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Relating Strain Accumulation to Microstructure in BCC Tantalum

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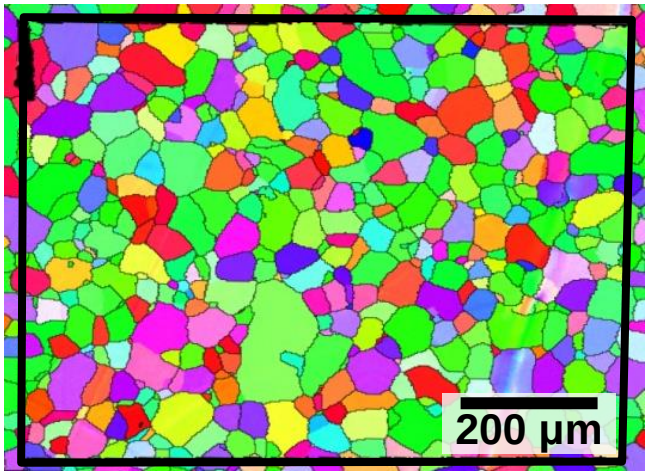
Motivation: Predict grain scale deformation behavior.

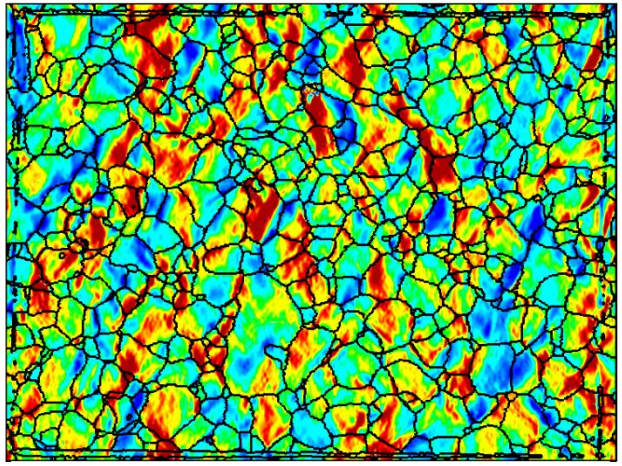
- Better predictions of material response.
- Better predictions of variability in deformation behavior.
- Better understanding of failure process.

- How well do current (and improved) crystal plasticity models predict behavior?
  - What parts of the models need work?

Microstructure

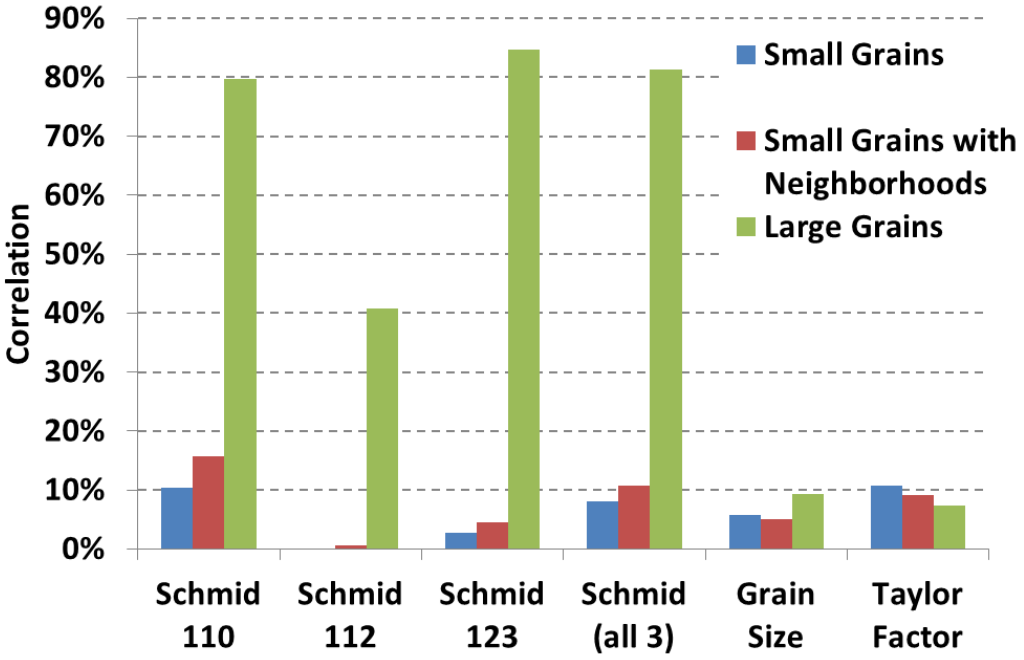


Strain



Special challenge with BCC models: Identifying active slip systems.

- {110} or {112} planes?
- No scientific consensus yet.
- Previous studies indicate {110} is the most common, but slip likely occurs on other planes as well.

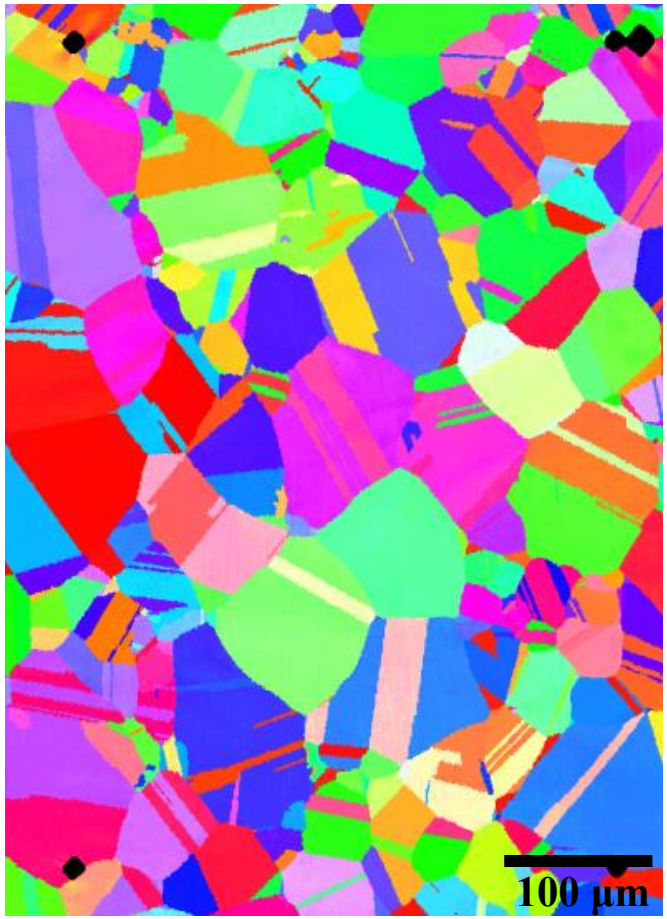


Material	Slip plane	...	References
Tungsten	{110}		118
Tungsten	{112}		118
α-iron	{110}		118
α-iron	{112}		118
Chromium	{112}		118
Vanadium	{112}		118
Tantalum	{112}		133
Tantalum	{112}		134
Tungsten	{110}		130
Molybdenum	{110}		130
Molybdenum	{110}		130
Molybdenum	{110}		130
Molybdenum	{110}		130
Niobium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

Carroll J.D., Clark B.G., Buchheit T.E., Boyce B.L., Weinberger C.R., Matls Sci. Eng. A (2013, in press)

Weinberger, C.R., Boyce, B.L., Battaile, C.C., International Materials Reviews (2013)

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



- Carroll J., Abuzaid W., Lambros J., Sehitoglu H., Rev. Sci Inst. 81 (2010)
- Carroll J.D., Abuzaid W., Lambros J., Sehitoglu H., *Int. J. Fatigue*, in press (2013)
- Carroll J.D., Abuzaid W.Z., Lambros J., Sehitoglu H., *Int. J. Fracture*, v. 180 (2013)

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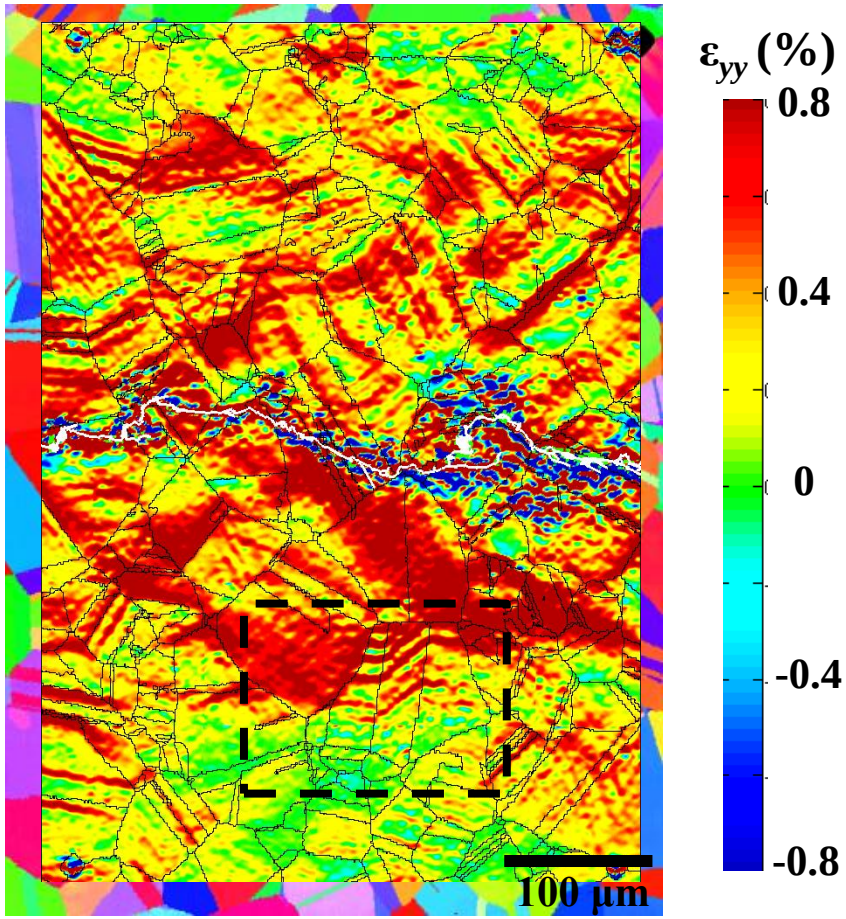

