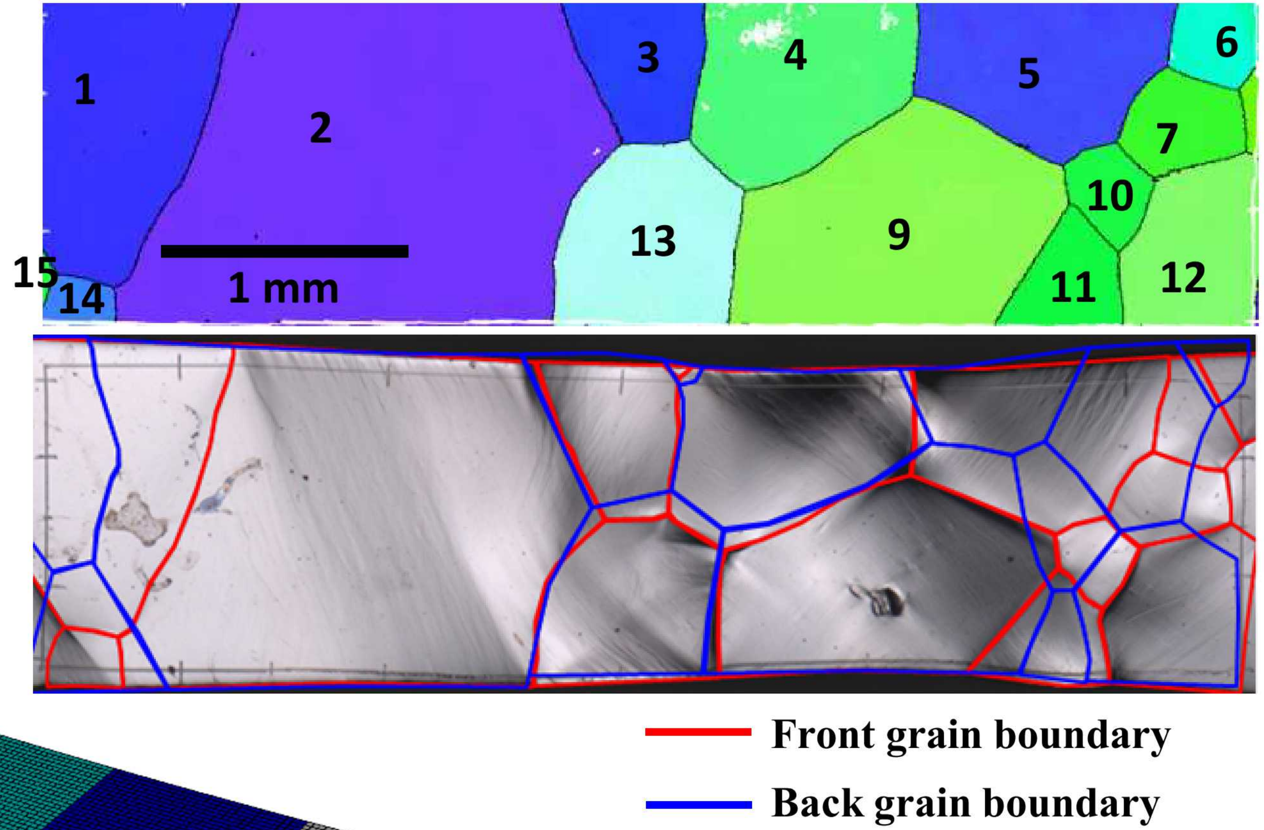
Strain accumulation agrees with Schmid factor for most grains.

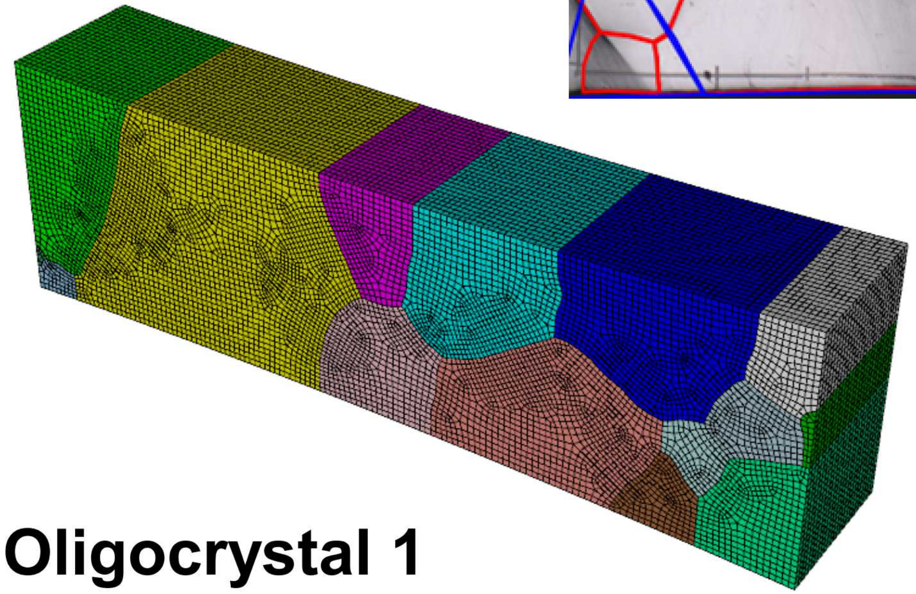


- 10 out of 13 grains have strain and Schmid agree (77%).
- Neighbor effects may explain the other cases.

