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Experimental Validation of Crystal Plasticity Models

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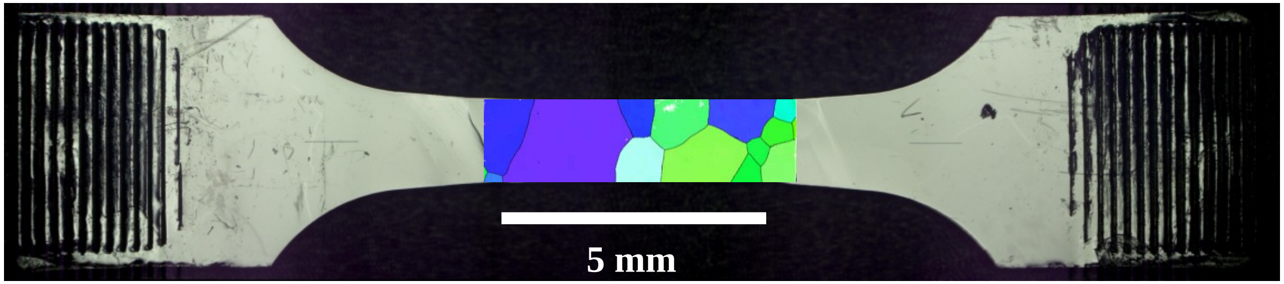
International Symposium on Plasticity
1/3/2014



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Outline

1. Background
2. Experimental setup
3. Model details
4. Model validation- strain fields
5. Model validation- crystal rotations
6. Conclusions

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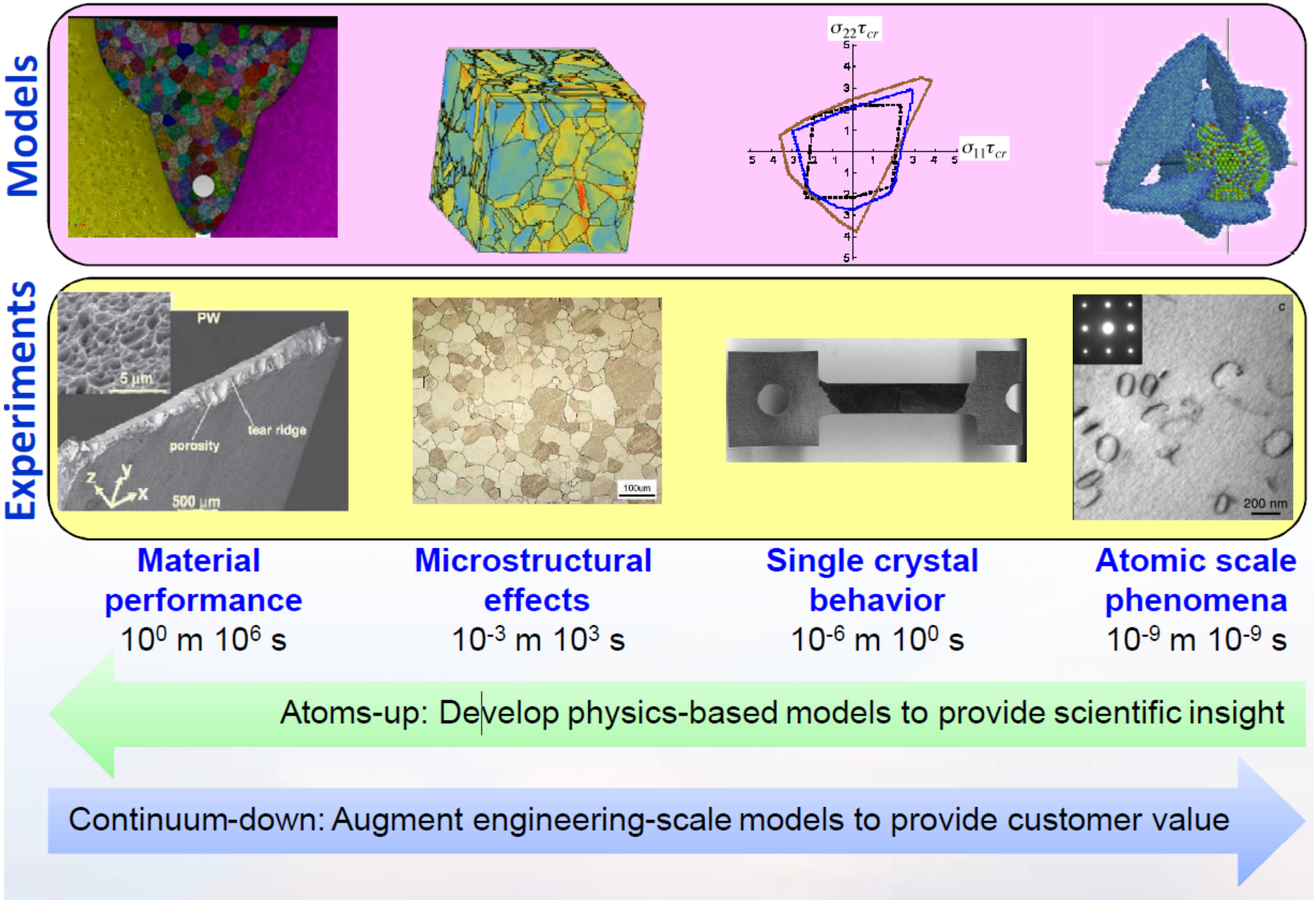
Relate variability in structural behavior to microstructural variability

- **Task 4: Modeling Processing Effects on Microstructure**
- **Task 3: Predict macroscale variability from microstructural statistical models.**
- **Task 2: Microscale effects on deformation behavior.**
- **Task 1: Atomic/nanoscale defects and dislocation effects.**



Models

Experiments

Material performance
10^0 m 10^6 s

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

Single crystal behavior
10^{-6} m 10^0 s

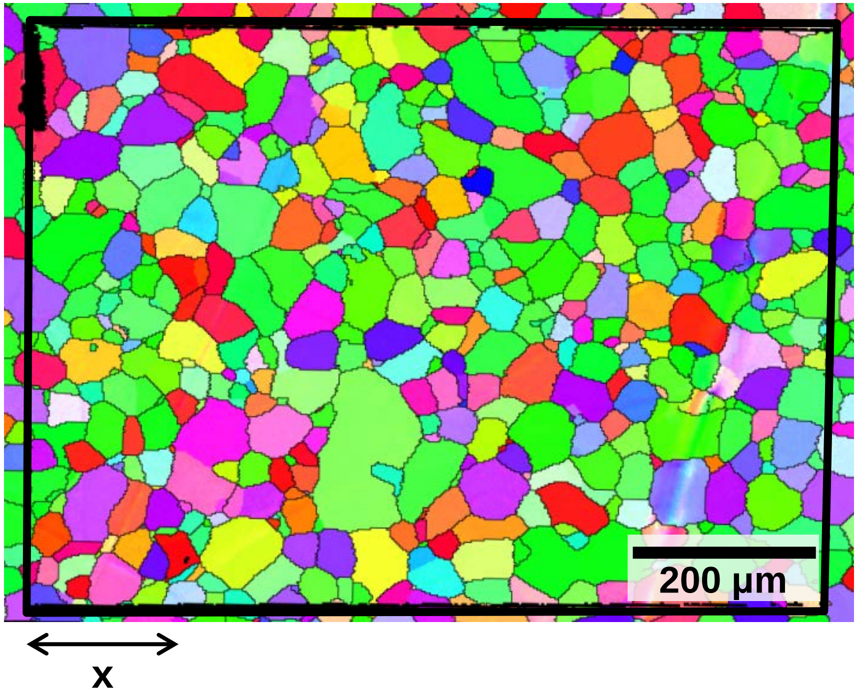
Atomic scale phenomena
10^{-9} m 10^{-9} s

Atoms-up: Develop physics-based models to provide scientific insight

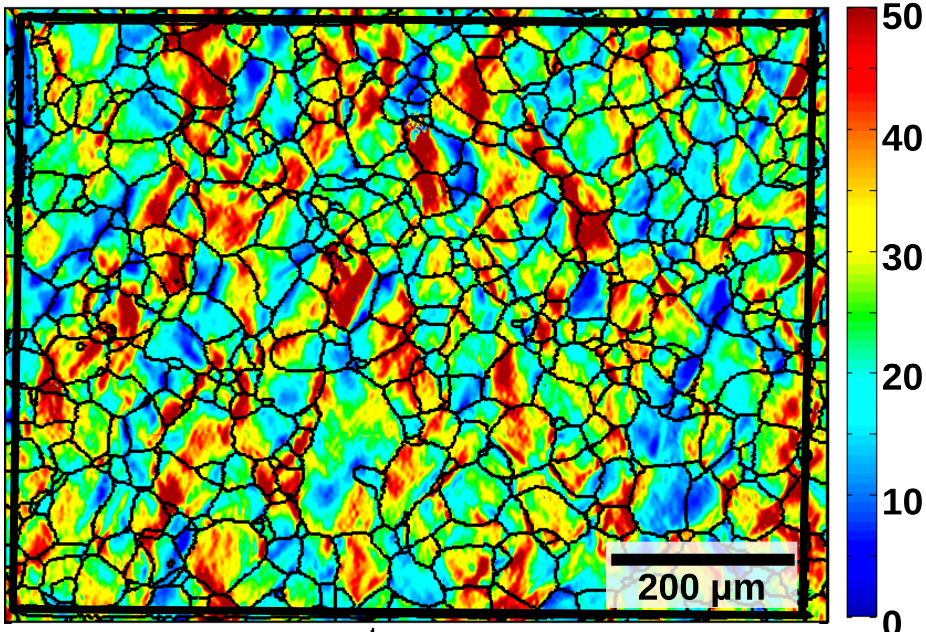
Continuum-down: Augment engineering-scale models to provide customer value

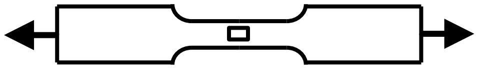
Local microstructure has significant effects on local deformation.

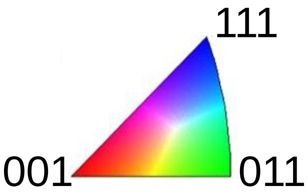
Microstructure (EBSD)

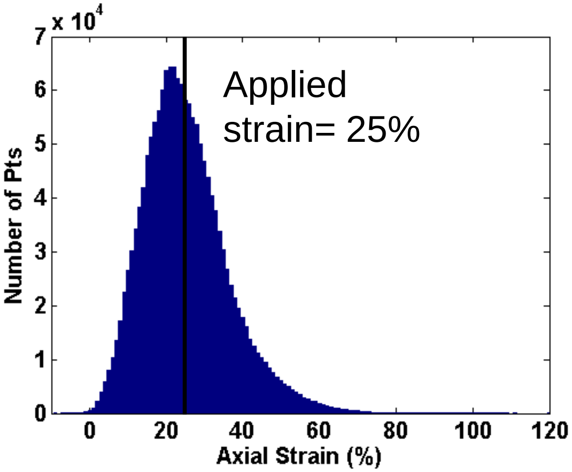


Effective Strain (%) (DIC)









Carroll JD, Clark BG, Buchheit TE, Boyce BL, Weinberger CR, Mat. Sci. Eng. A, v. 581 (2013)

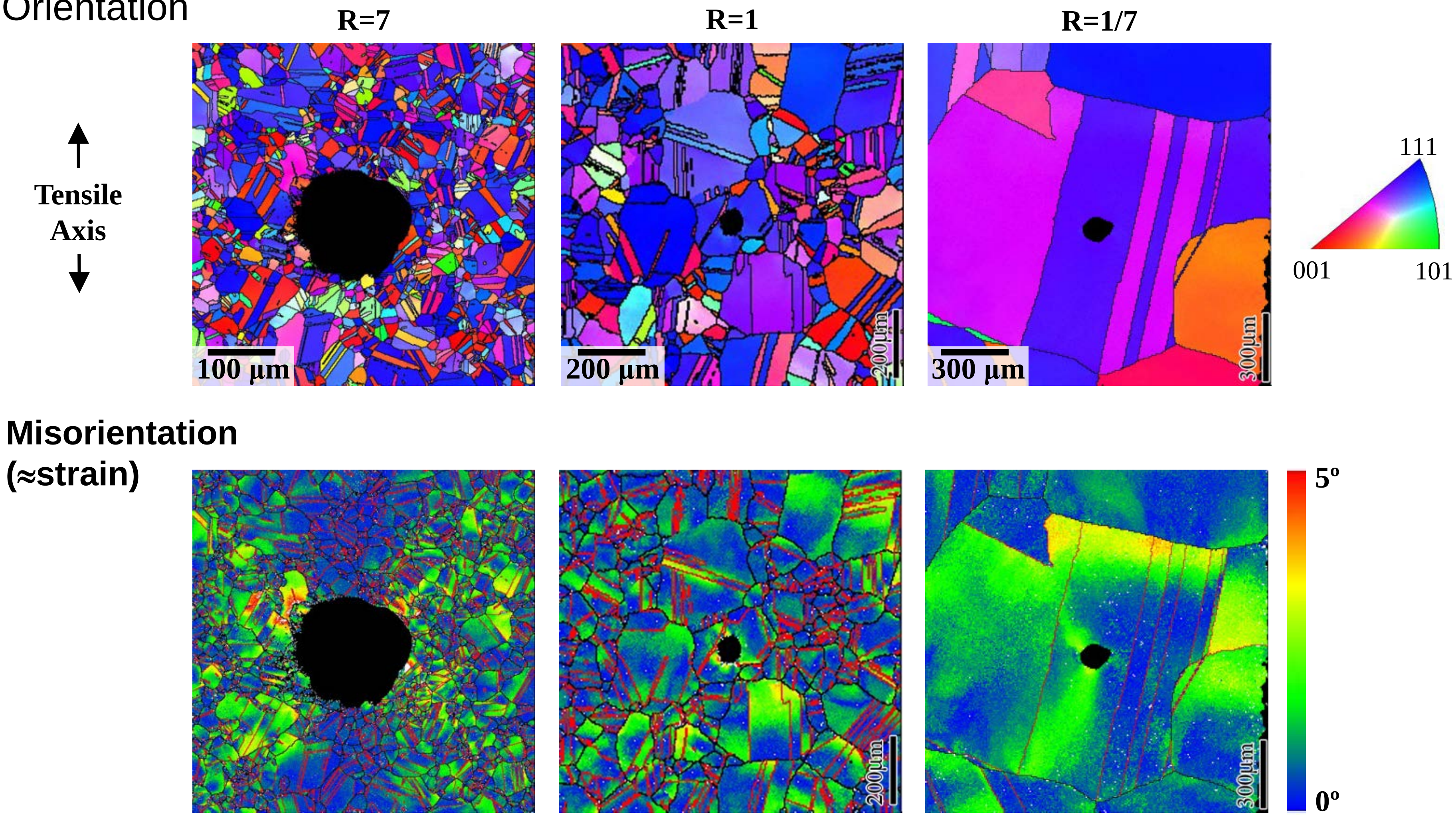
For small features, microstructure can be more important than the stress concentrator.