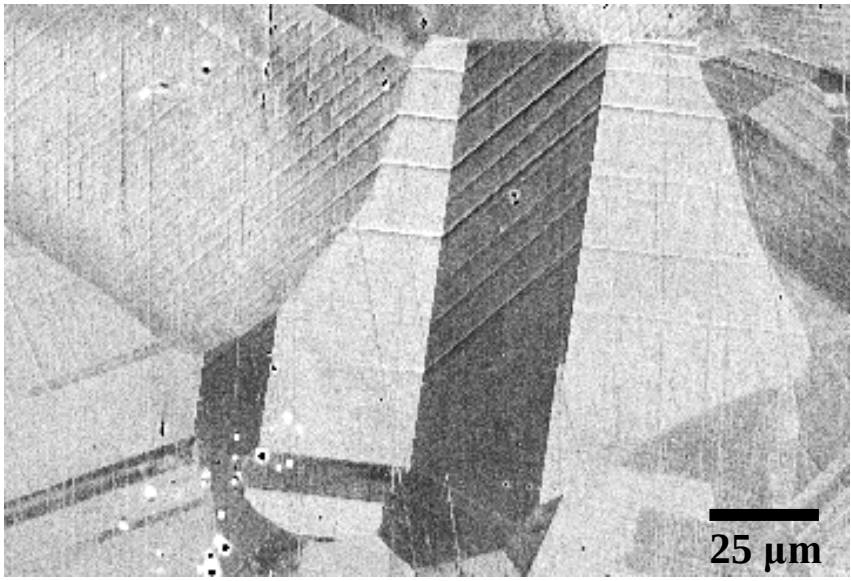

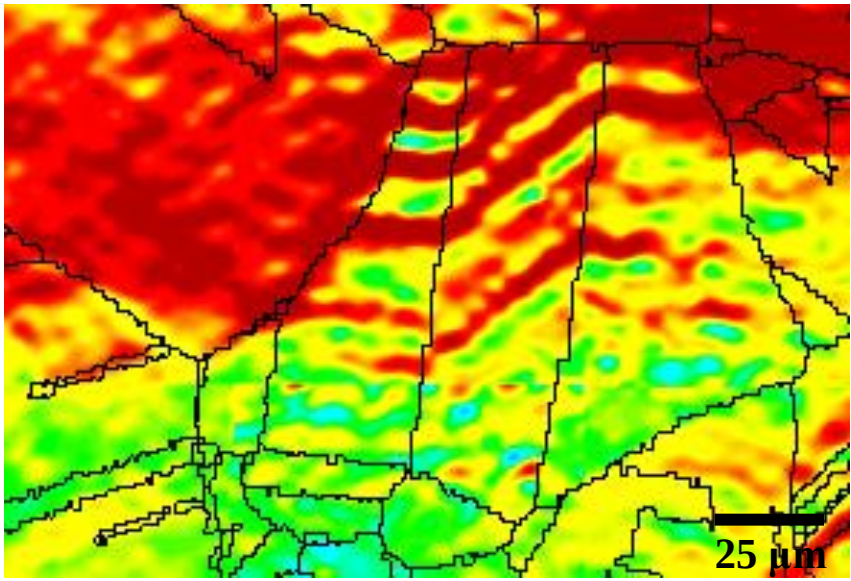

- Carroll J., Abuzaid W., Lambros J., Sehitoglu H., Rev. Sci Inst. 81 (2010)
- Carroll J.D., Abuzaid W., Lambros J., Sehitoglu H., *Int. J. Fatigue*, in press (2013)
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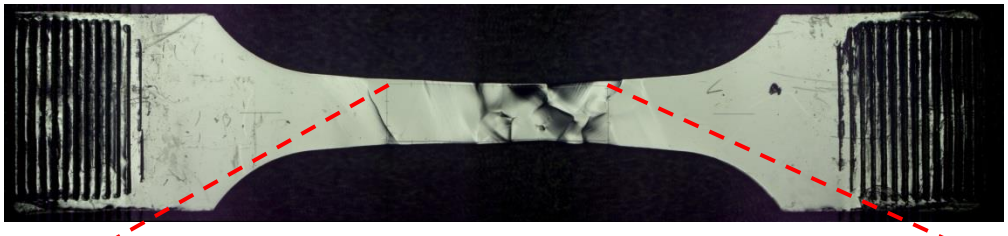
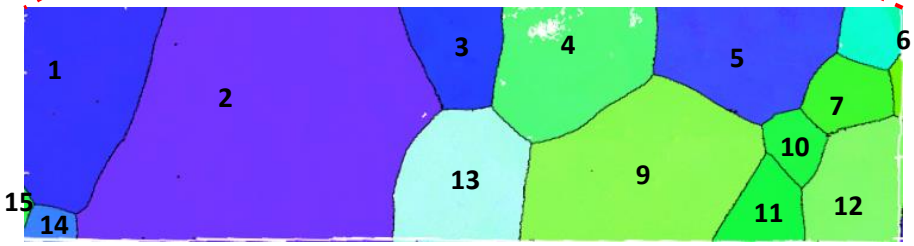
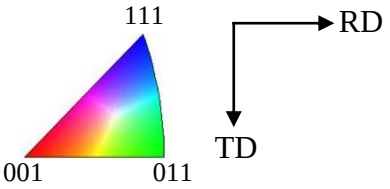
Oligocrystal specimens with pseudo-2D grains allow a comparison between models and experiments.

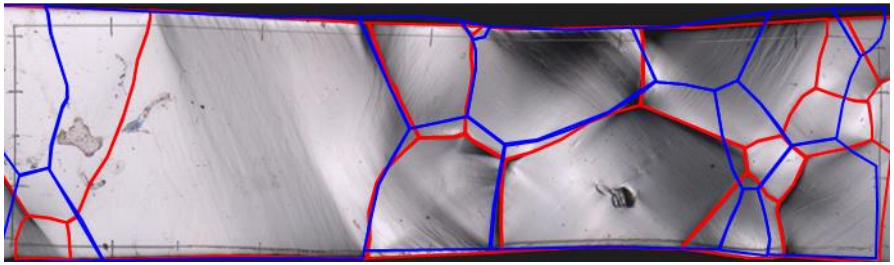


Specimen 1

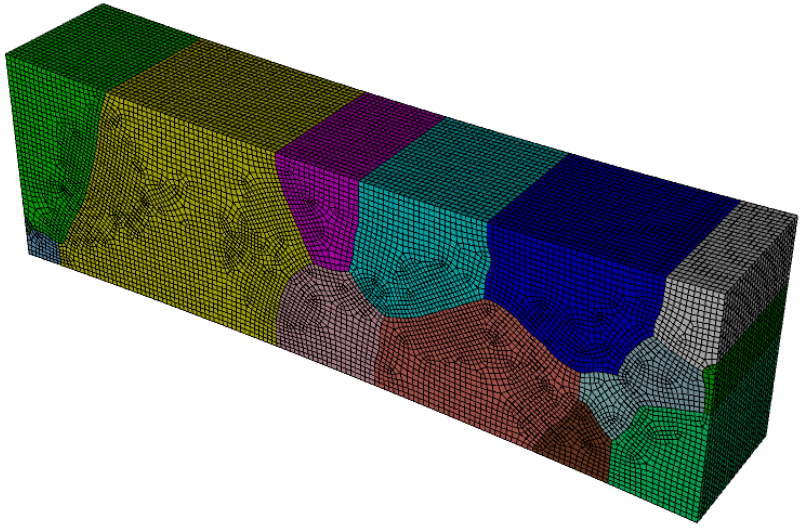


1 mm





Grain boundary (Front) Grain boundary (Back)



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)

Lattice friction

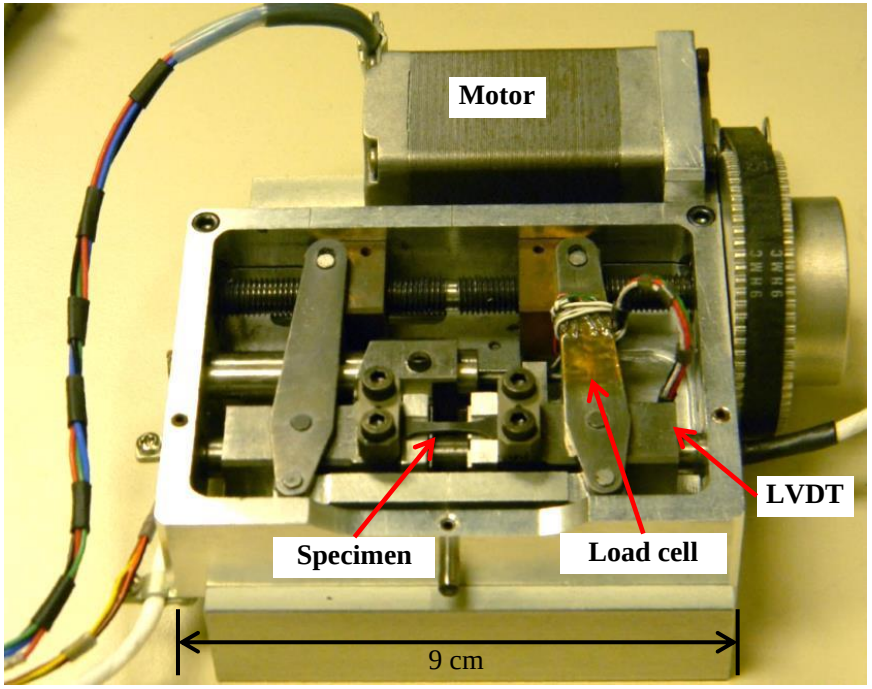
Obstacle stress

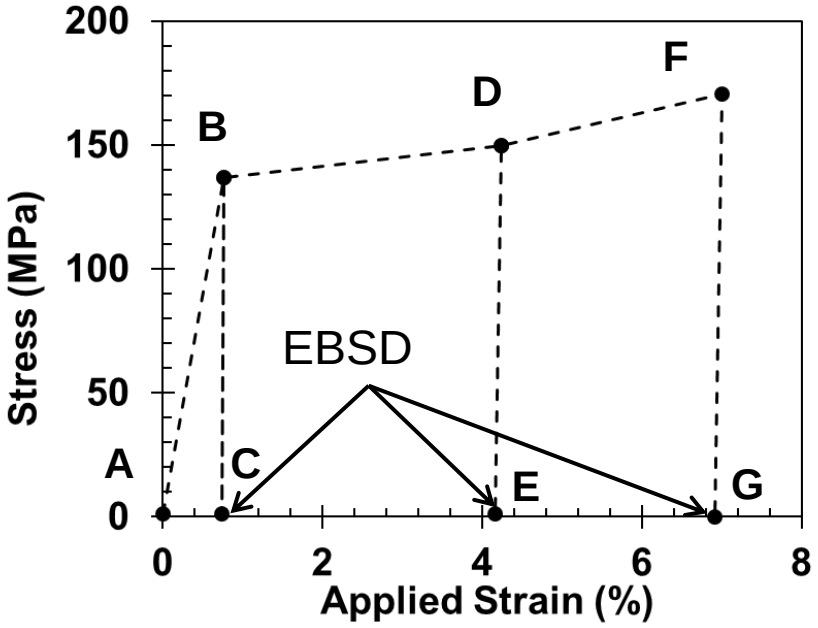
Obstacle stress: $\tau_{\text{obs}}^\alpha = \alpha \mu b \sqrt{\sum_{\beta=1}^{NS} \rho^\beta}$ (Taylor, 1934)

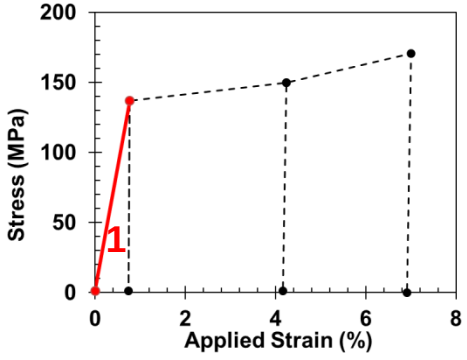
$$\rho^\alpha = \left(\kappa_1 \sqrt{\sum_{\beta=1}^{NS} \rho^\beta} - \kappa_2 \rho^\alpha \right) \cdot |\gamma^\alpha| \quad \text{(Kocks, 1976)}$$

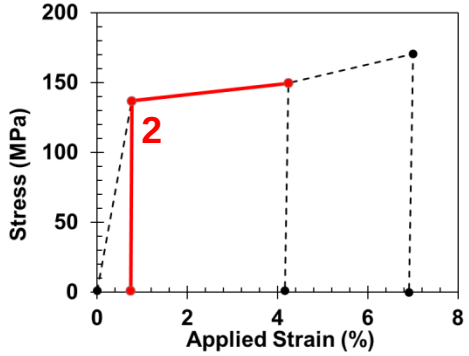
- Incorporates temp and strain rate effects
- FEM code (JAS-3D) developed at Sandia
- 50 elements through thickness, total of 1,426,650 and 1,664,150 elements for oligo 1 and 2.
- 8 element h exahedral elements.
- One orientation per element, pixelated grain boundaries.