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

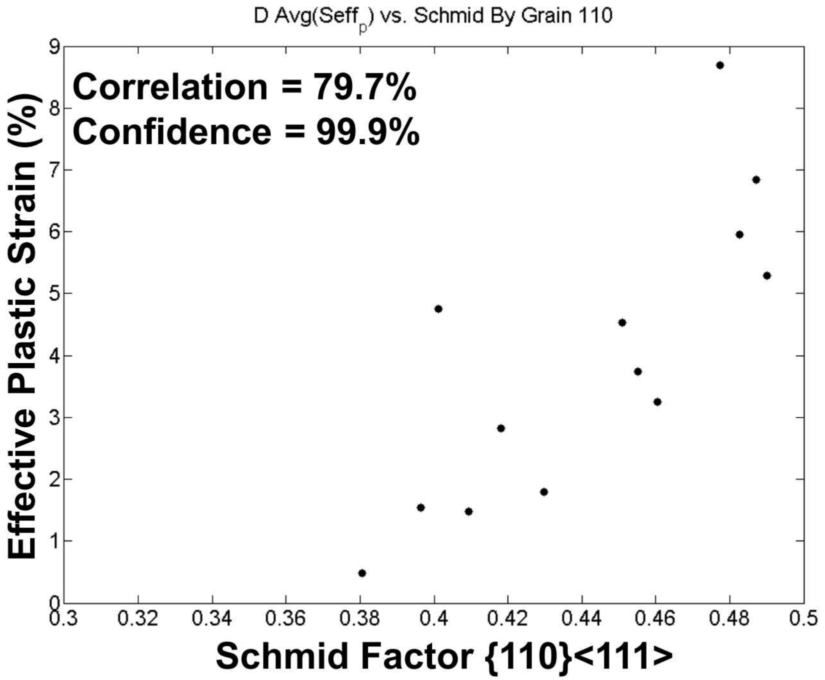


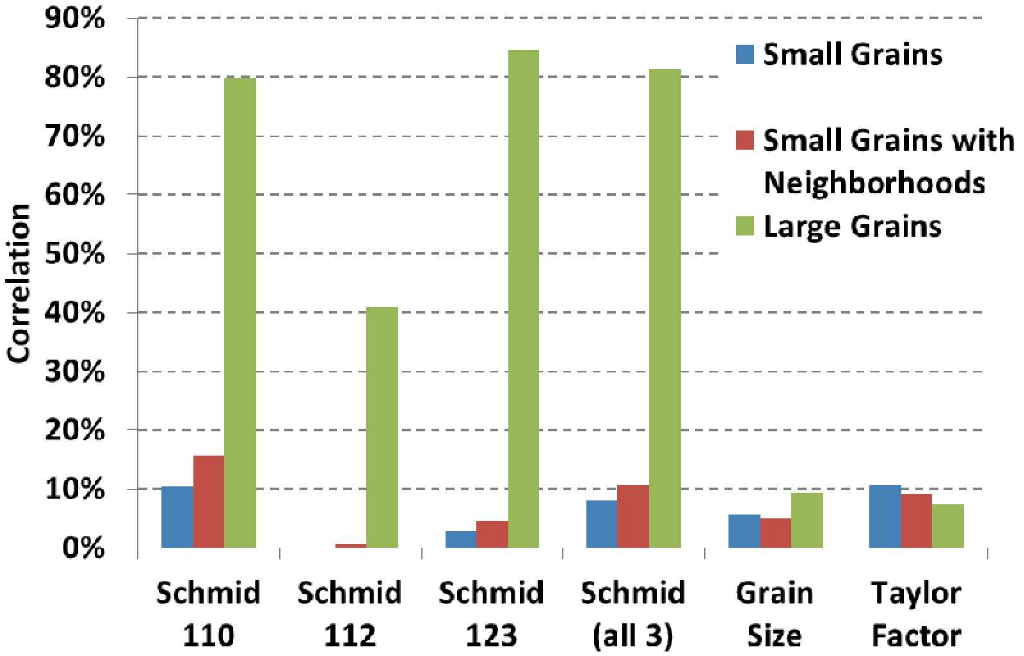




Oligocrystal 1

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!