- **Experimental measurements**

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

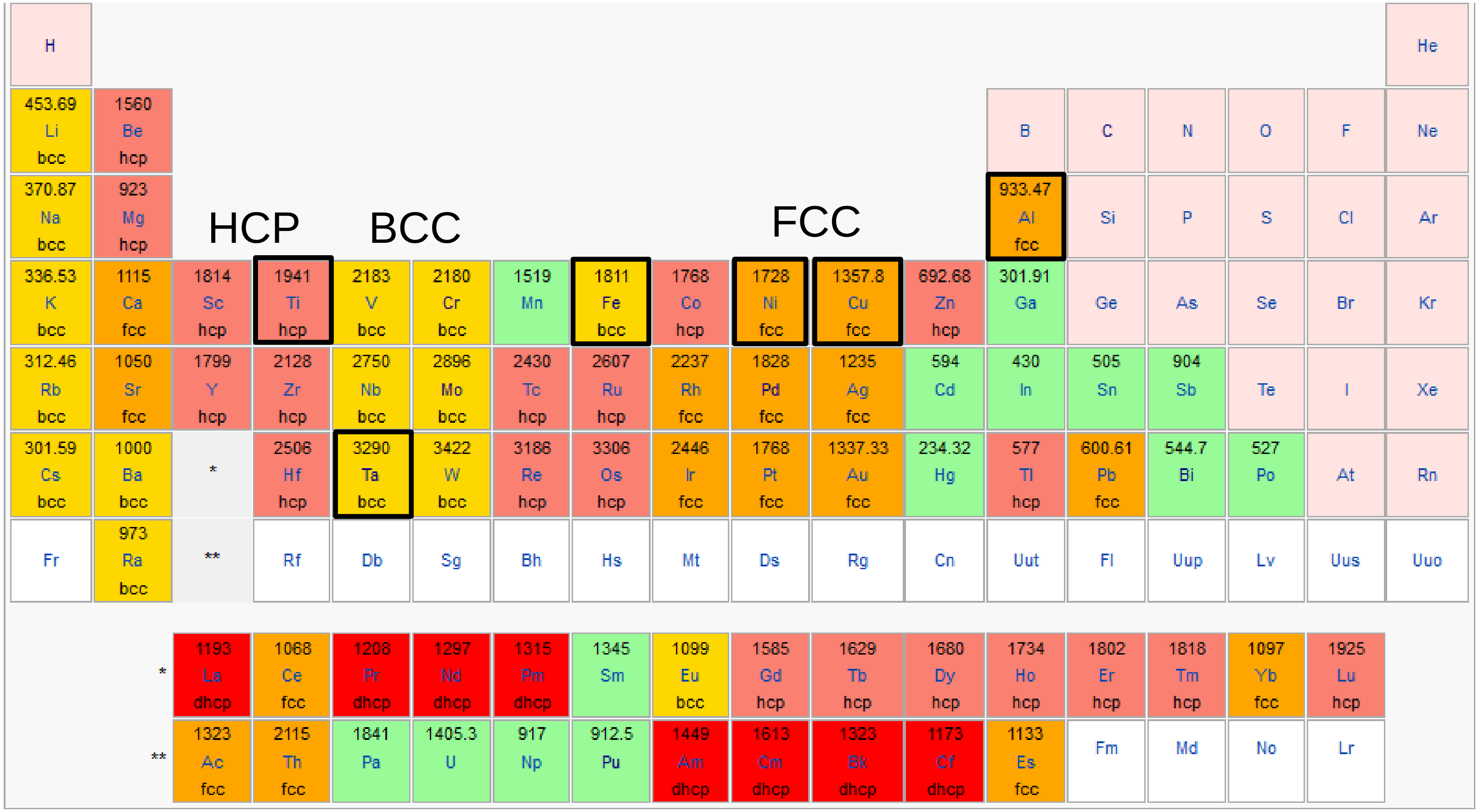
Orientation

Misorientation (≈strain)

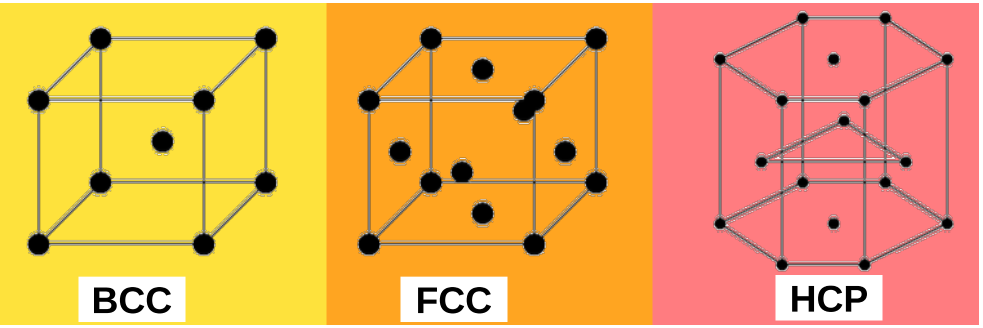


Carroll JD, Brewer LN, Battaile CC, Boyce BL, Emery JM, Int. J. Plasticity, v. 39 (2012).

Several important structural metals are BCC.

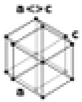


H																	He
453.69 Li bcc	1560 Be hcp											B	C	N	O	F	Ne
370.87 Na bcc	923 Mg hcp											933.47 Al fcc	Si	P	S	Cl	Ar
336.53 K bcc	1115 Ca fcc	1814 Sc hcp	1941 Ti hcp	2183 V bcc	2180 Cr bcc	1519 Mn	1811 Fe bcc	1768 Co hcp	1728 Ni fcc	1357.8 Cu fcc	692.68 Zn hcp	301.91 Ga	Ge	As	Se	Br	Kr
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

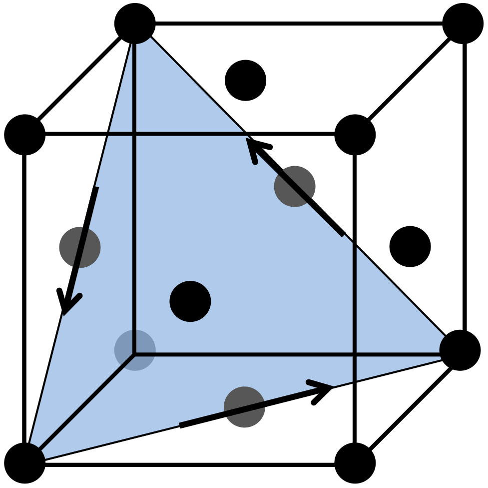
▨ nonmetal

☐ unknown or uncertain

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

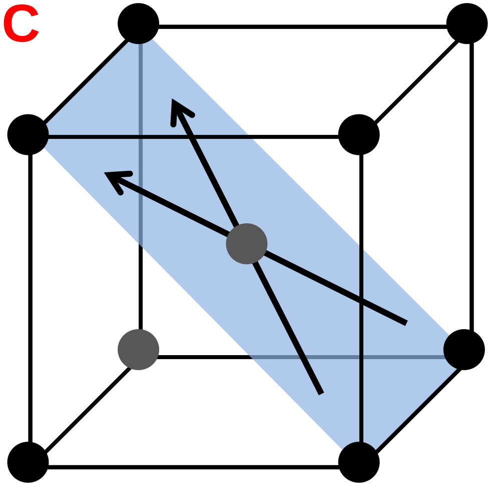
Images showing slip planes and directions in FCC and BCC unit cells.

FCC

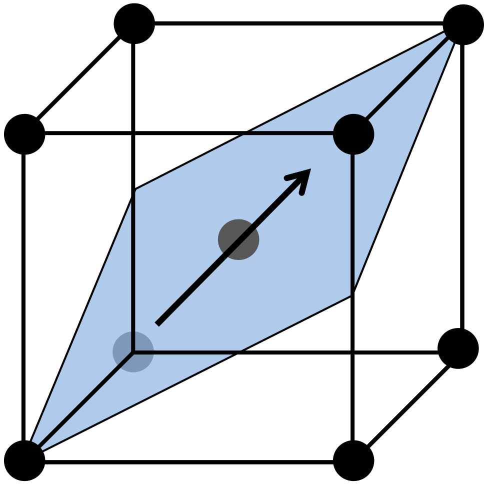


12 Slip systems:
Four {111} Planes each with
three <110> Slip directions

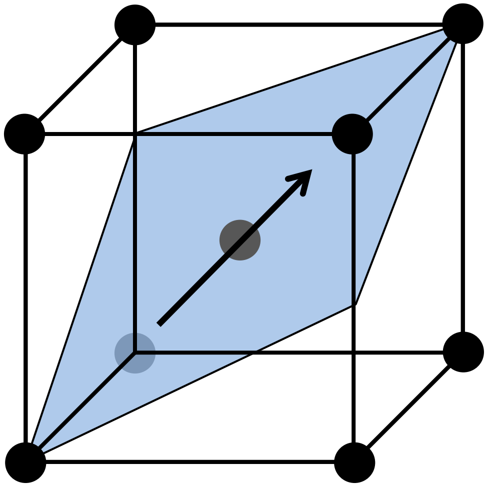
BCC



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

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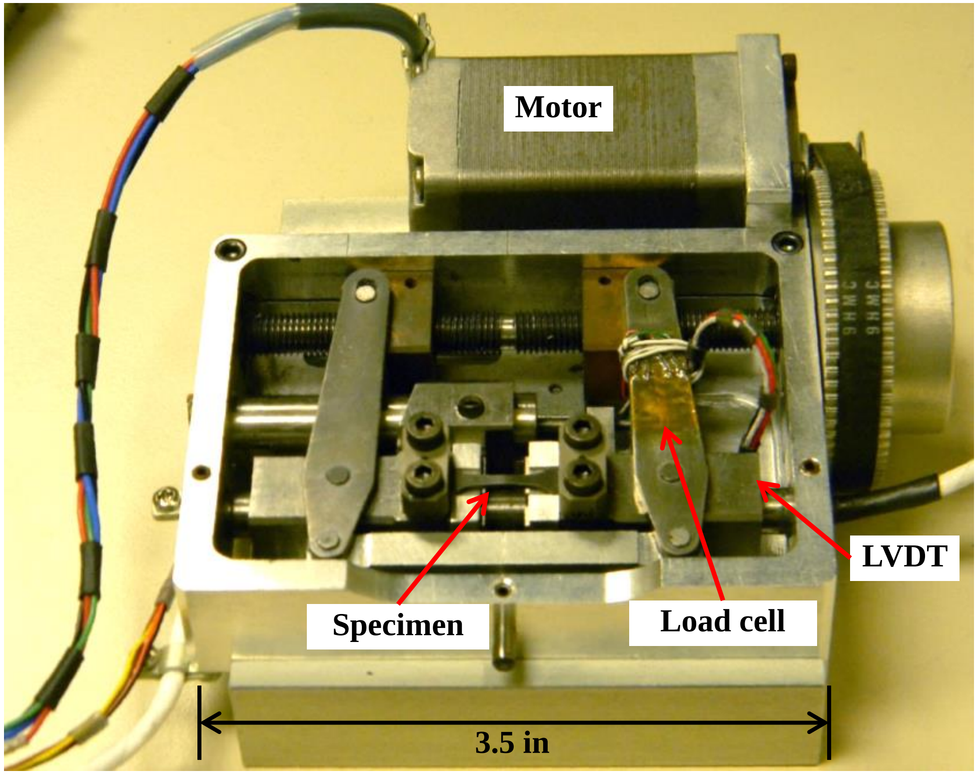
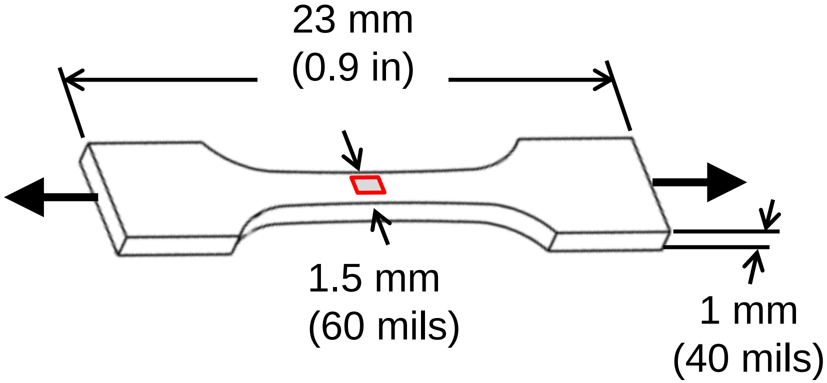
An in situ load frame developed at Sandia allows loading inside the SEM.