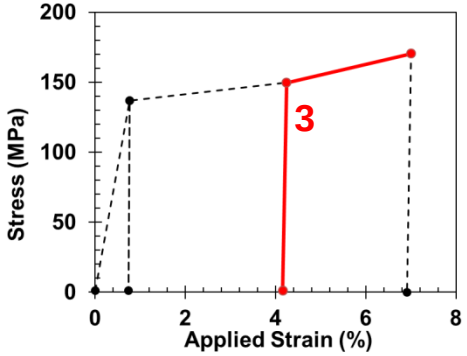
Specimen 1 was loaded incrementally with EBSD measurements between increments.







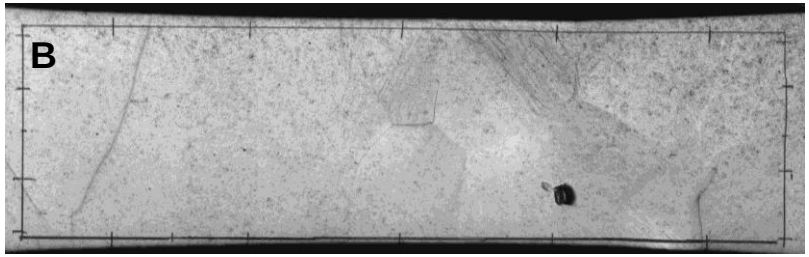




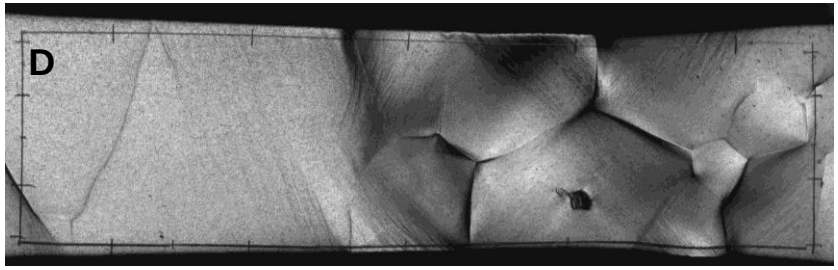
Deformation in specimen 1 was concentrated in <110> grains.

Undeformed

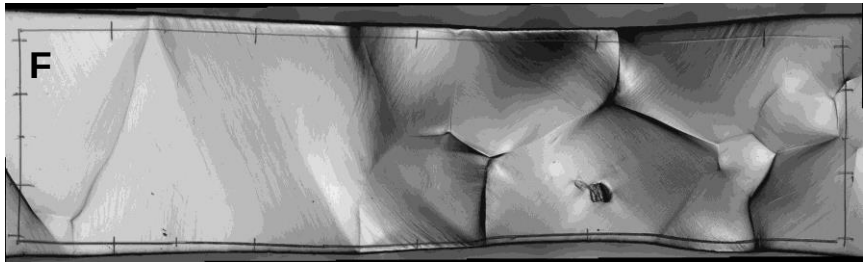
Strain 1:
0.75% Inc.
0.75% Total



Strain 2:
3.4% Inc.
4.2% Total



Strain 3:
2.6% Inc.
6.8% Total



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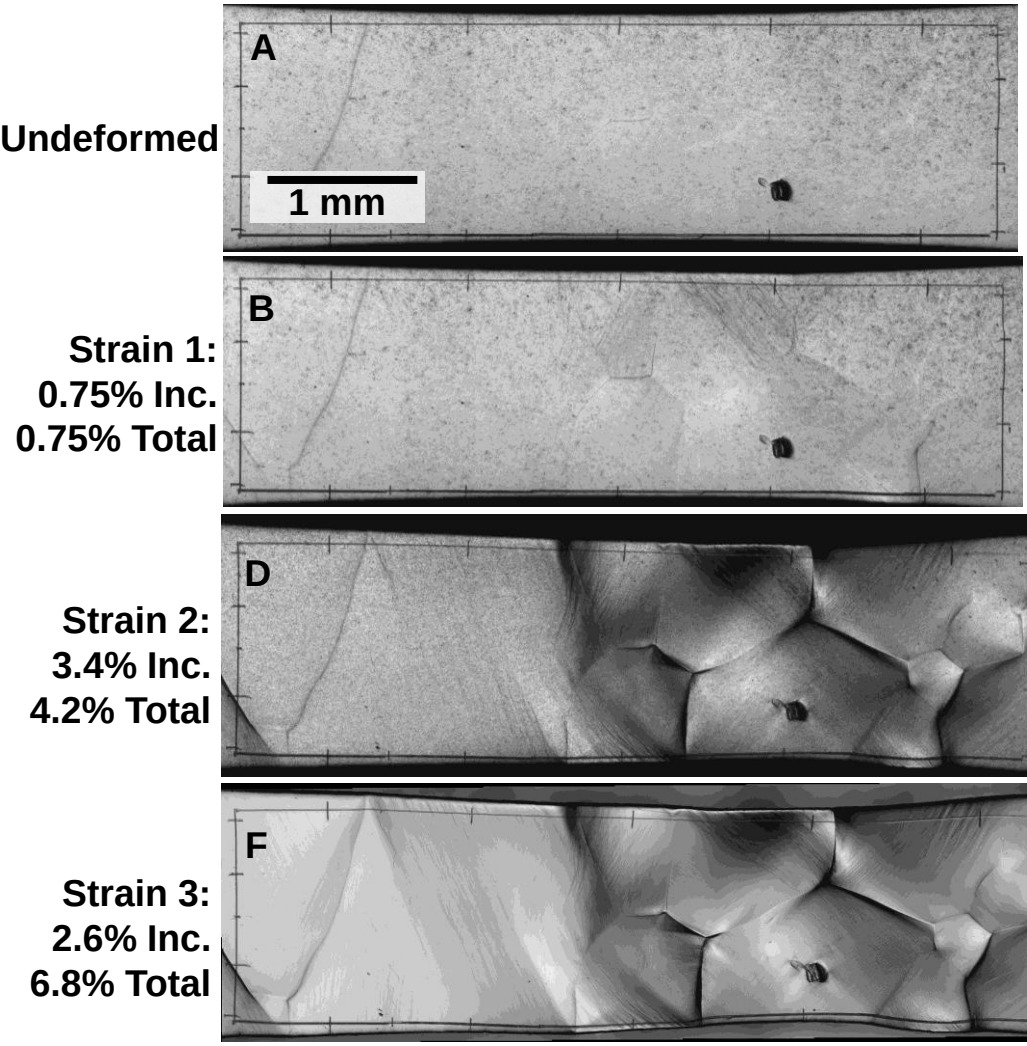

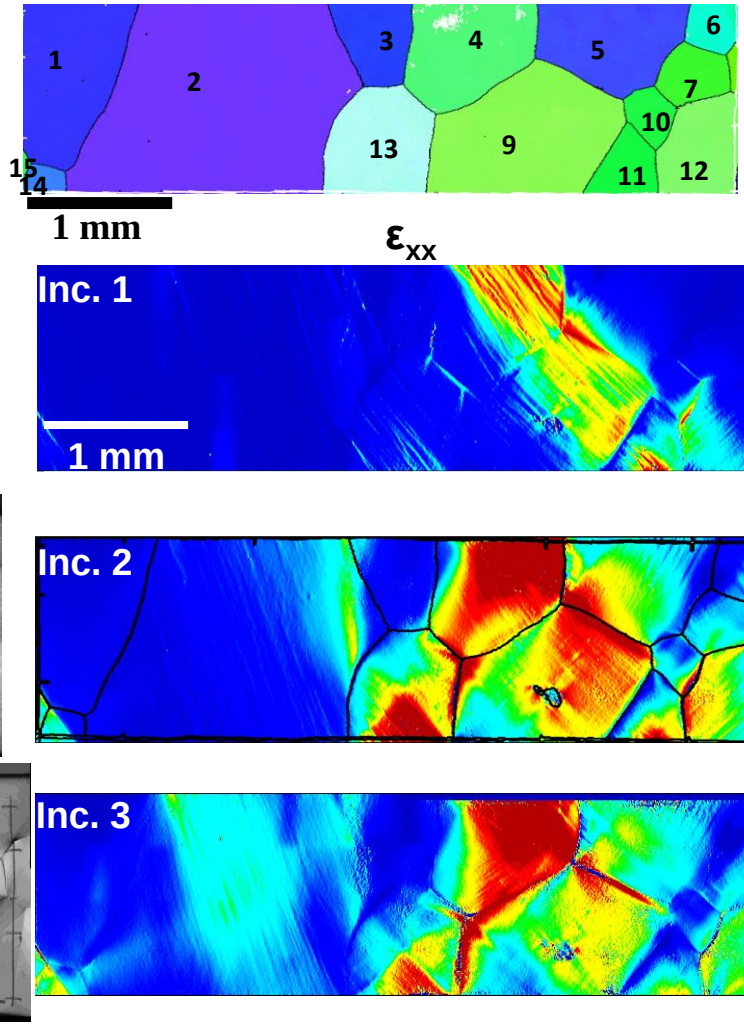

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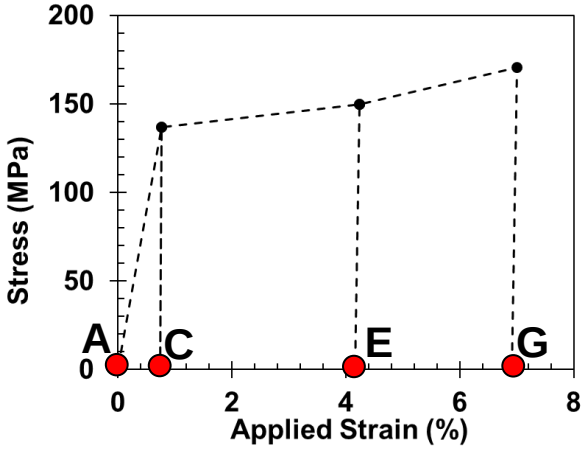
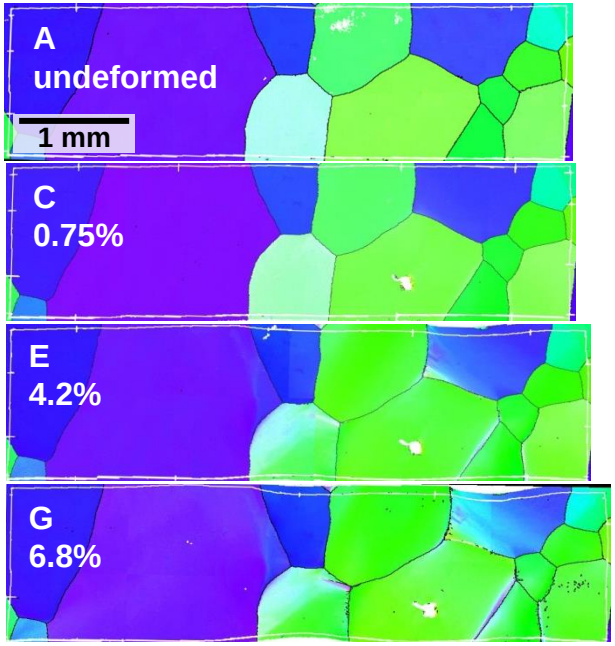
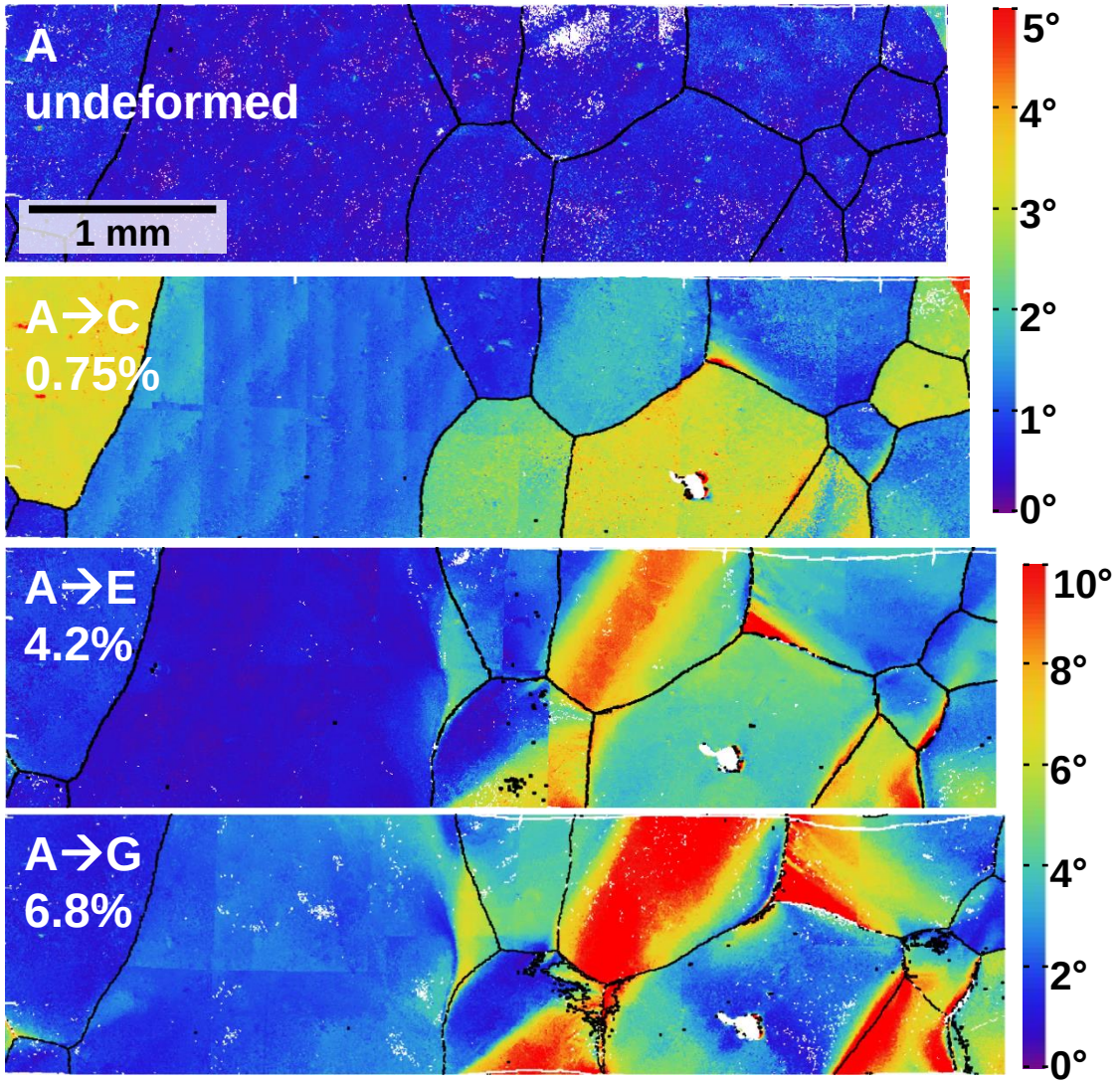
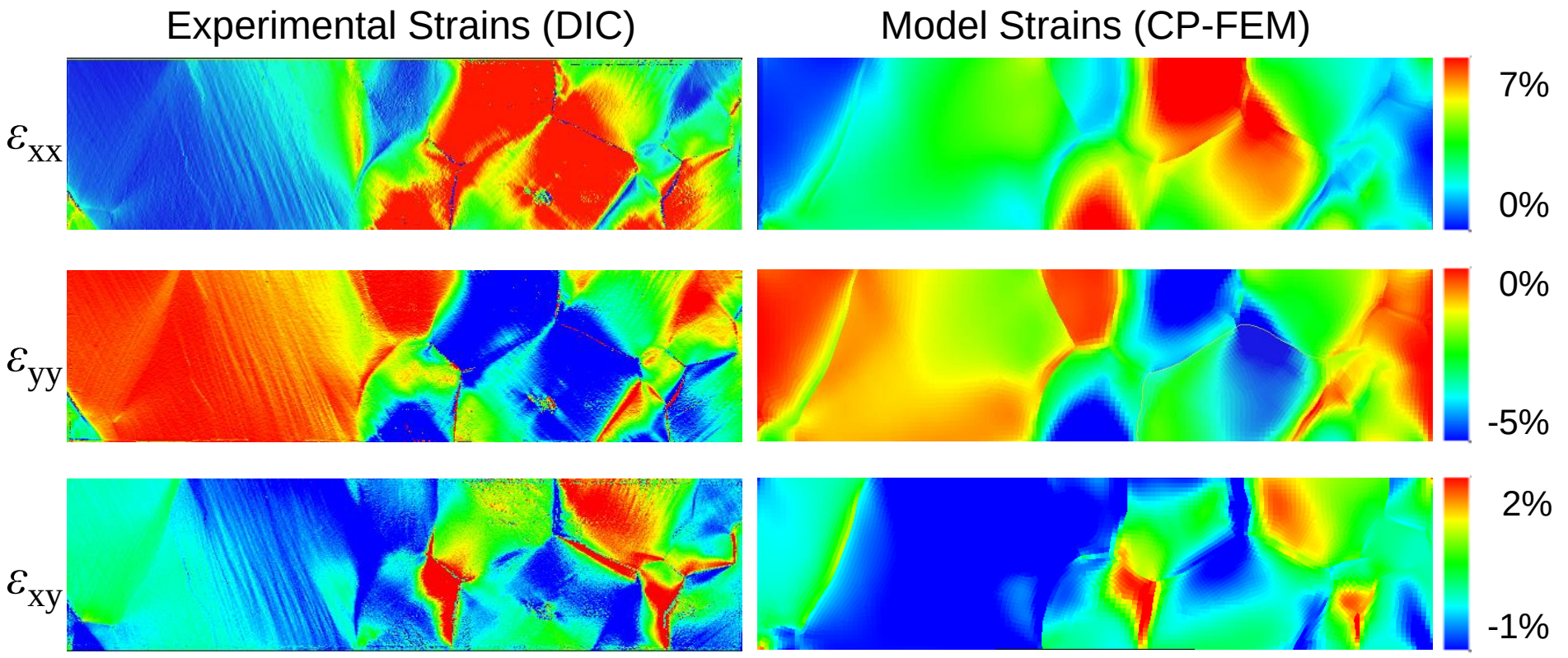
Intragrain misorientation at each strain level was calculated from repeated EBSD measurements.



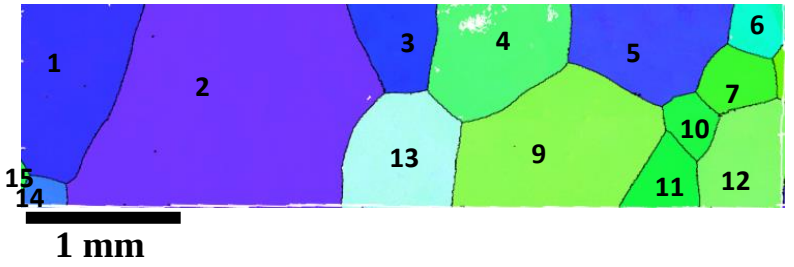




Model predictions of strain agree well with experimental measurements.



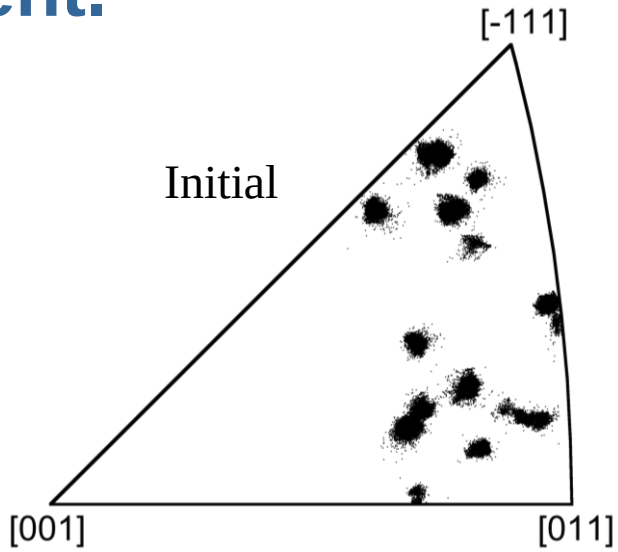
Model only considers slip on {110} planes.