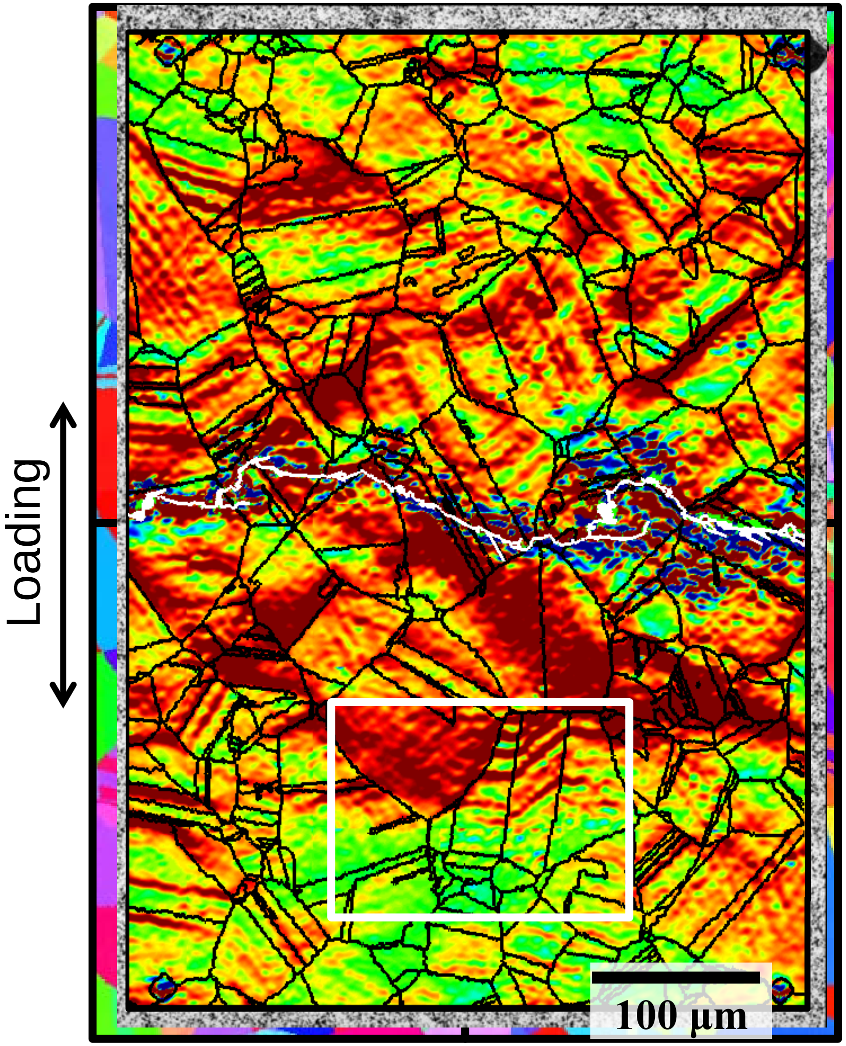


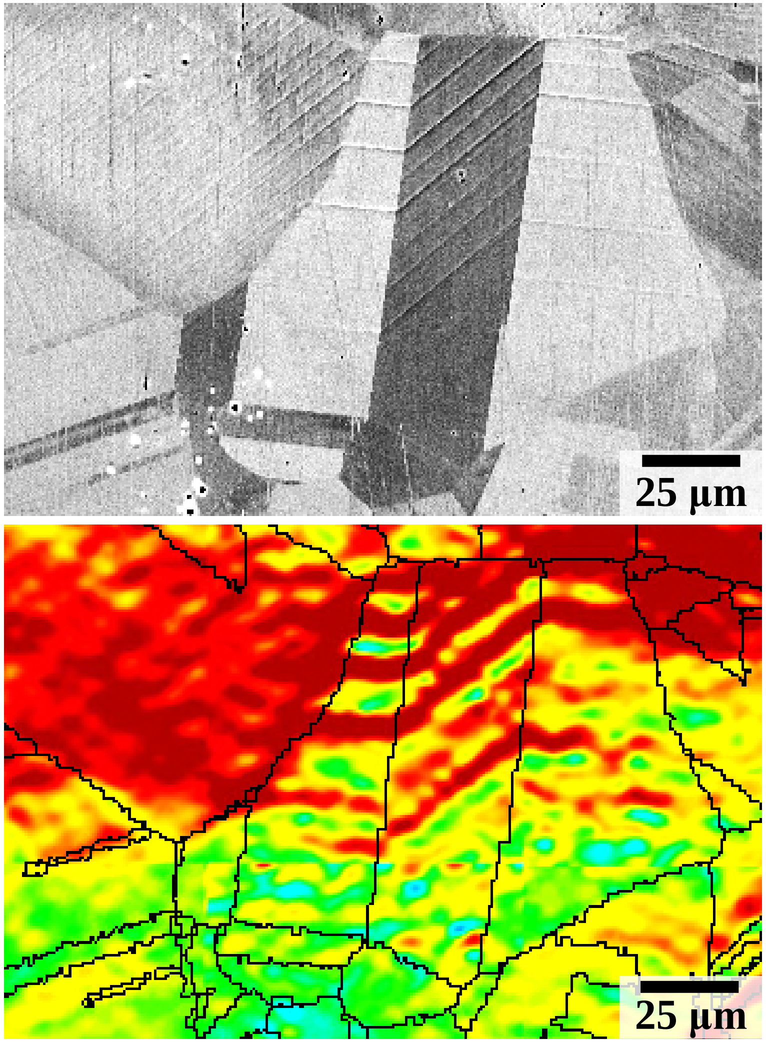
- **Can make DIC and EBSD measurements at load.**



Tapered gage section is narrower at center.

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

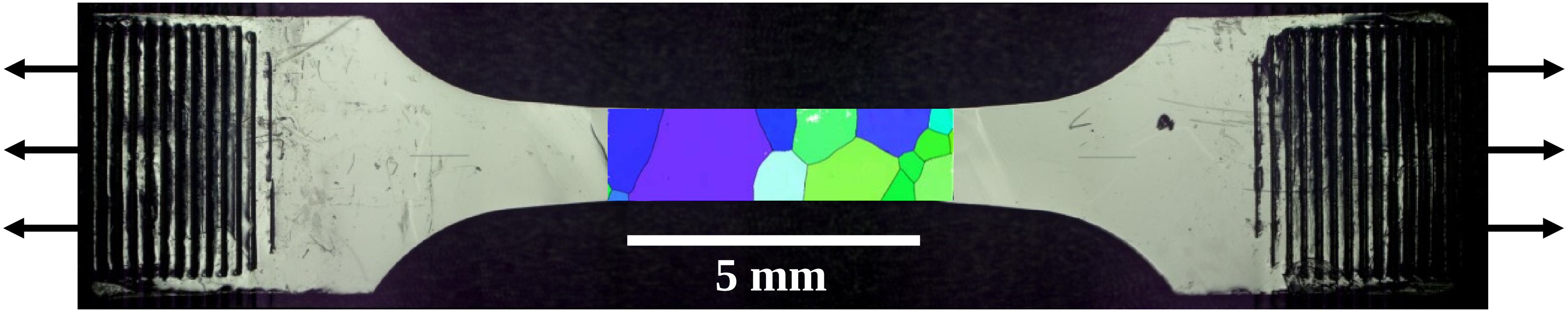




- Carroll JD, Abuzaid W, Lambros J, Sehitoglu H, *Int. J. Fatigue*, v. 57 (2013).
- Carroll JD, Abuzaid W, Lambros J, Sehitoglu H, *Int J. Fracture*, v. 180 (2012).
- Carroll JD, Abuzaid W, Lambros J, Sehitoglu H, *Rev. Sci Inst.,* v. 81 (2010).

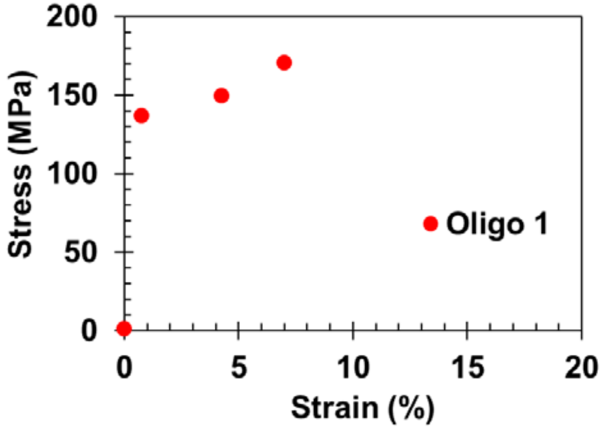
Oligocrystals

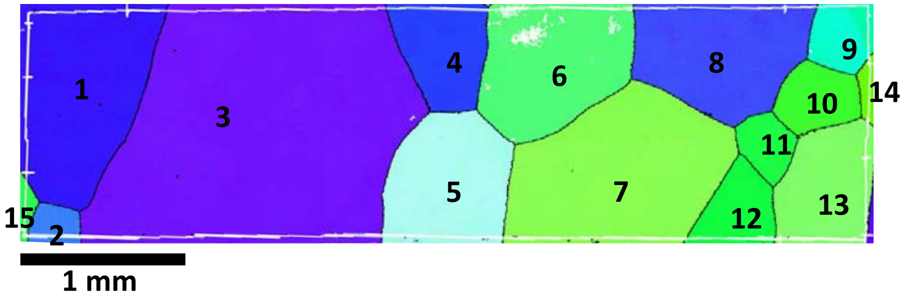
Specimens where deformation is controlled by a few grains (3–20).

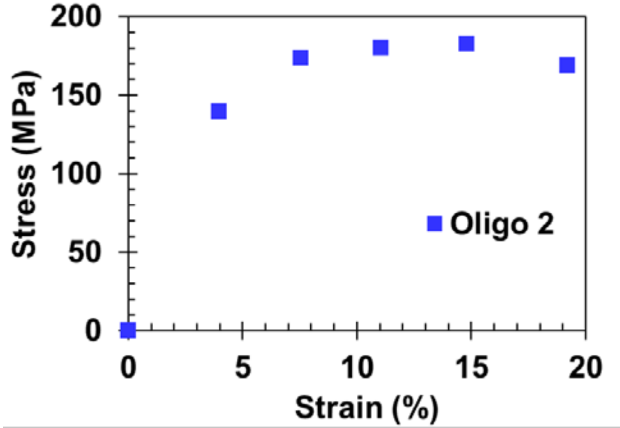


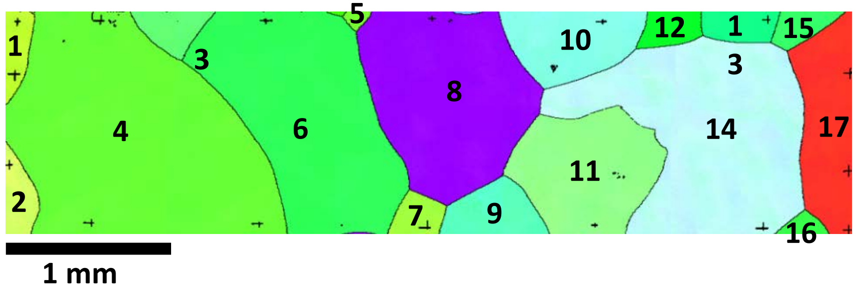
- **Ta oligocrystals were made by annealing.**
- **Mostly columnar, 2D grain structure.**

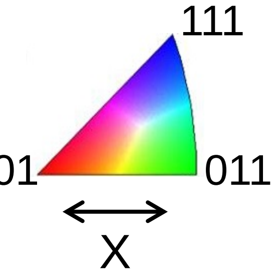
Loaded three oligocrystal specimens

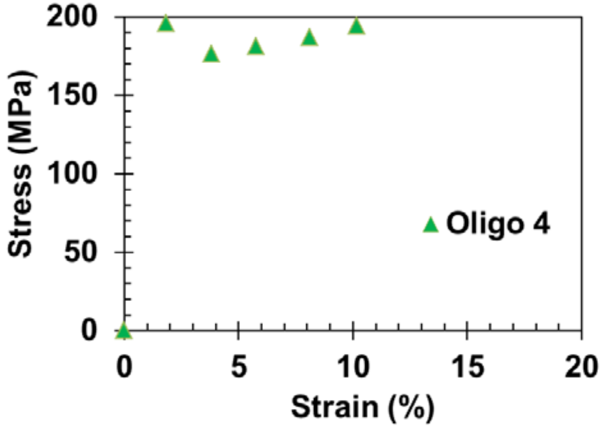


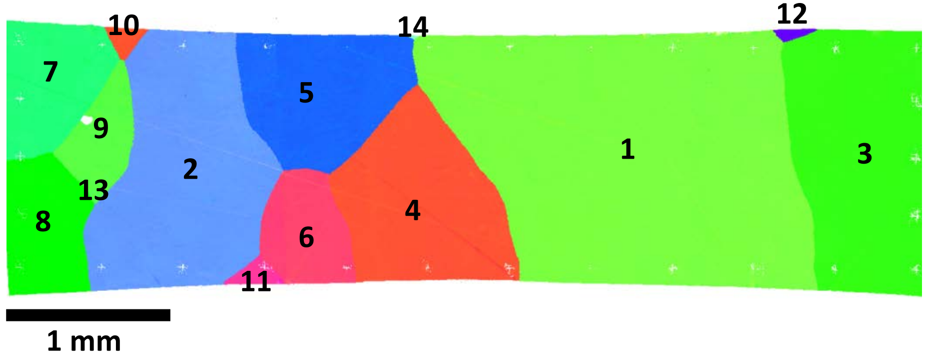






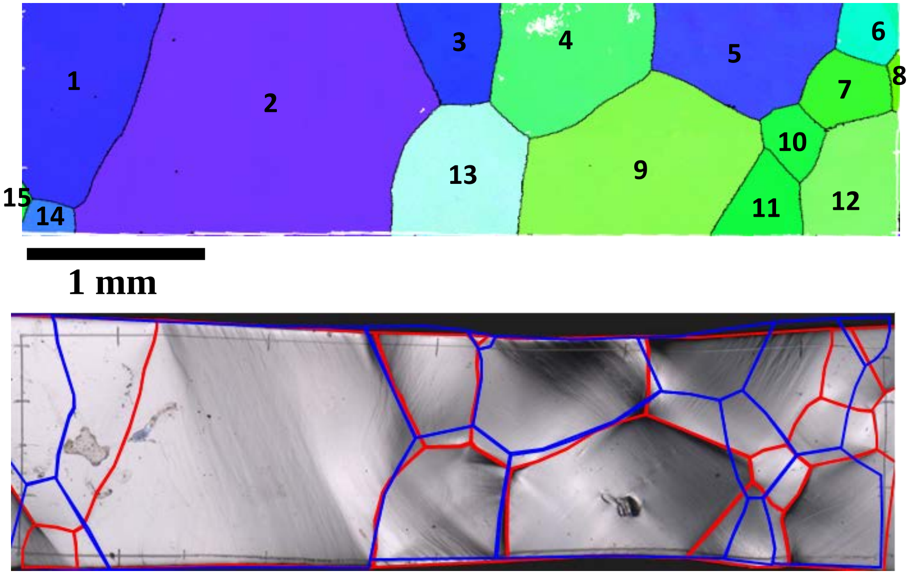




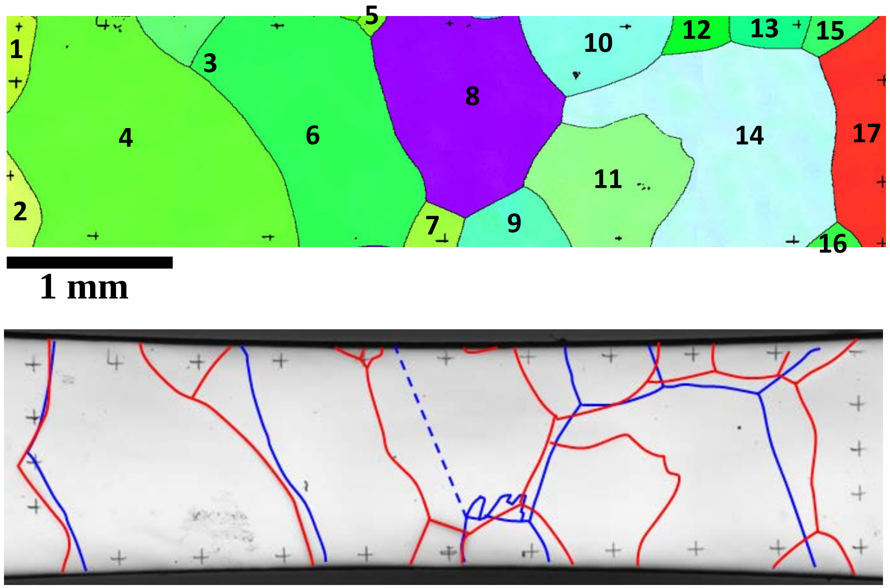


Grain structure in specimens is pseudo-2D. Most grains are nearly columnar.