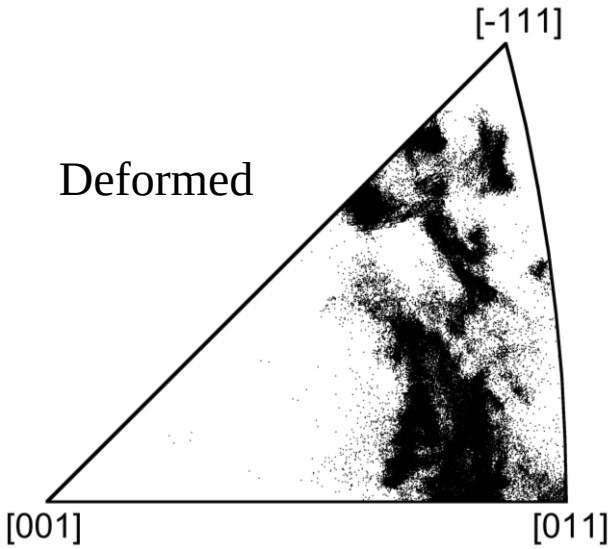
Compare grain orientations of model and experiment.

Specimen 1

EBSD

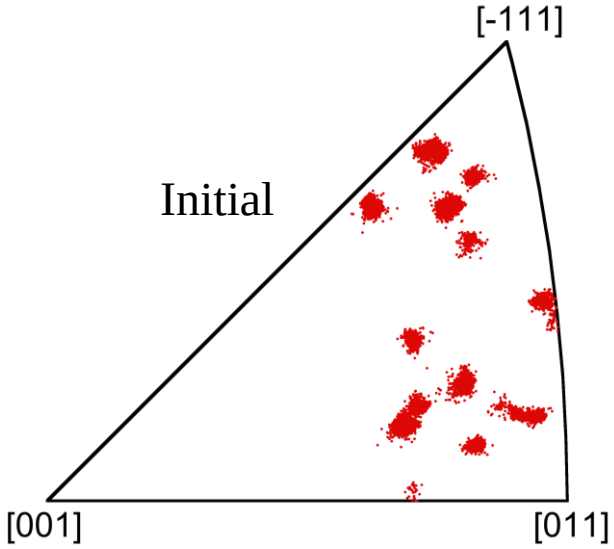


Initial

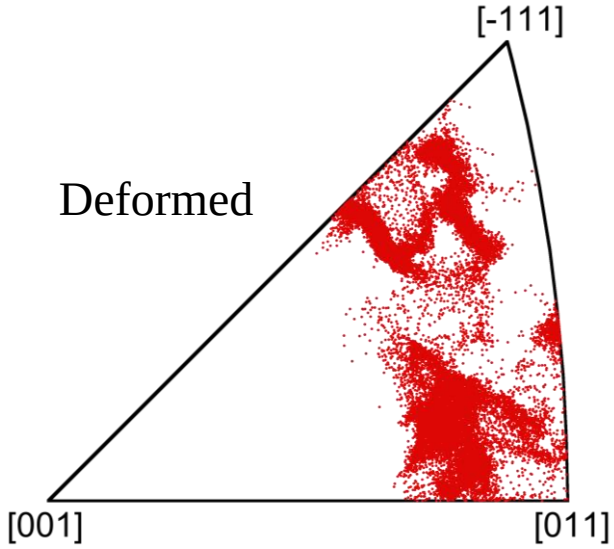


Deformed

CP-FEM



Initial

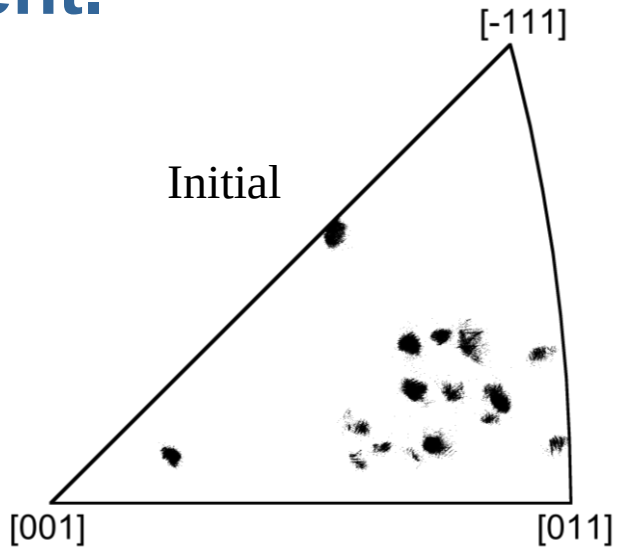


Deformed

Compare grain orientations of model and experiment.

Specimen 2

EBSD



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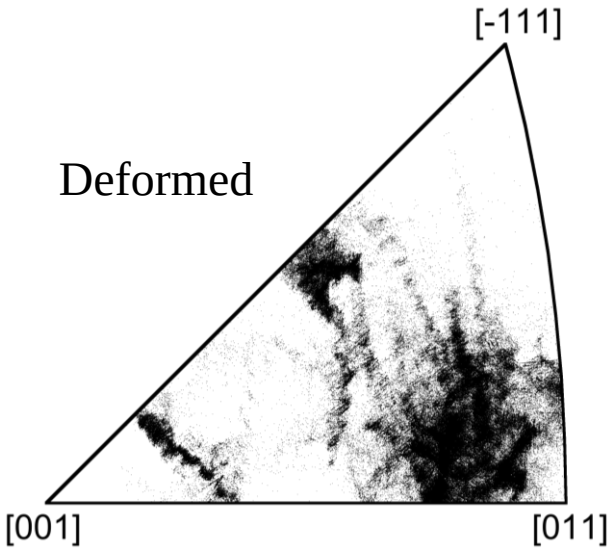
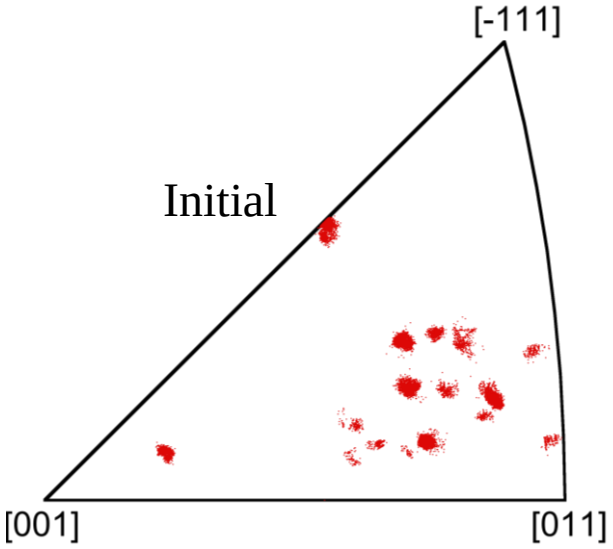


Deformed

CP-FEM



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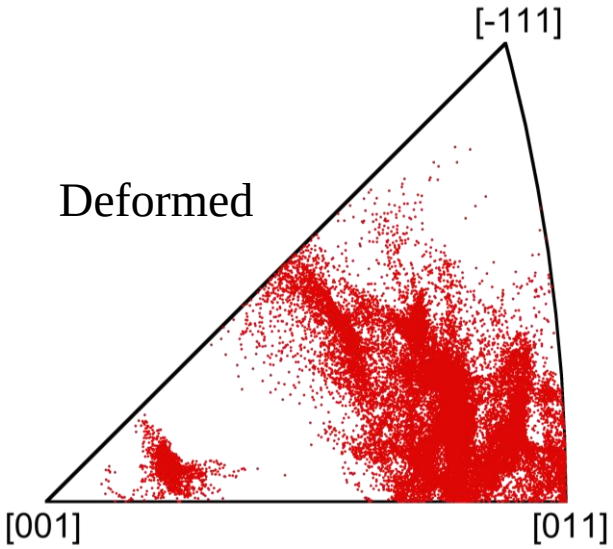
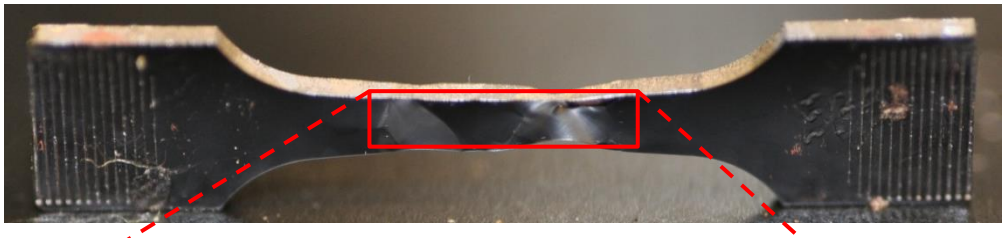
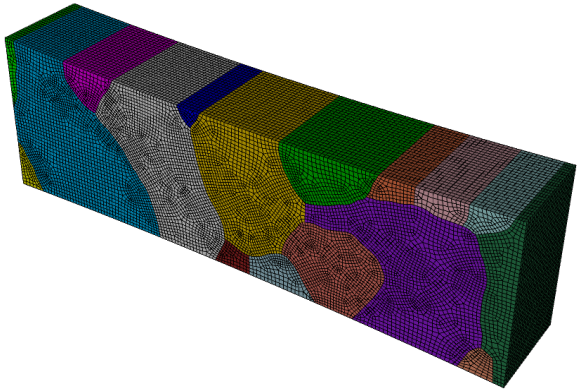
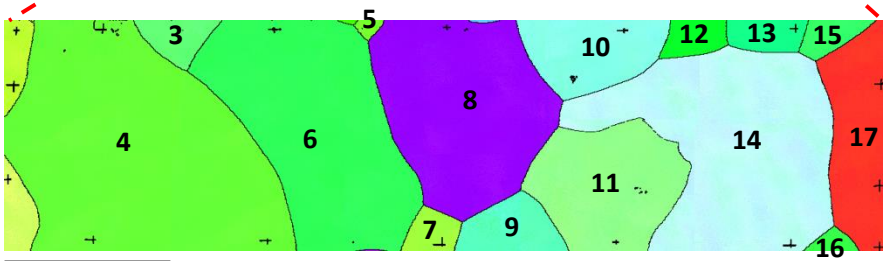


Deformed

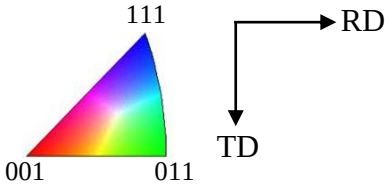
Compare model and experiment for a second oligocrystal specimen.

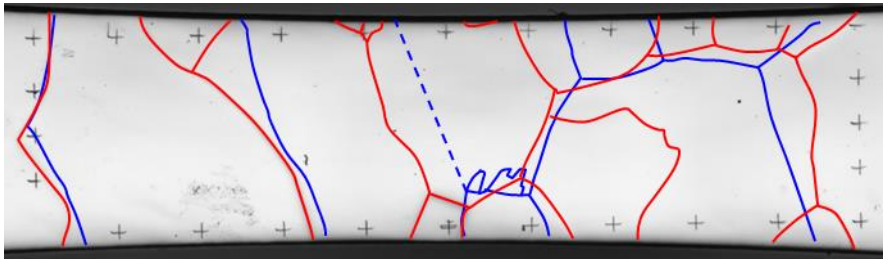




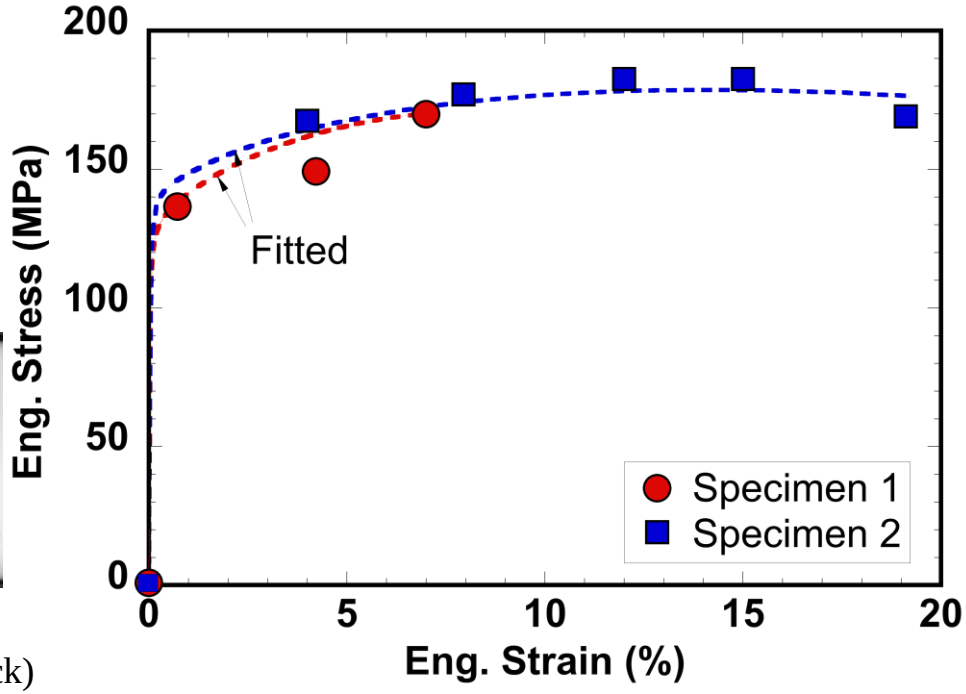


1 mm

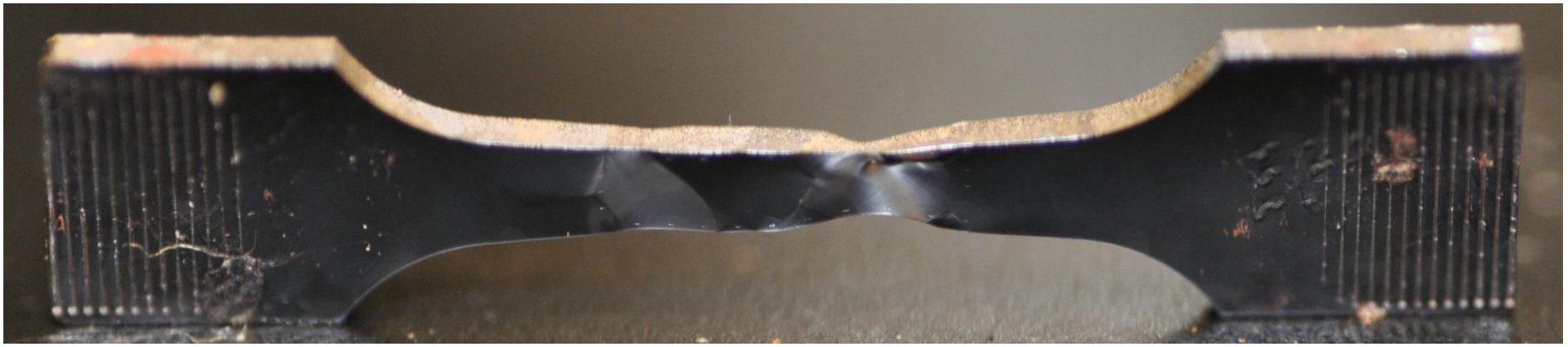




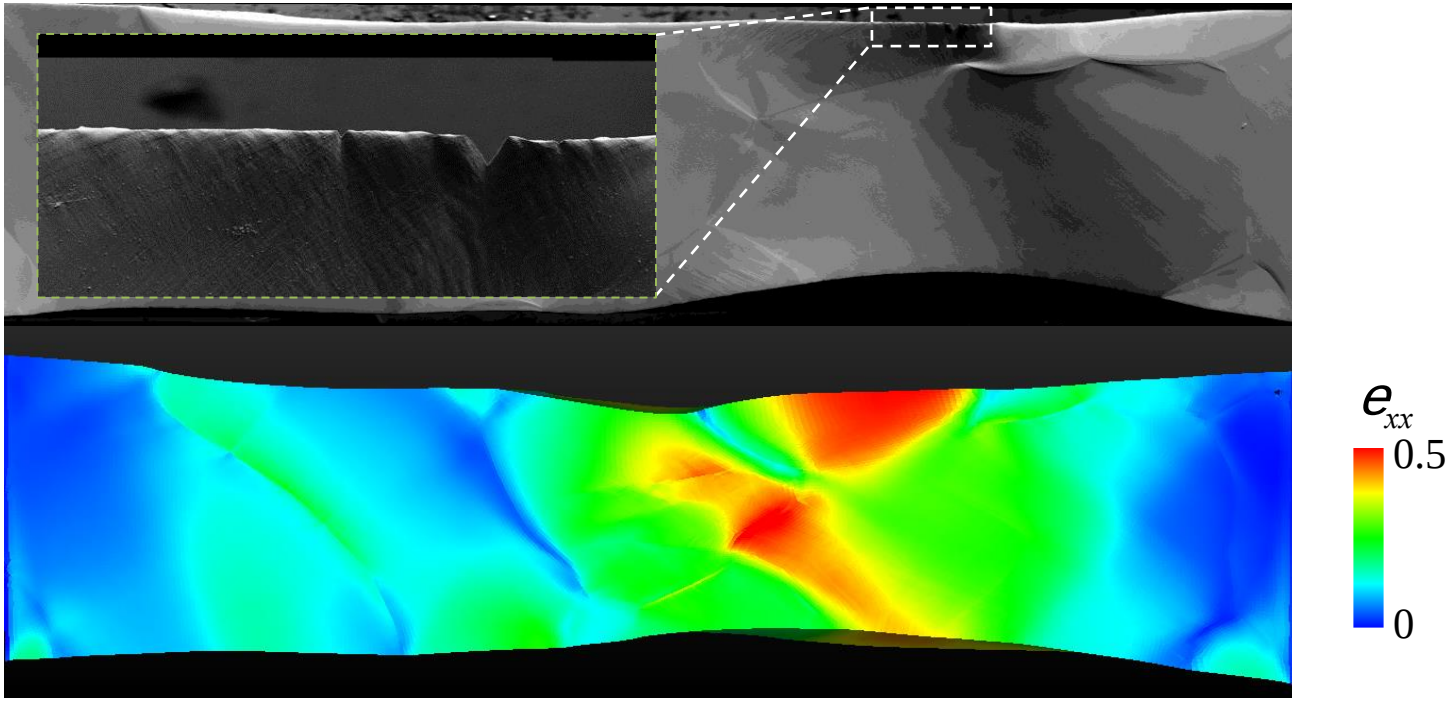
Grain boundary (Front) Grain boundary (Back)



Model predicts maximum strain at location where failure initiated in experiment.



{110} slip



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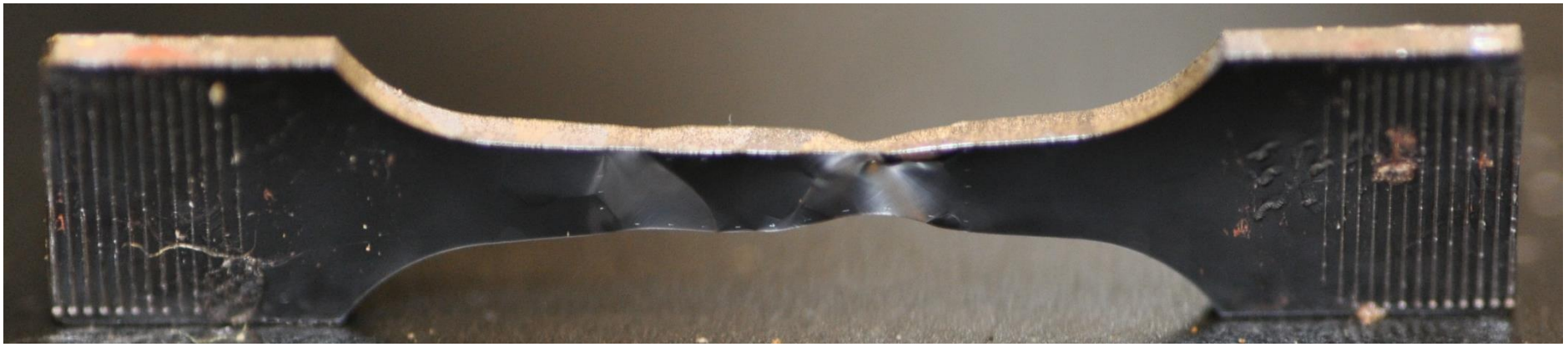
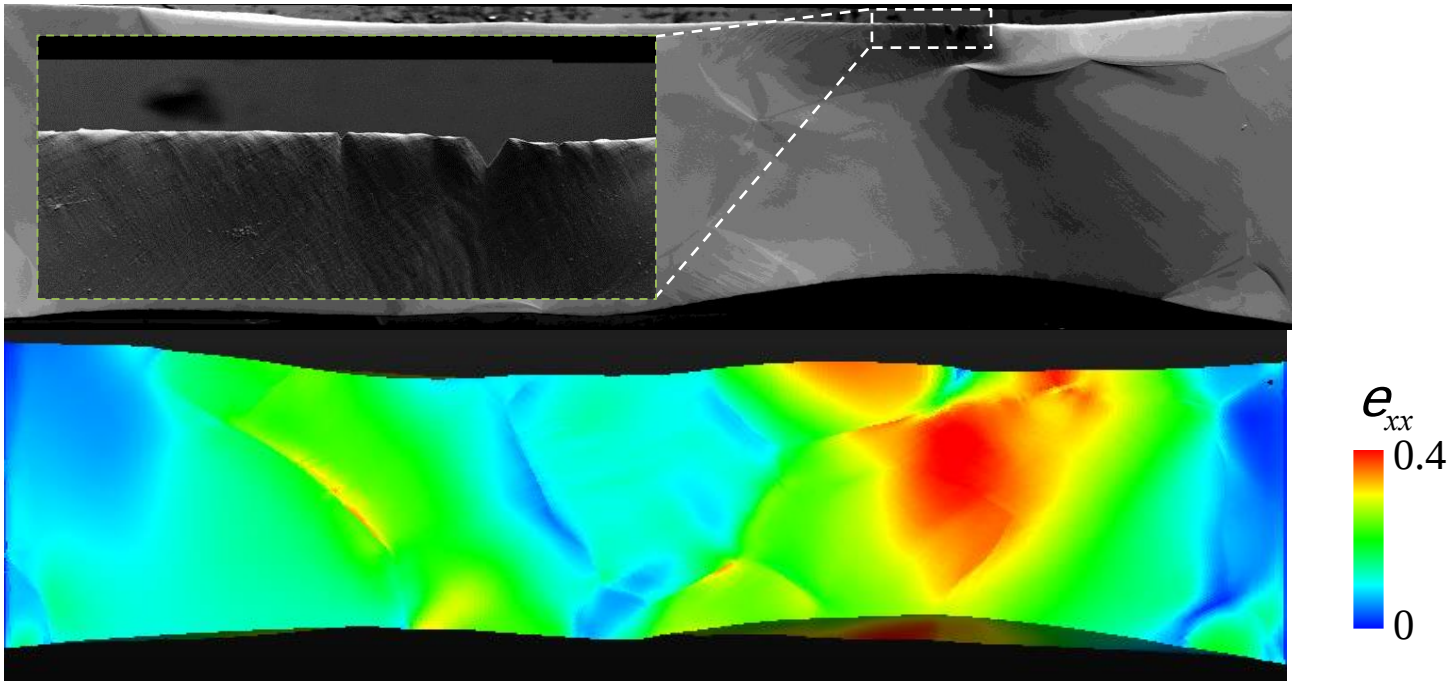