Oligo 1



Oligo 2



🟥 Grain boundary (Front) 🟦 Grain boundary (Back)

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Crystal Plasticity Model Equations

- 24 {110}<111> slip systems
- **Slip rate:** $\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \left(\frac{\tau^{\alpha}}{g^{\alpha}} \right)^{1/m}$ (Hutchinson, 1976)
- **Slip resistance:** $g^{\alpha} = \min\left(\tau_{EI}^{*\alpha}, \tau_{LT}^{*\alpha} \right) + \tau_{obs}^{\alpha}$

  Obstacle stress

  Lattice friction
- **Obstacle stress:** $\tau_{obs}^{\alpha} = A \mu b \sqrt{\sum_{\beta=1}^{NS} \rho^{\beta}}$ (Taylor, 1934)

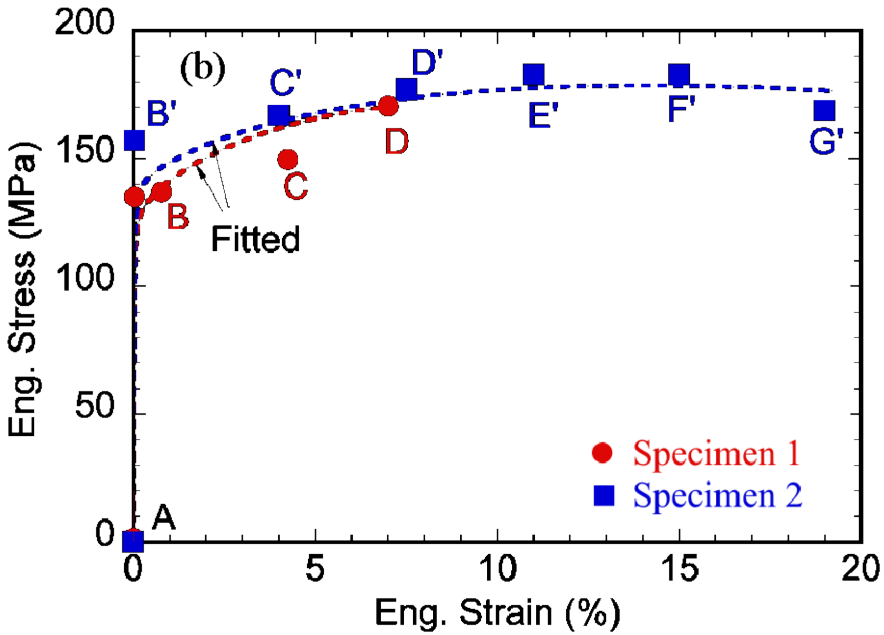
$$\dot{\rho}^{\alpha} = \left(\kappa_1 \sqrt{\sum_{\beta=1}^{NS} \rho^{\beta}} - \kappa_2 \rho^{\alpha} \right) \cdot \left| \dot{\gamma}^{\alpha} \right|$$

(Kocks, 1976)

For more model details, see Lim et al. “Temperature and Strain Rate Effects on the Dislocation Plasticity of BCC Transition Metals” in room xx at time xx.

Lim H, Battaile CC, Carroll JD, Boyce BL, Weinberger CR, “A physically based temperature and strain rate dependent crystal plasticity model for BCC metals” (submitted).

Crystal plasticity finite element model.



Slip Rate Obstacle Strength		Lattice Resistance		Elastic Coefficients		Obstacle Strength	
Parameters	Values	Parameters	Values	Parameters	Values	Parameters	Values
m	0.012	τ_0^{LT}	406 MPa	C_{11}	267 GPa	κ_1	$1.4 \times 10^6\ m^{-1}$
$\dot{\gamma}_0$	$0.001\ \mathrm{s}^{-1}$	τ_0^{EI}	320 MPa	C_{12}	161 GPa	κ_2	14
A	0.4	$2H_k$	0.85 eV	C_{44}	82.5 GPa	$\tau^1_{\mathrm{obs},0}$	27 MPa
b	2.87 Å	$\dot{\epsilon}_0$	$2.99{\times}10^6\ \mathrm{s}^{-1}$	μ	70.7 GPa	$\tau^2_{\mathrm{obs},0}$	37 MPa

From literature

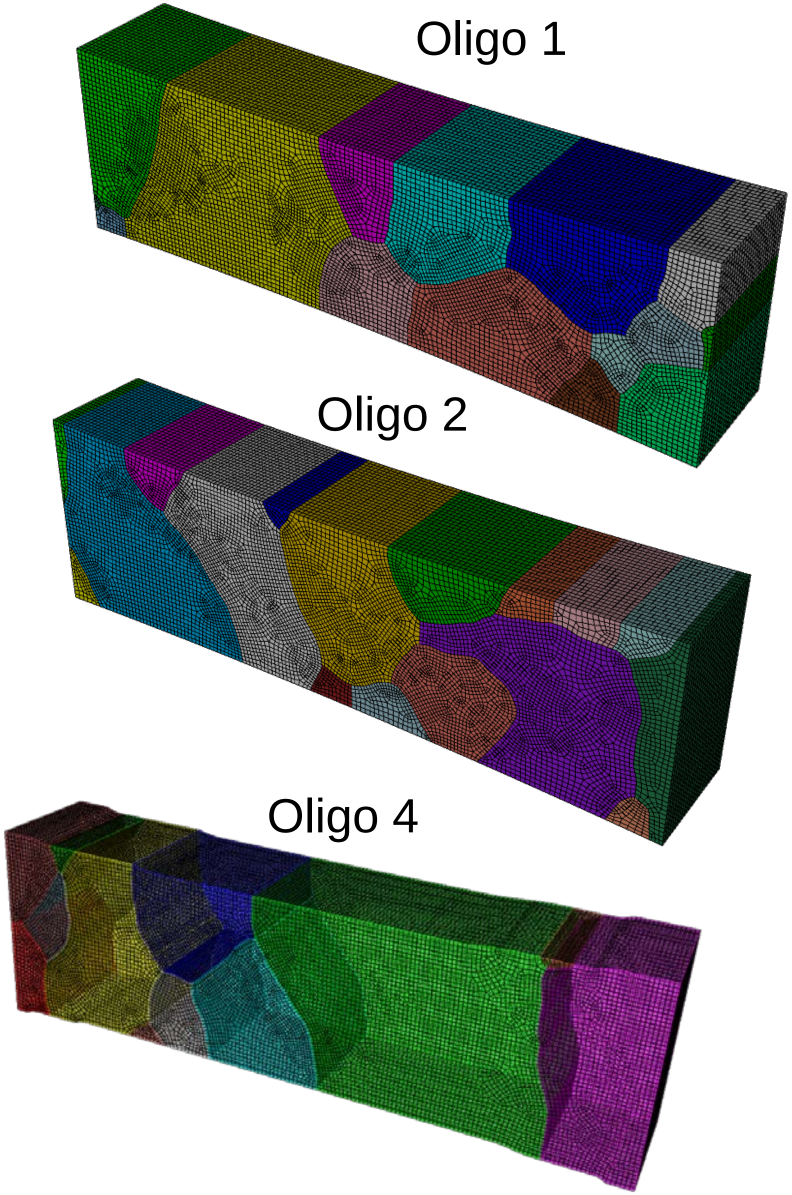
From fits to single crystal experiments

From literature

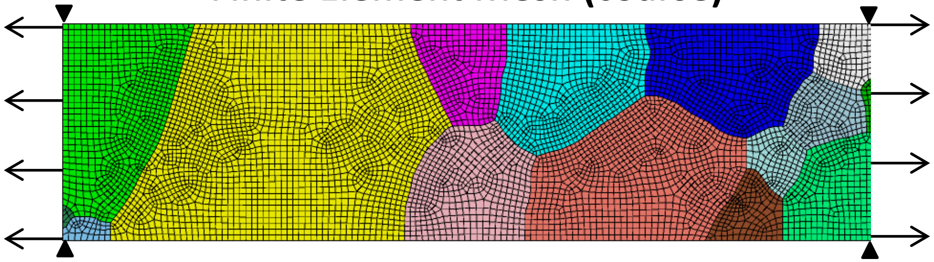
Fitting stress-strain data for each specimen

Finite element meshes for each specimen cover most of the gage section with pseudo-3d mesh.

- FEM code (JAS-3D) developed at Sandia.
- Dislocation density based hardening.
- Hexahedral elements (8 nodes).
- One orientation per element.
- 50 elements through specimen thickness.
  - ~1.5 million total elements
  - ~30,000 surface elements



Finite Element Mesh (coarse)



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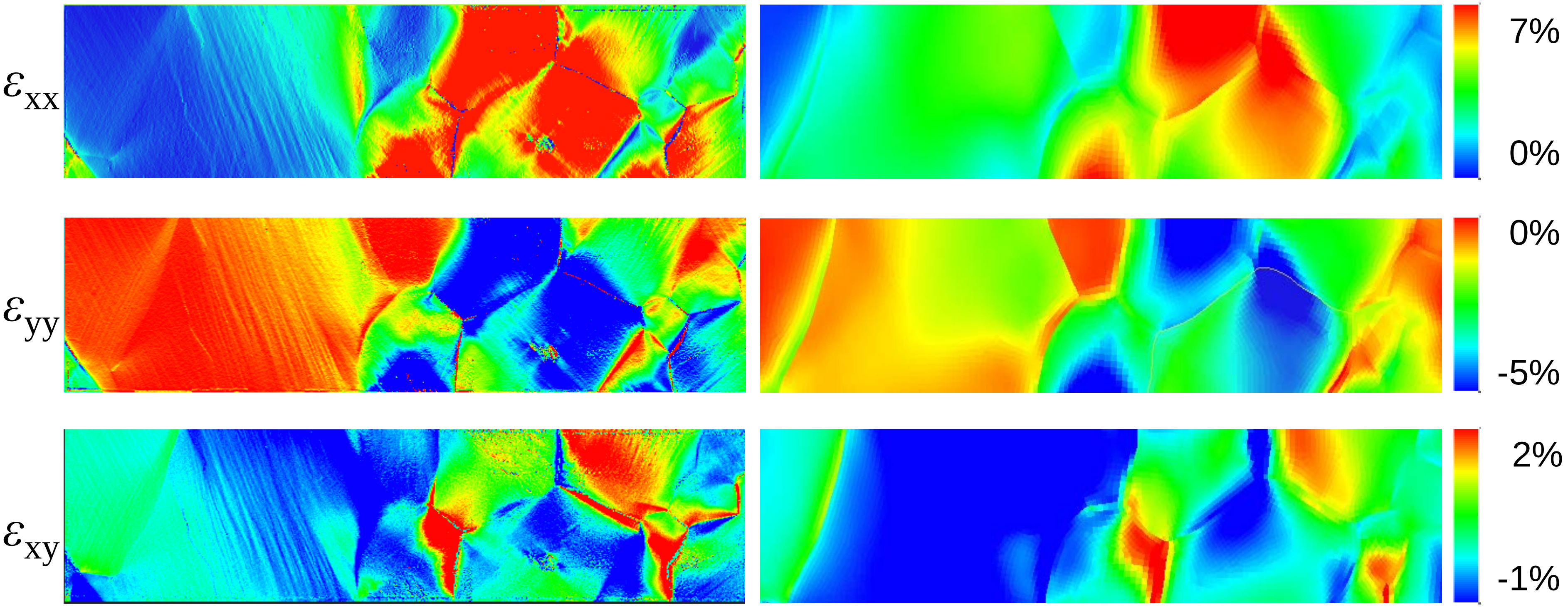
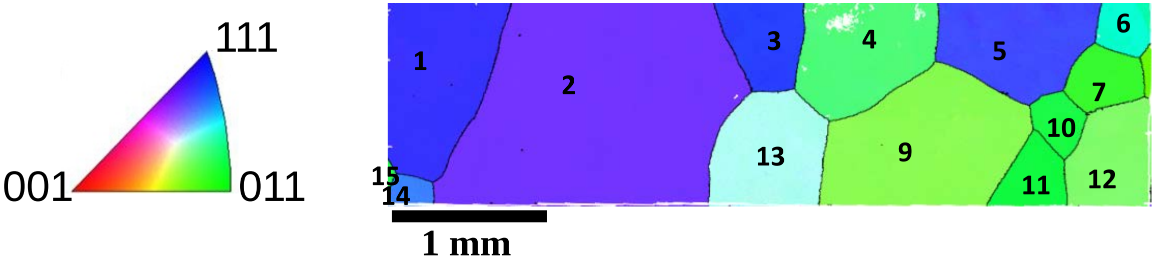
Oligo 1 Strain fields agree in most places.



Experimental Strains (DIC)

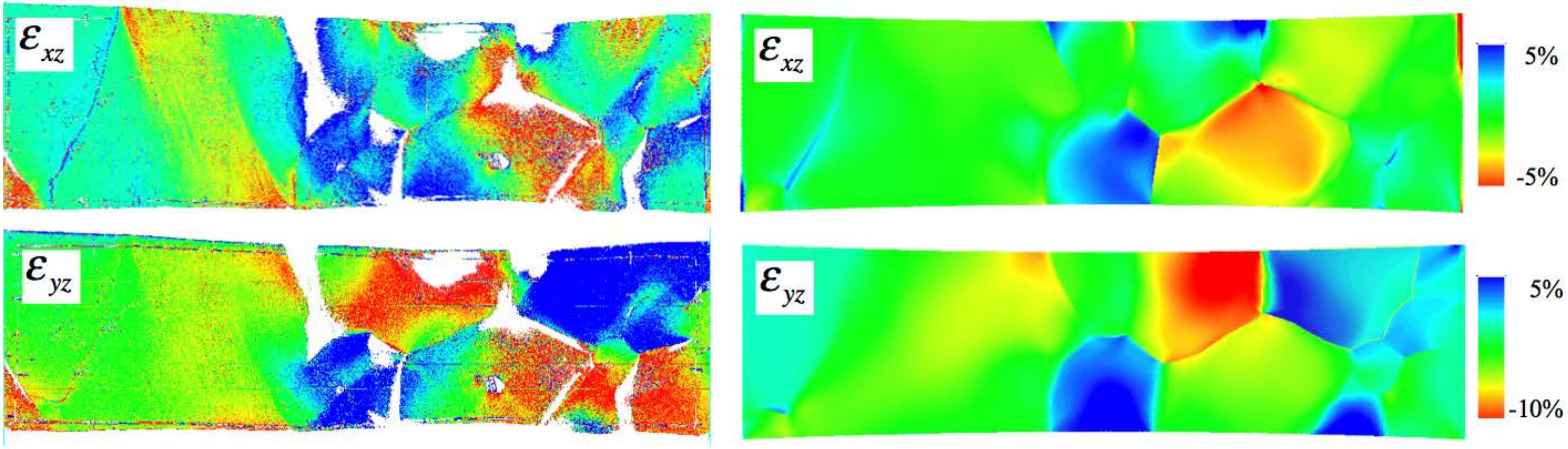
Model Strains (CP-FEM)

Model only considers slip on {110} planes.



Out-of-plane strain fields agree within most grains.