{112} slip



Conclusions

- Promising BCC CP-FEM model was developed.
- Improvements needed in model validation.
  - As always, general qualitative agreement was found.
  - In future work, a pointwise comparison will be used for error quantification.
- <111> grains rotate the most, but <110> grains experience the highest strains.
- Many different modeling approaches attempted
  - Accuracy of results was related to effort expended.

Extra Slides

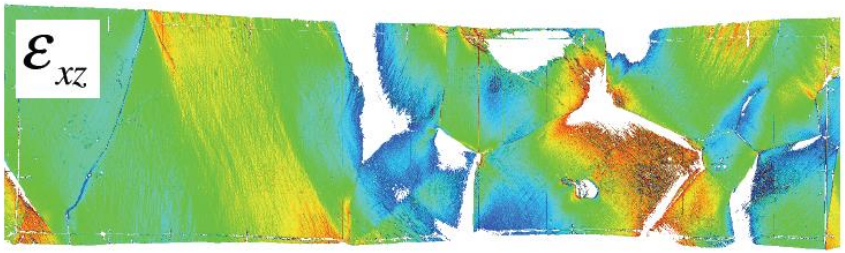
Profilometry comparisons

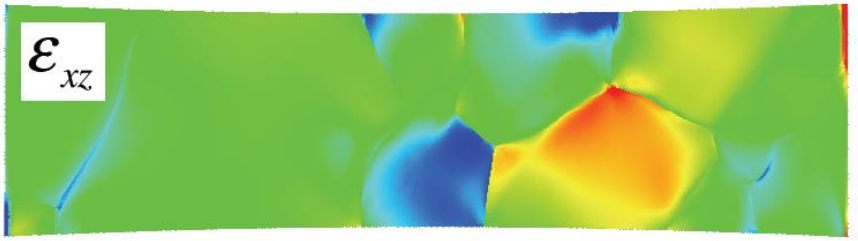
Out-of-plane Strain Maps

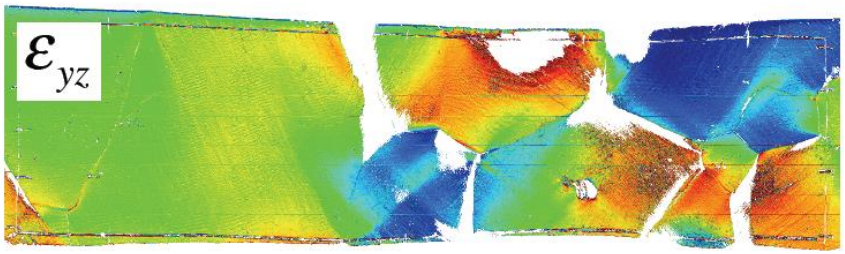
Ta oligocrystal specimen 1 (7% deformation)

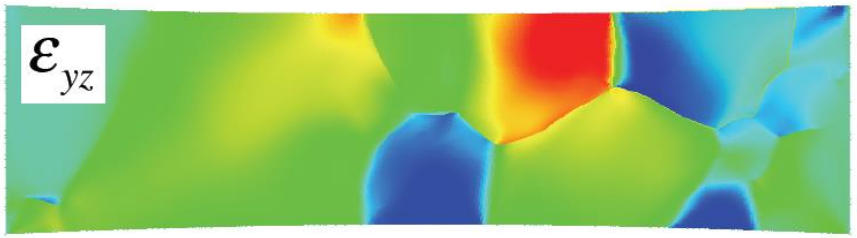
Profilometry Measurements

CP-FEM Predictions



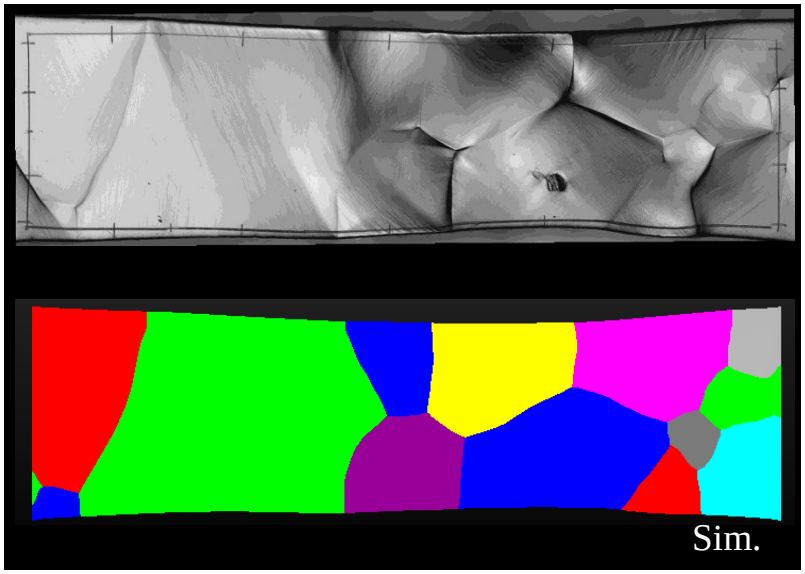




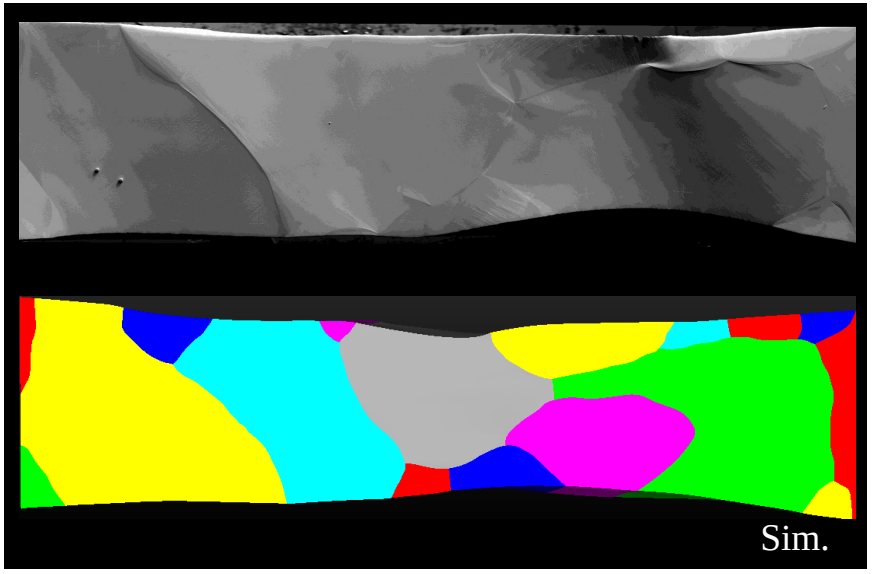


They agree well qualitatively but note that they have different contour levels (Measured exz and eyz are plotted with -10 to 10.)