Specimen 1 (6.8% applied strain)



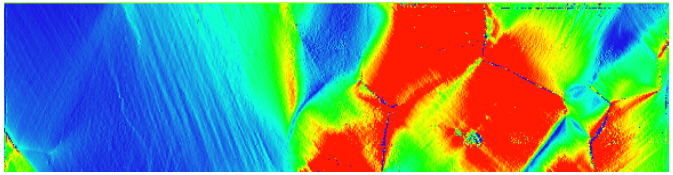
Profilometry Measurements

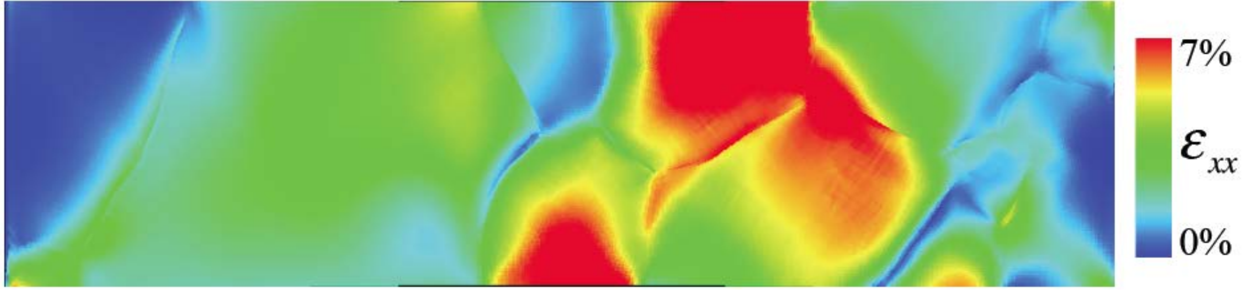
CP-FEM Predictions

- **Many grain boundaries have large strains not captured by model.**

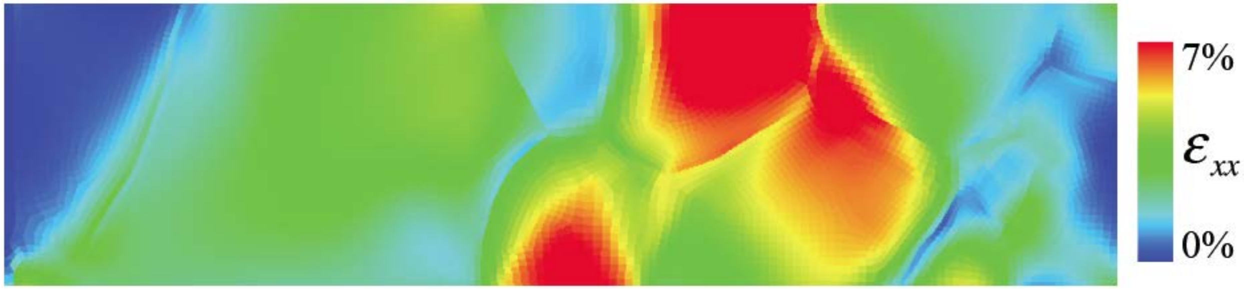
Mesh refinement has a slight affect on strain field. Including a pseudo-3d mesh has a significant effect.

Experiment

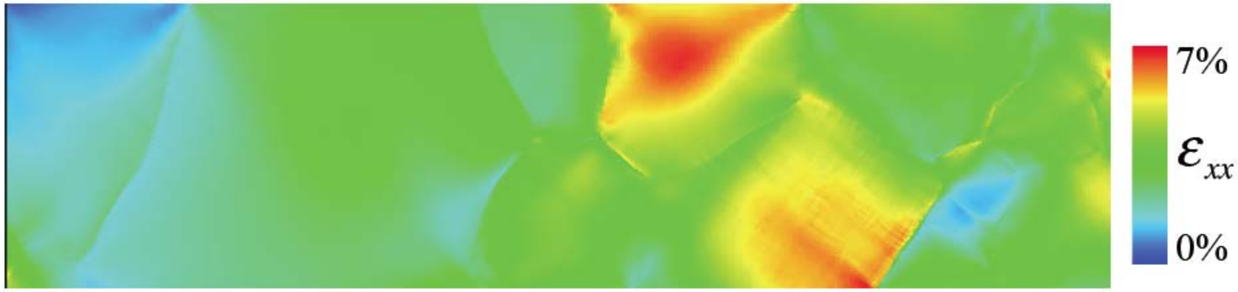




Medium Mesh
(1,664,150 elements)

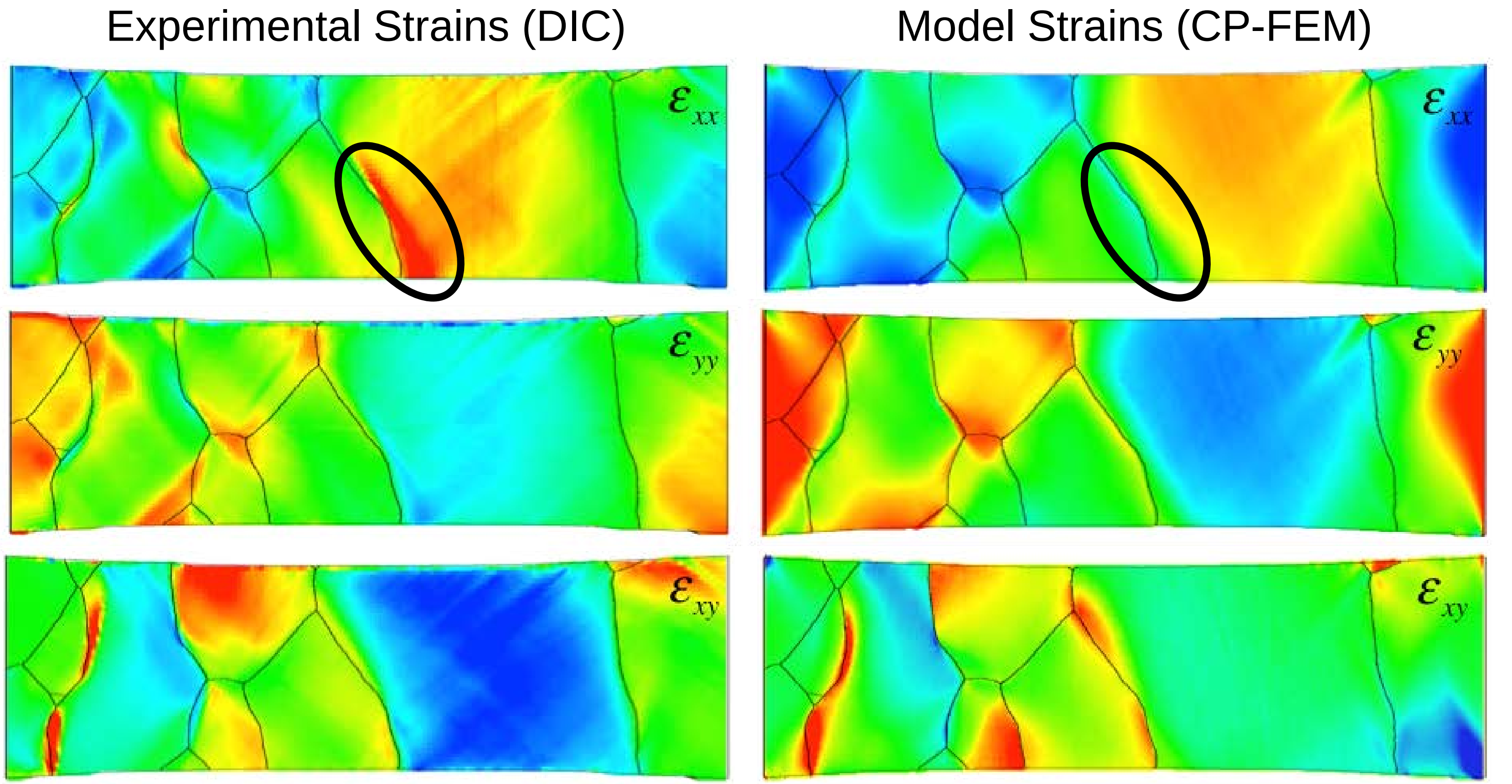


Coarse Mesh
(207,200 elements.)



Medium Mesh
1 element through thickness

Oligo 4 Strain fields agree in most places.

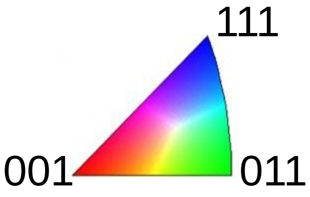


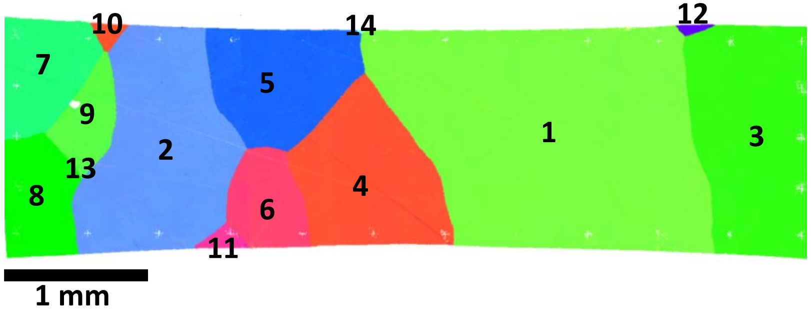
Experimental Strains (DIC)

Model Strains (CP-FEM)

(10% global strain).

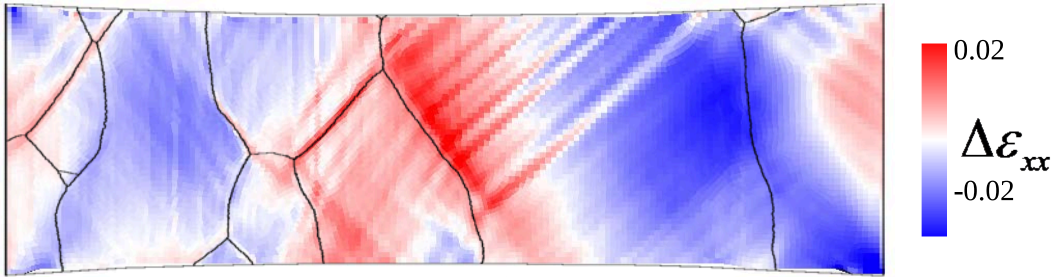
Model only considers slip on {110} planes.





Quantitative, pointwise comparison of measured and predicted strains.

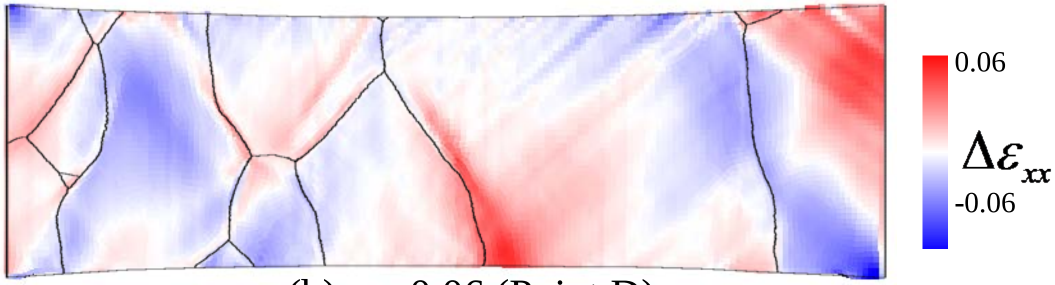
$$\Delta\varepsilon = \varepsilon_{measured} - \varepsilon_{predicted}$$



$$\Delta\varepsilon_{xx}(\max) = 0.024$$

$$\Delta\varepsilon_{xx}(\min) = -0.038$$

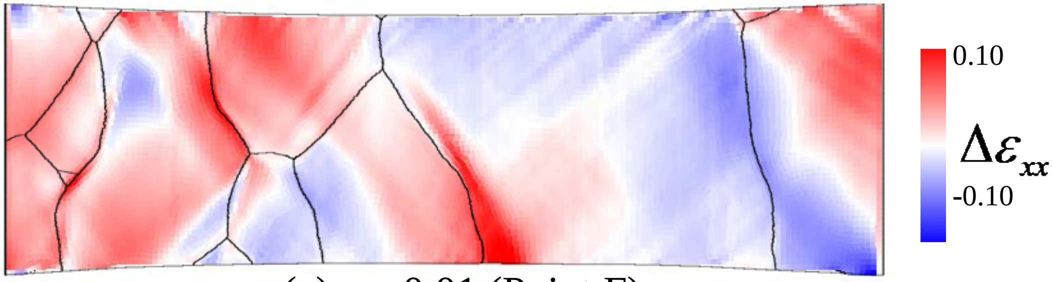
(a) $\varepsilon = 0.02$ (Point B)



$$\Delta\varepsilon_{xx}(\max) = 0.052$$

$$\Delta\varepsilon_{xx}(\min) = -0.074$$

(b) $\varepsilon = 0.06$ (Point D)

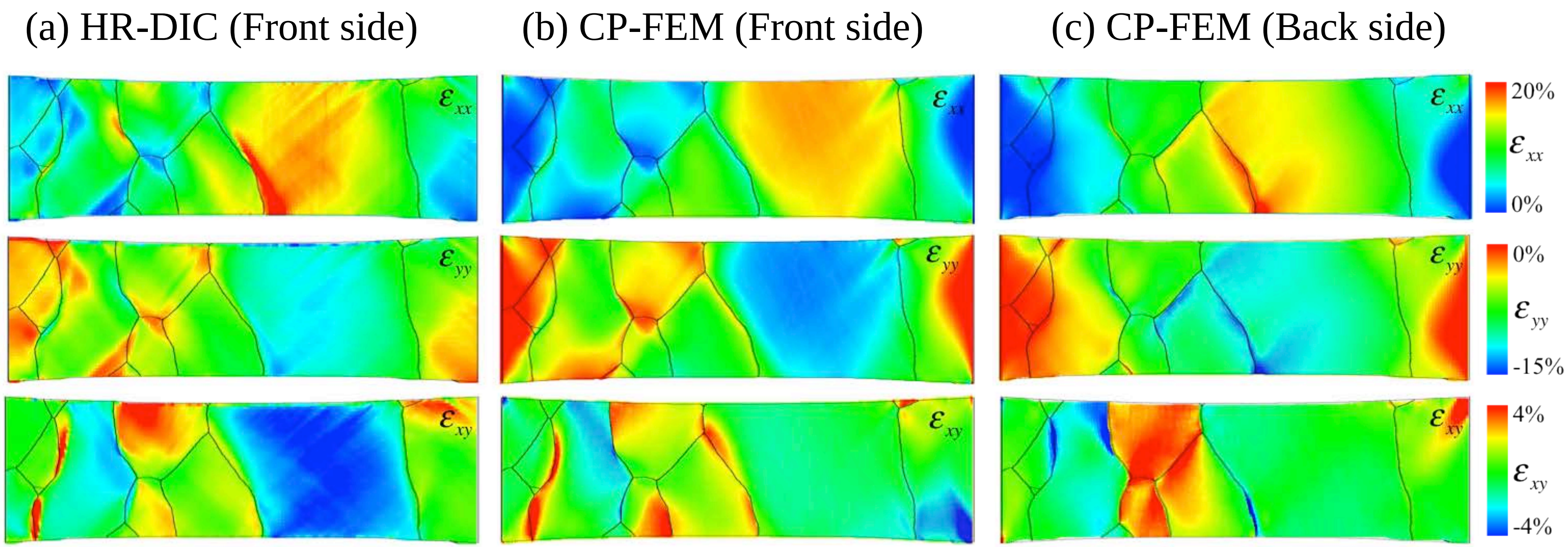


$$\Delta\varepsilon_{xx}(\max) = 0.153$$

$$\Delta\varepsilon_{xx}(\min) = -0.106$$

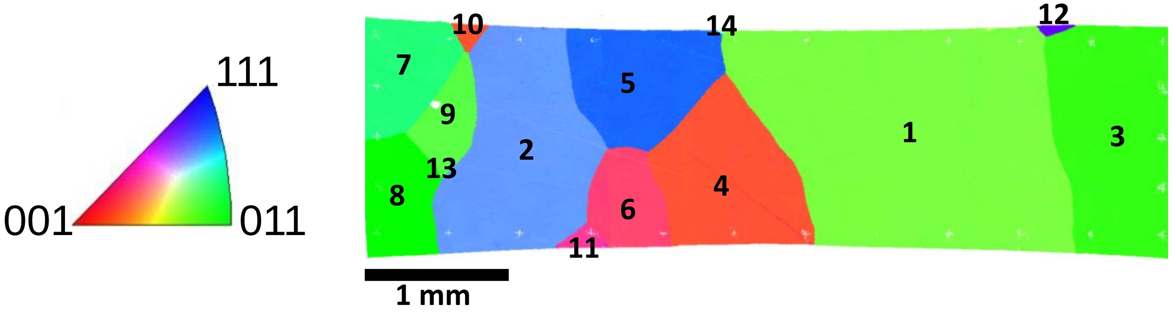
(c) $\varepsilon = 0.01$ (Point F)

Oligo 4 Disagreement between measured and predicted strain fields is explained by 3d effects.



(10% global strain).

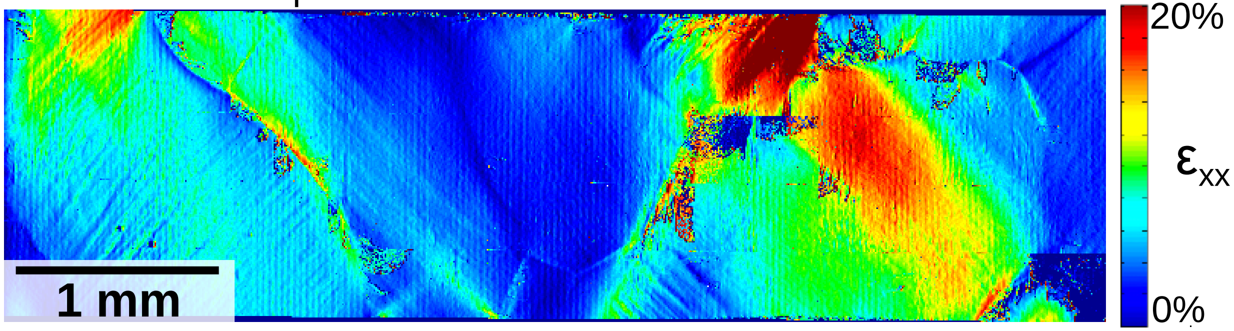
Model only considers slip on {110} planes.



Oligo 2: Modeling with {110} and {112} slip planes give different results, but with roughly the same accuracy.

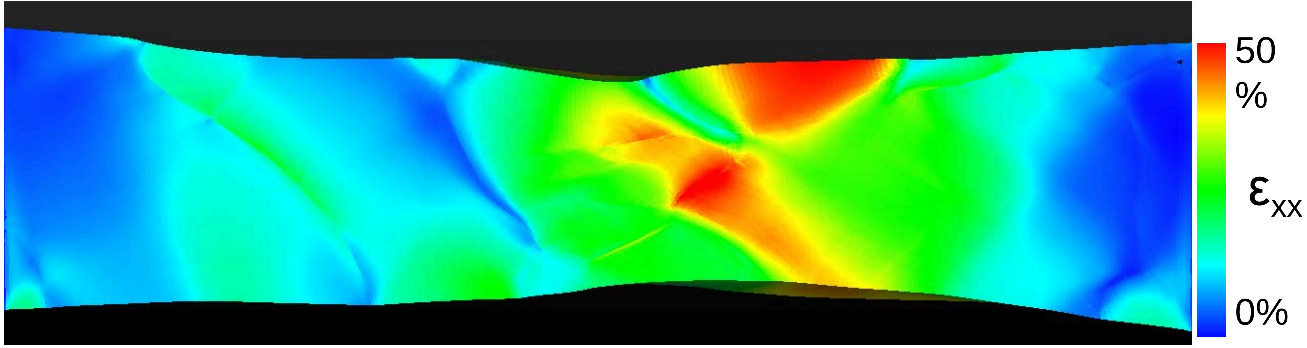
Experiment DIC ~10% strain

15.1 million DIC points

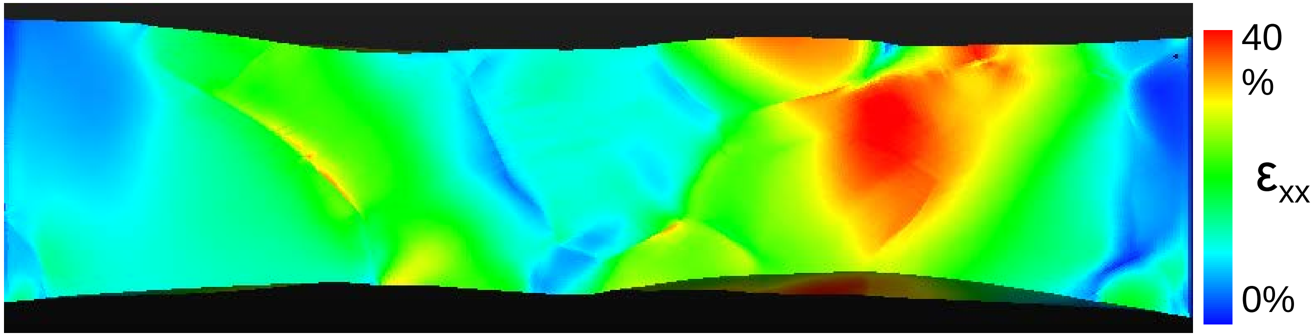


Model {110} slip 19% strain

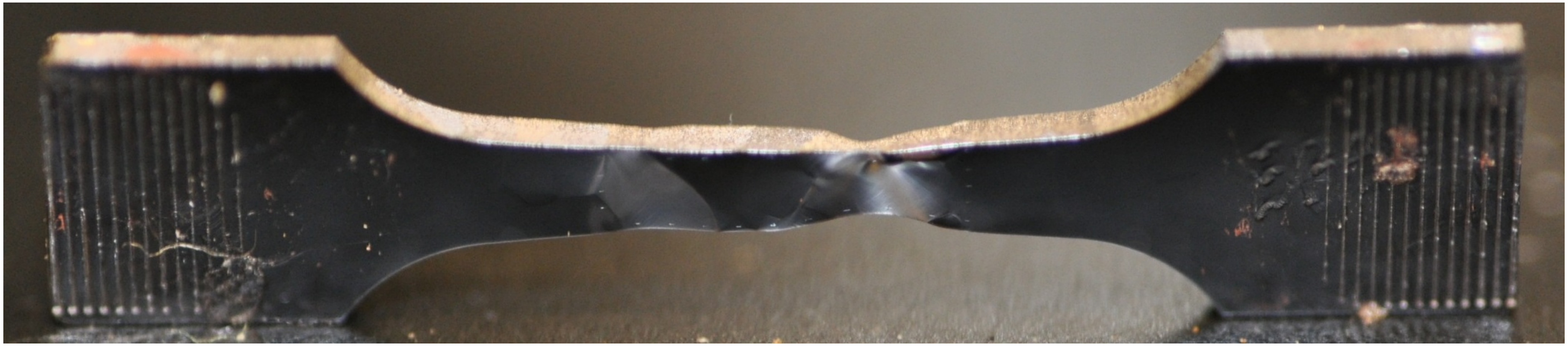
32,800 Surface Elements

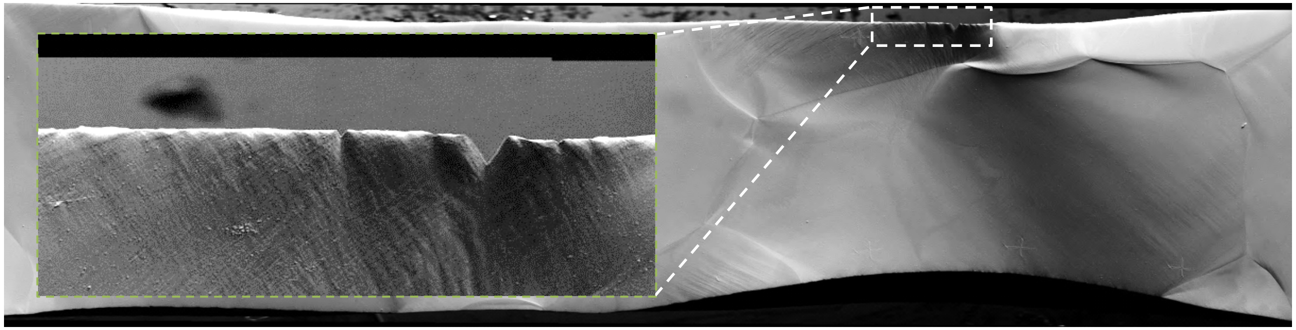


Model {112} slip 19% strain

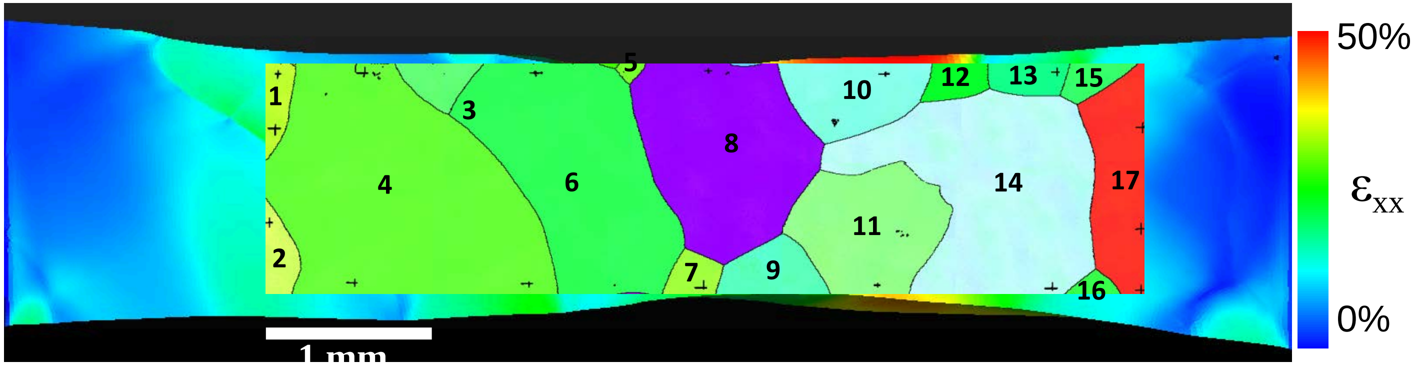


Model predicts high strain at location of observed crack initiation.