Deformed shape

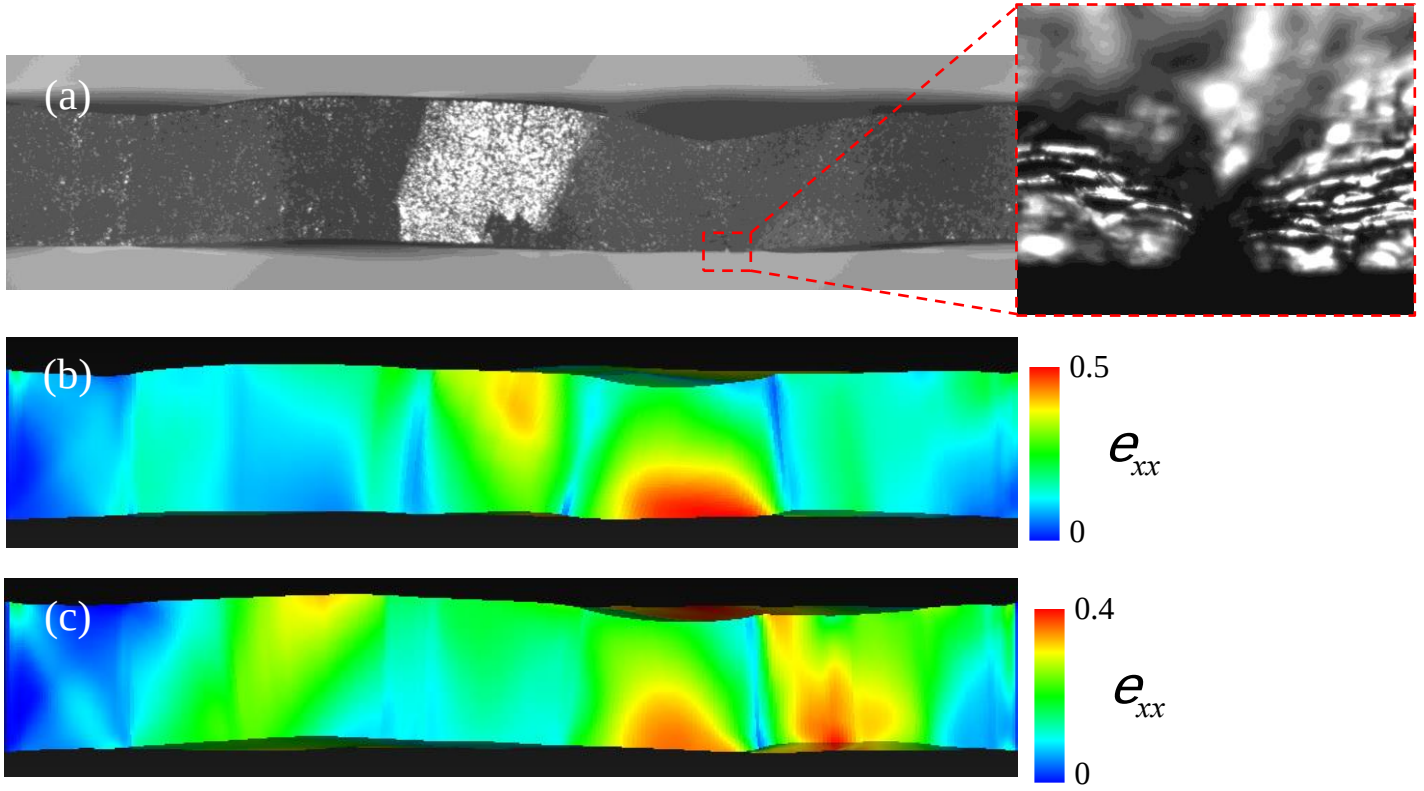


(a) Specimen 1 (e=6.8%)



(b) Specimen 2 (e=19.2%)

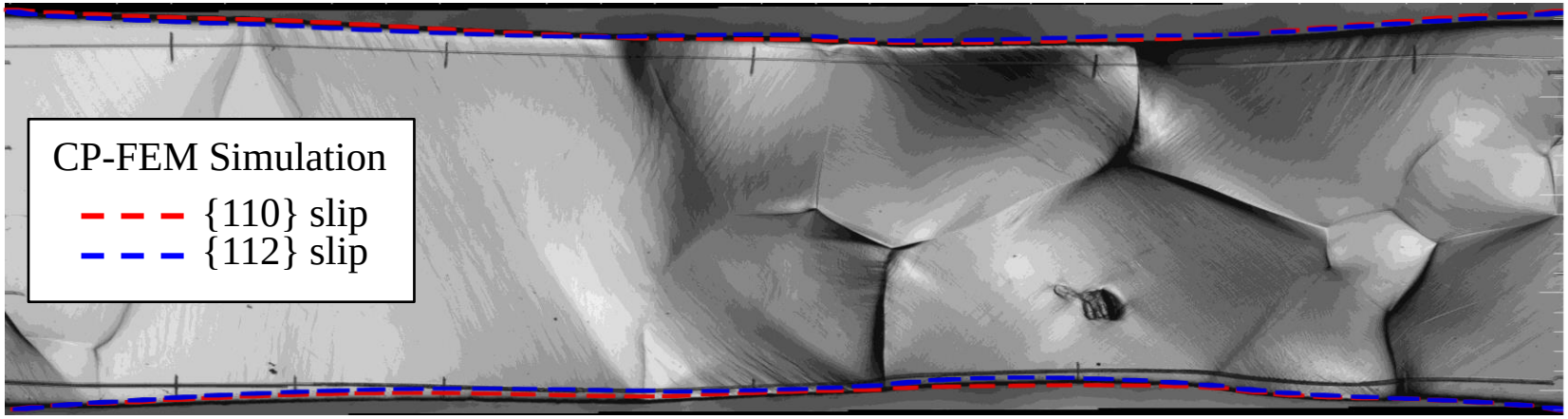
Deformed shape and strains on side of specimen. Compare model to observations.



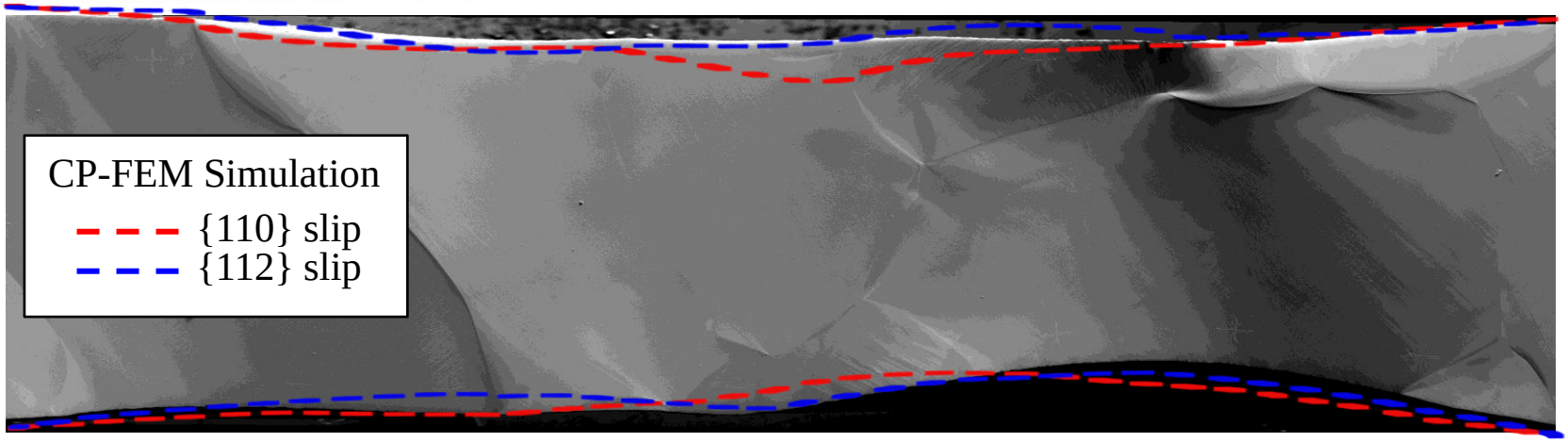
{110} slip

{112} slip

Deformed shape and strains on side of specimen. Compare model to observations.

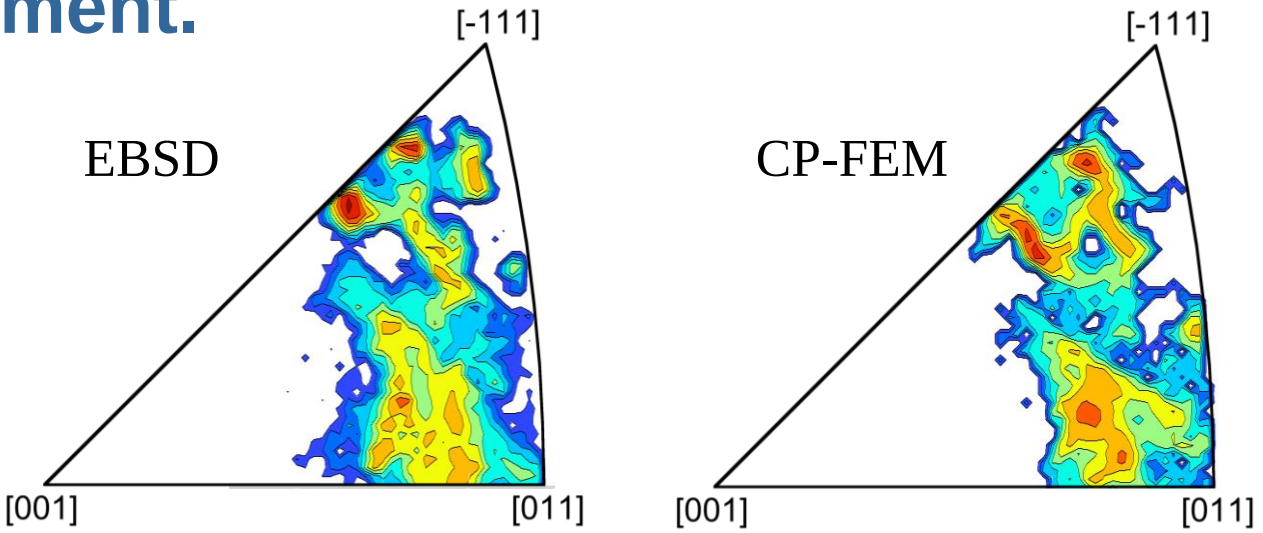


(a) Specimen 1

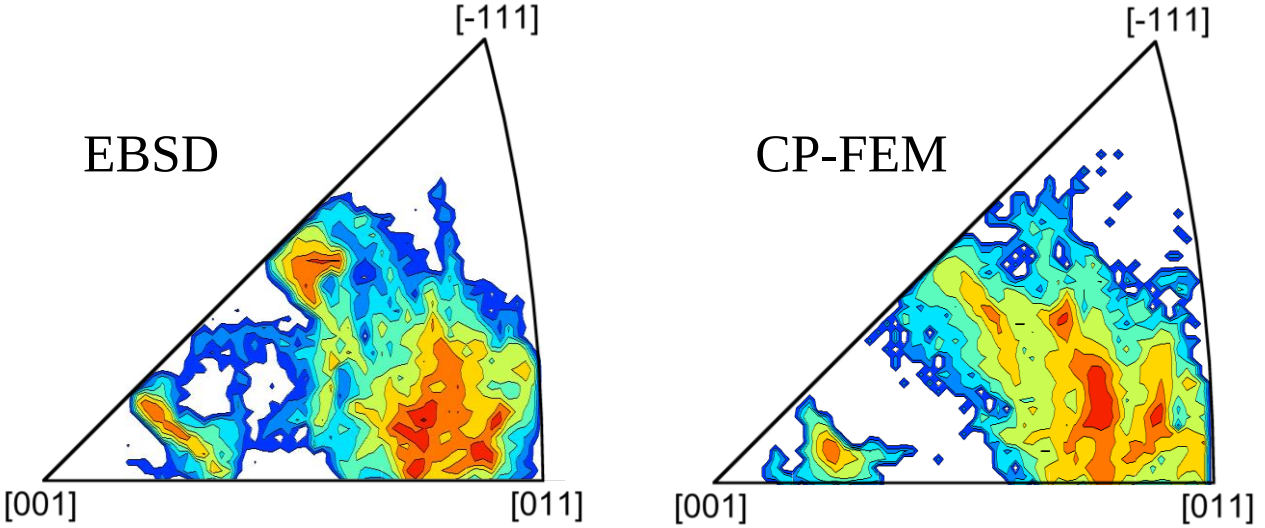


(b) Specimen 2

Compare grain orientations of model and experiment.



(a) Specimen 1 (e=6.8%)



(b) Specimen 2 (e=19.2%)