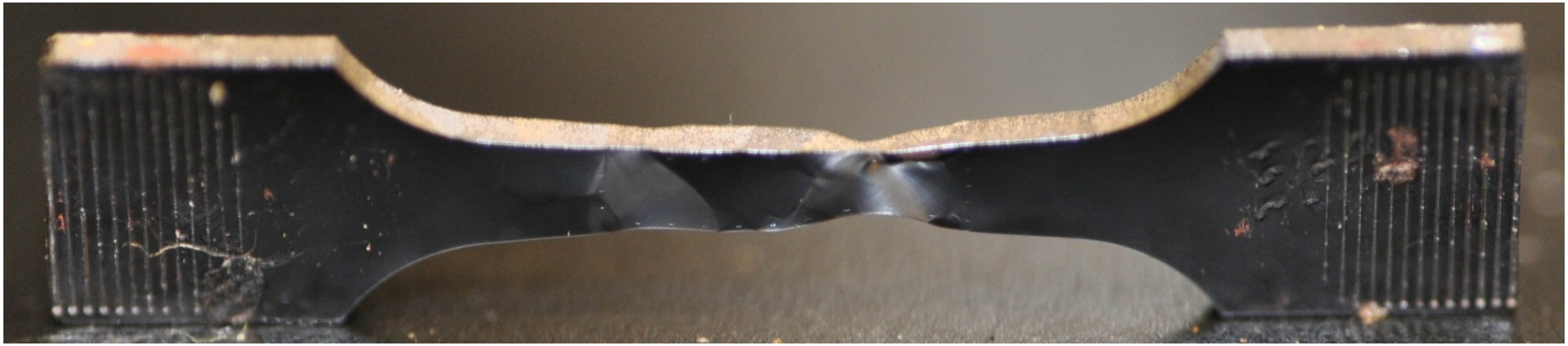


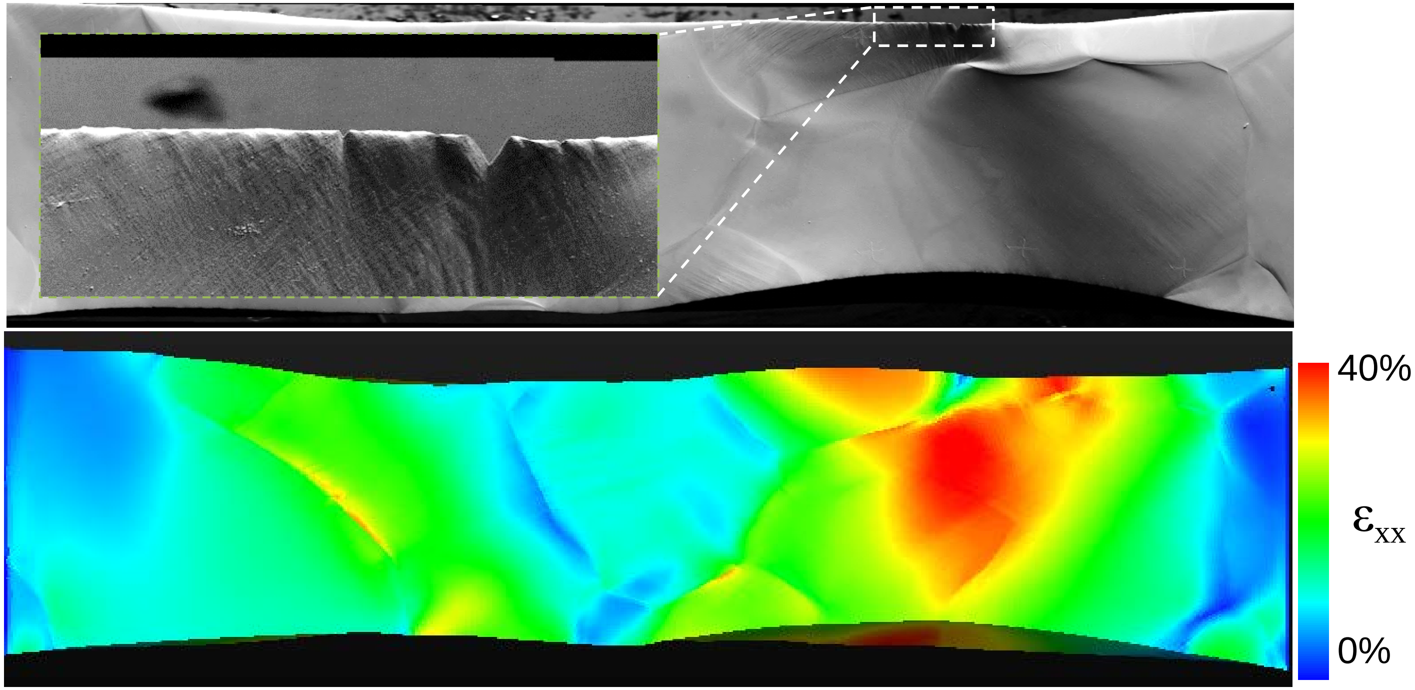


{110} slip

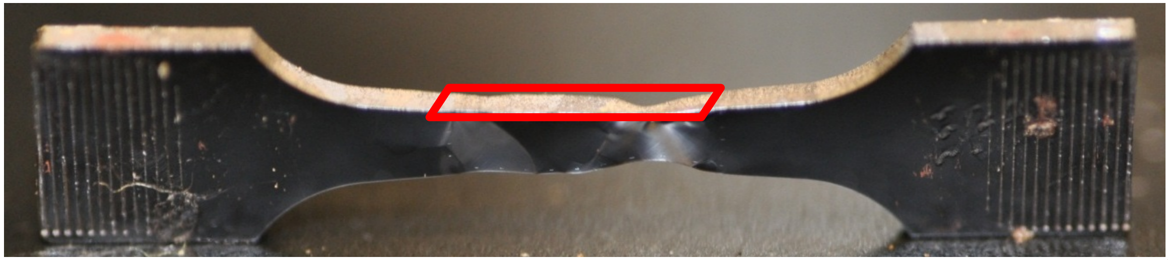


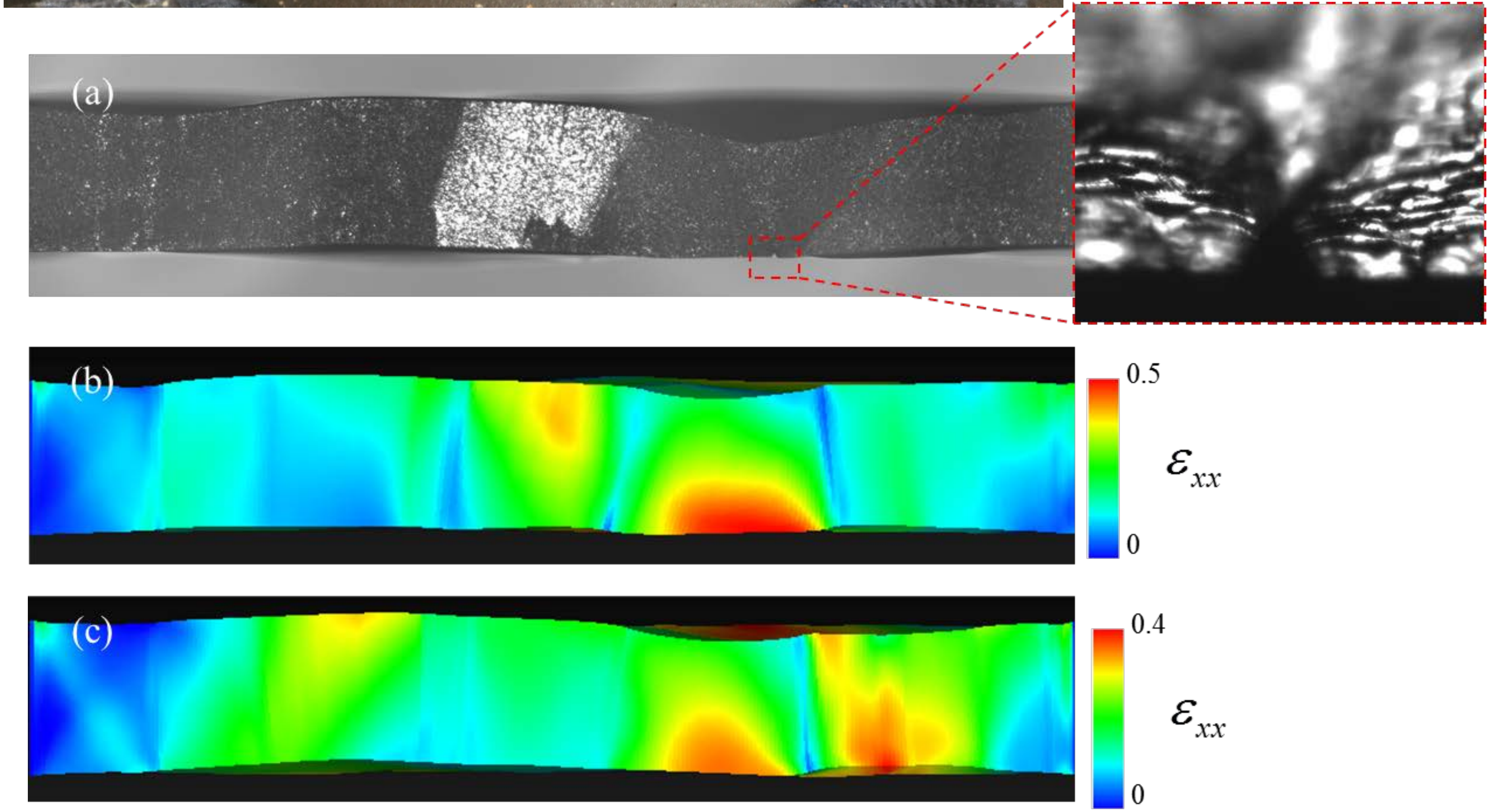
Model predicts high strain at location of observed crack initiation.





In 3D, model predicts failure initiation on front surface.





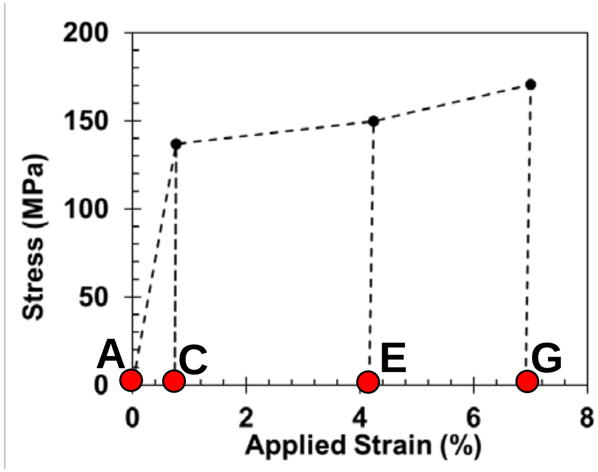
{110} slip

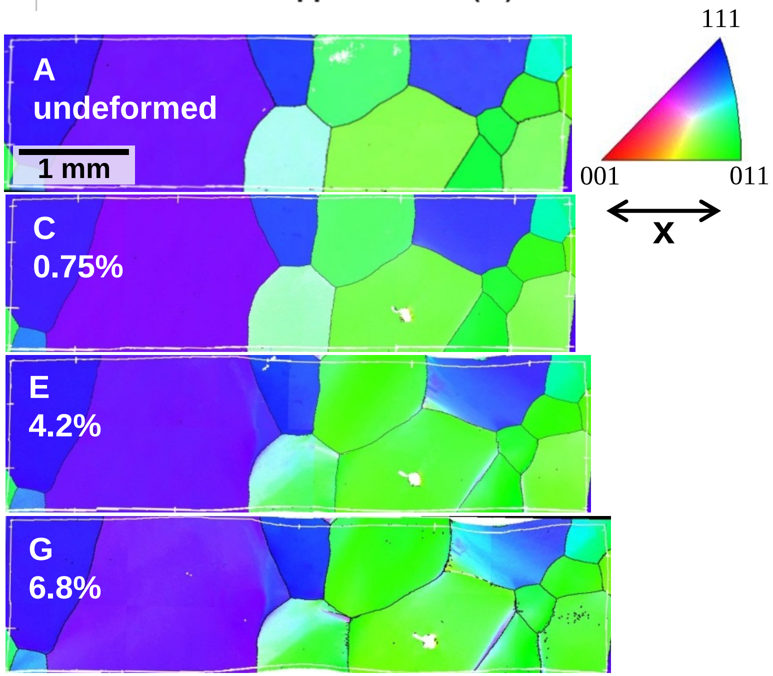
{112} slip

Outline

1. Background
2. Experimental setup
3. Model details
4. Model validation- strain fields
5. Model validation- crystal rotations
6. Conclusions

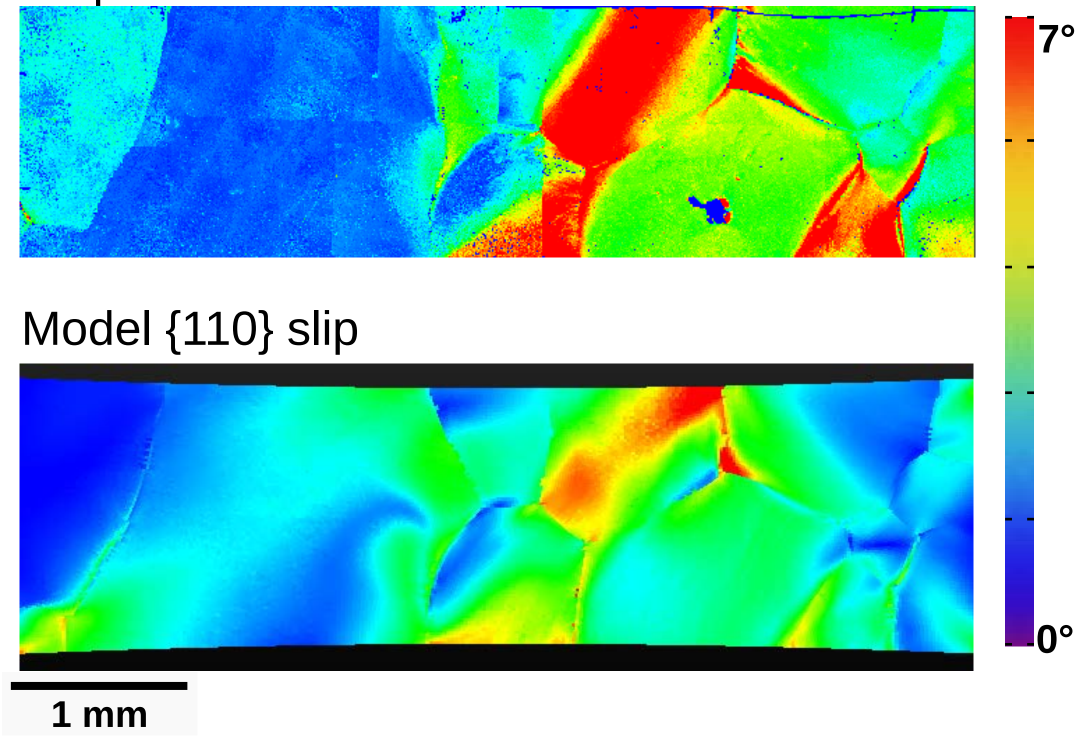
Oligo 1 grain rotation: model and experiment show good qualitative agreement.





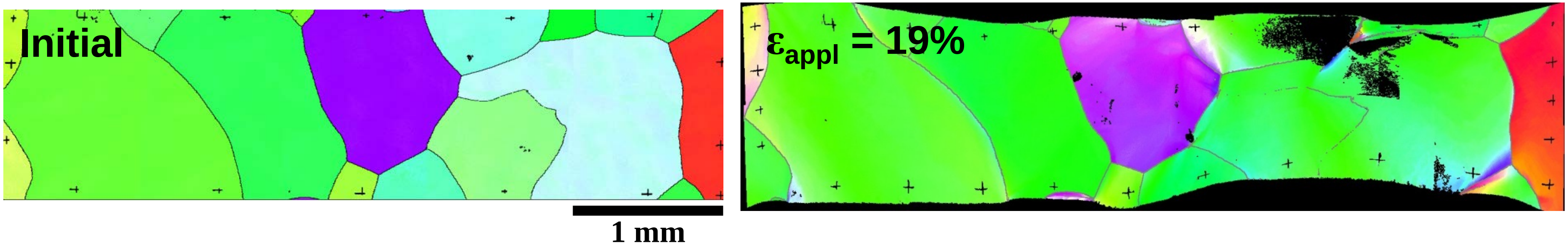
Grain rotation at 4.2% applied strain

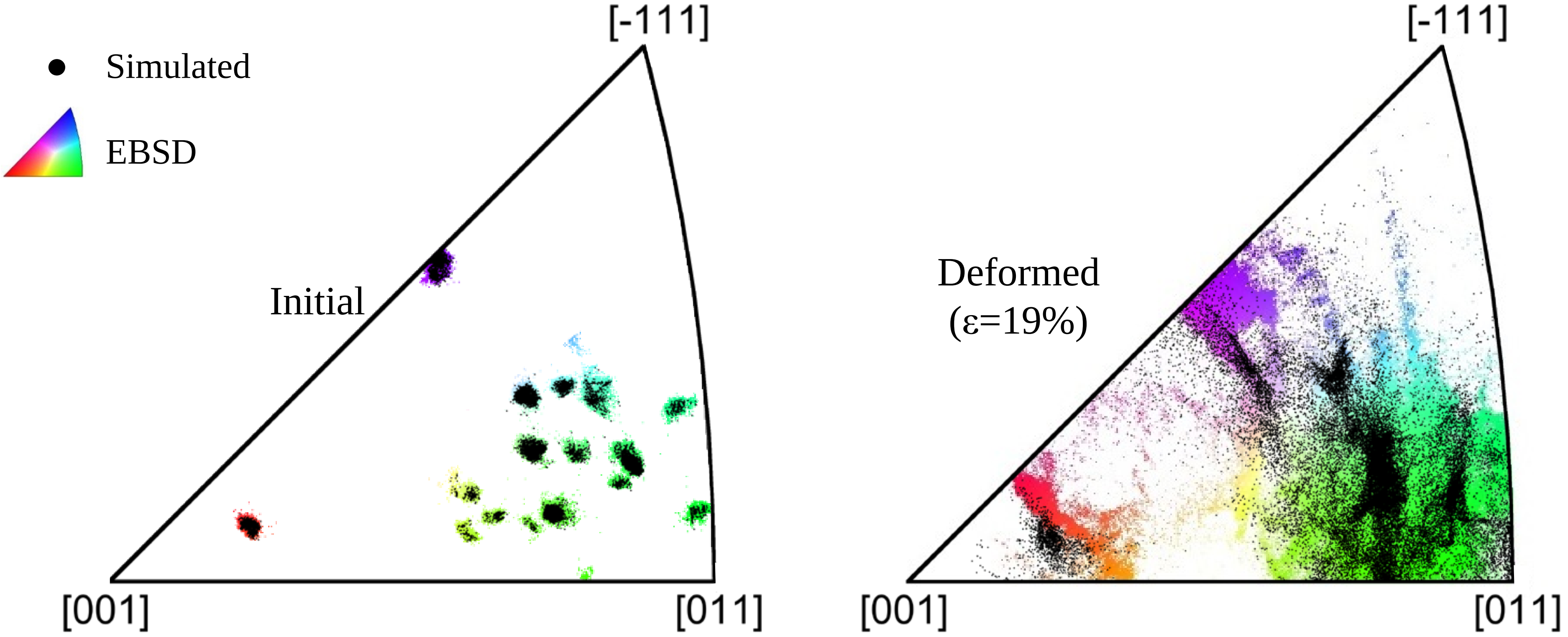
Experiment



Model {110} slip

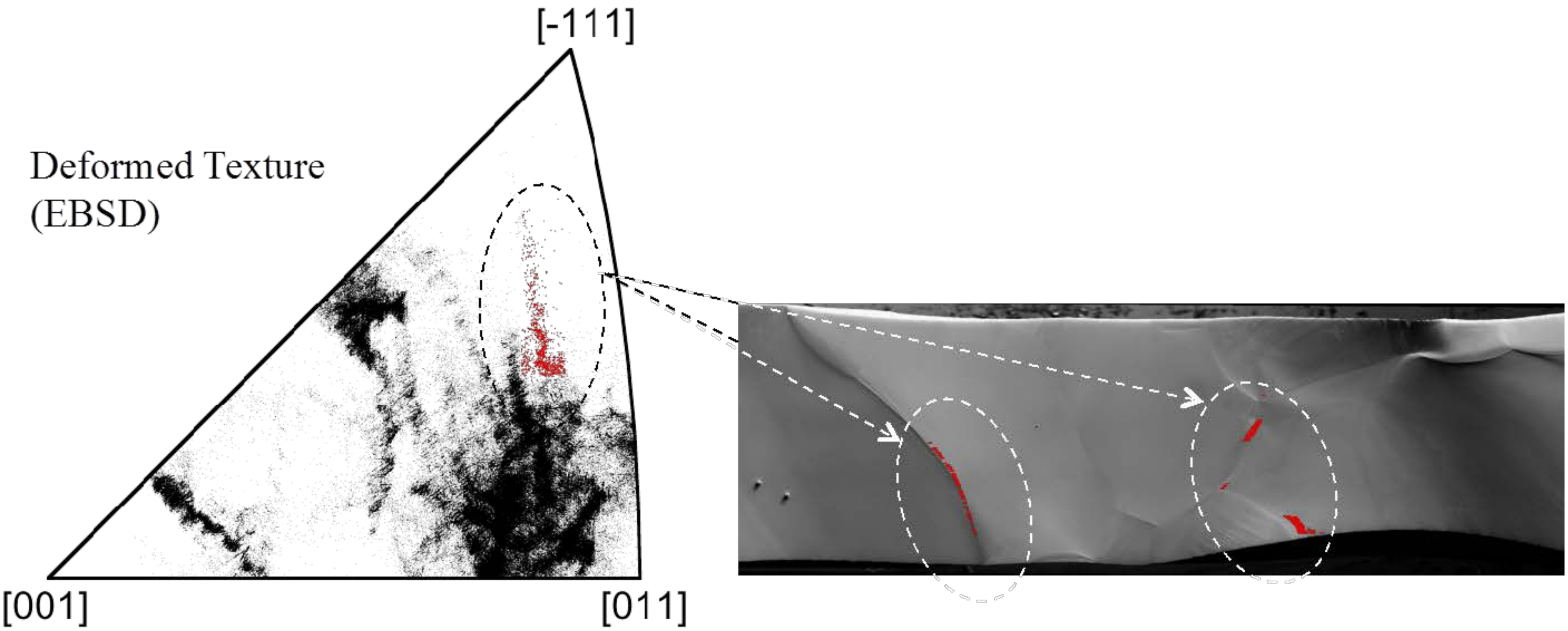
Oligo 2: Compare texture evolution.





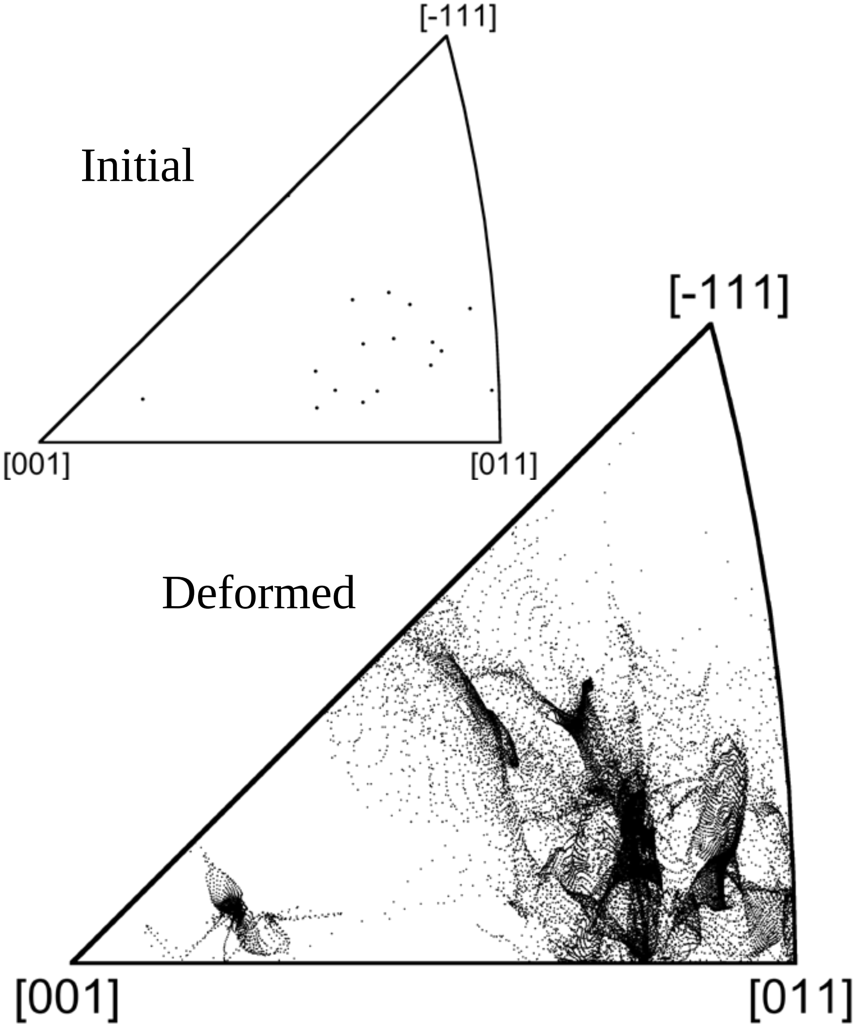
Medium mesh, orientation per element

Streaks in inverse pole figure (from experiment) are at grain boundaries.

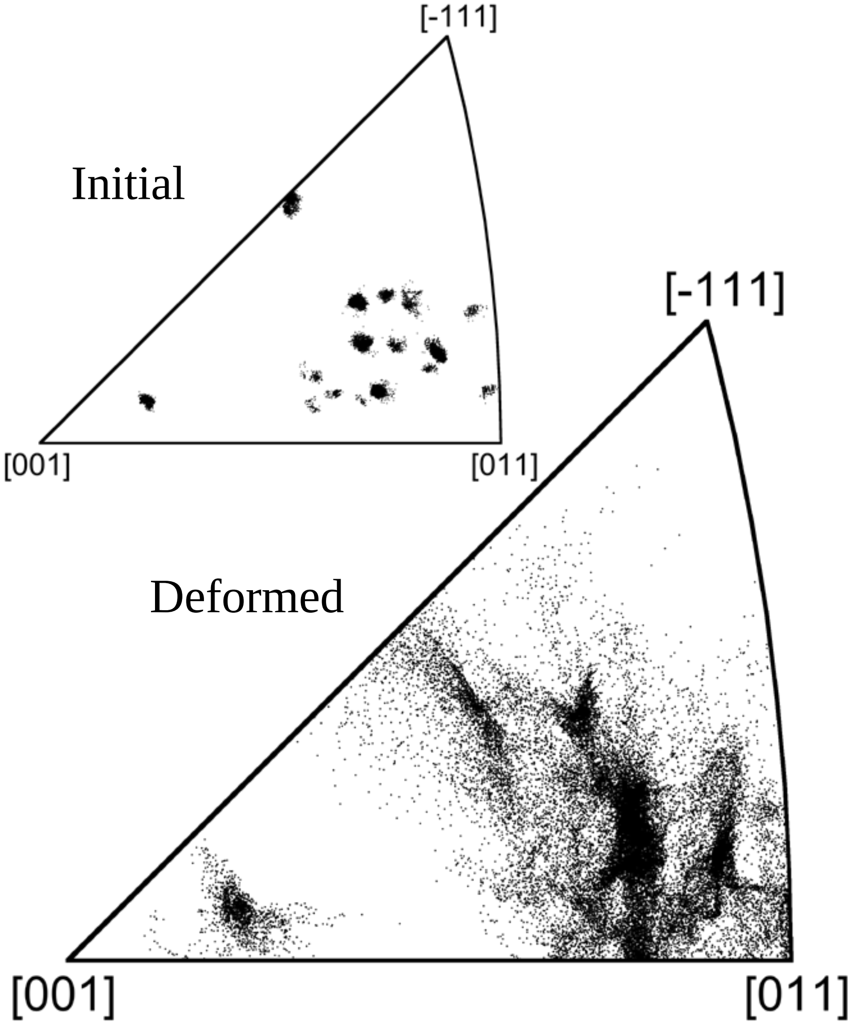


Defining orientations per element (instead of an orientation per grain) gives more realistic inverse pole figures.

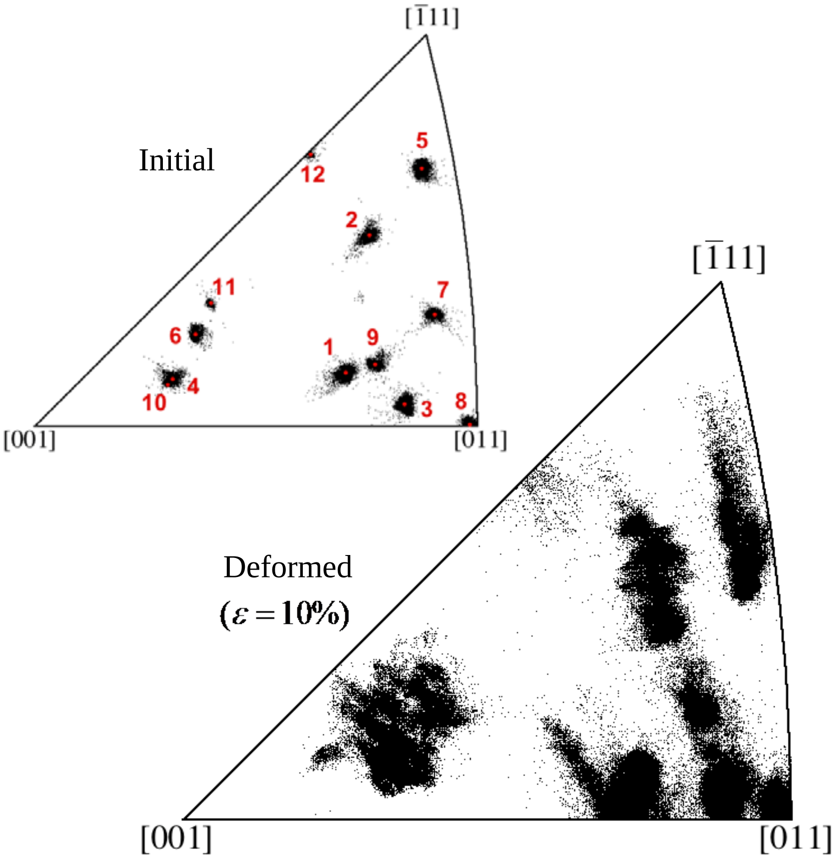
Orientation per grain



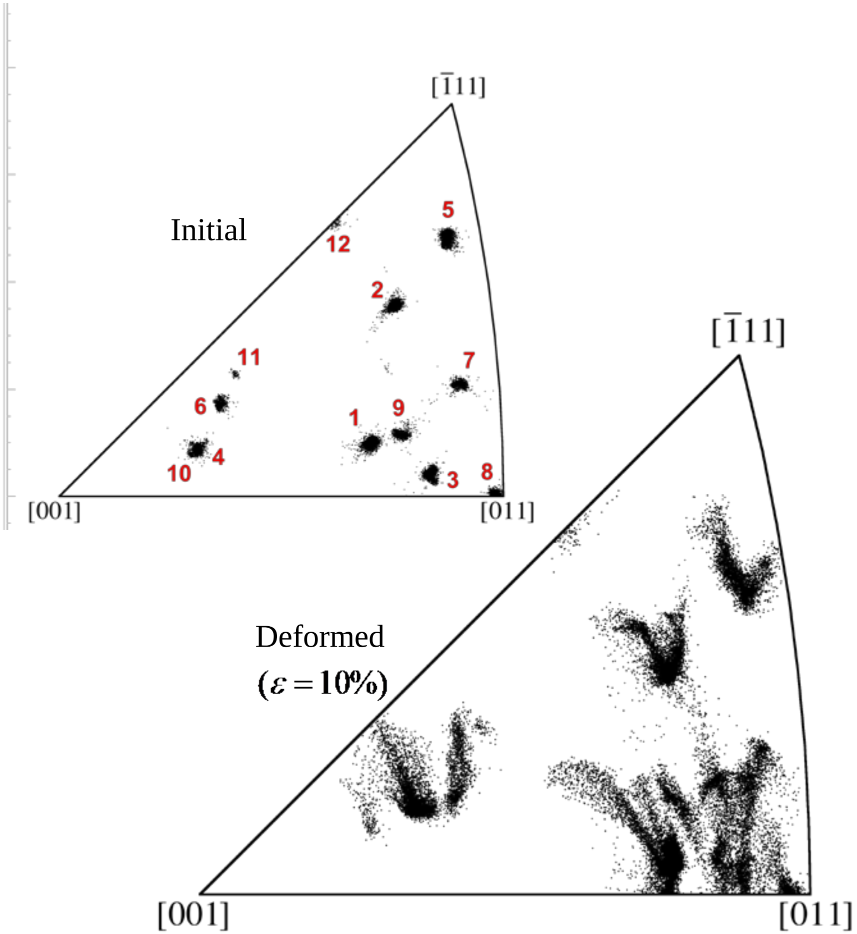
Orientation per element



Oligo 4: Grain rotations



(a) Measured (EBSD)



(b) Predicted (CP-FEM)

Outline

1. Background
2. Experimental setup
3. Model details
4. Model validation- strain fields
5. Model validation- crystal rotations
6. Conclusions

Conclusions

- Strain predictions show good agreement with experiments.
  - Quantitative pointwise agreement within ~3% strain.
  - Results affected by 3d issues
  - Fracture initiation observed at location of highest predicted strain.
- Grain rotations are more challenging.
  - Improved grain boundary modeling has promise.
- Effects of model parameters
  - Still unclear whether {110} or {112} (or combination) is better.
  - Pseudo 3D model is much more accurate than 2D.
  - Defining orientations element-wise makes grain rotations look more realistic.