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Grain-scale Experimental Validation of Crystal Plasticity Finite Element Simulations of Tantalum Oligocrystals

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U.S. DEPARTMENT OF ENERGY | NNSA National Nuclear Security Administration

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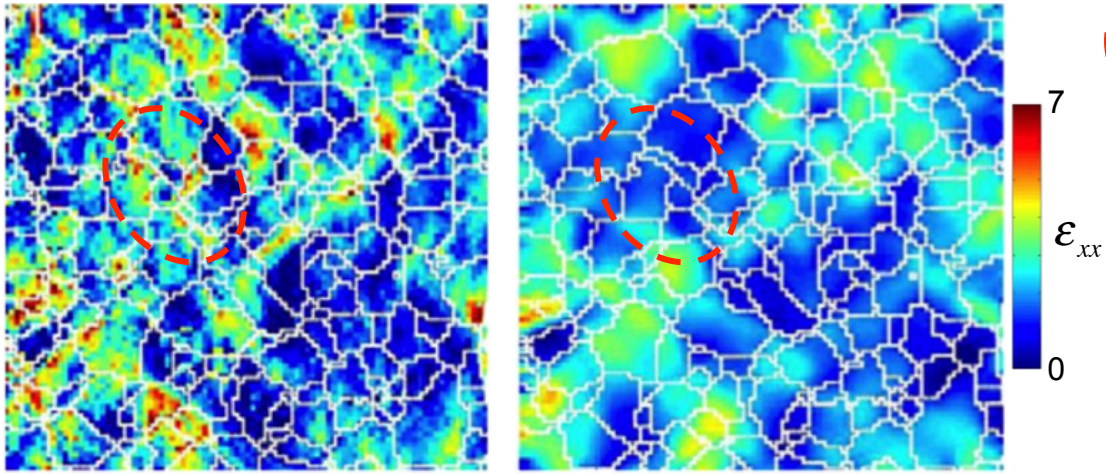
Outline

- **Introduction**
- **Strain Field Analysis: HR-DIC vs. CP-FEM**
- **Texture Analysis: EBSD vs. CP-FEM**
- **Summary**

Previous Work on Sim.- Exp. Comparison

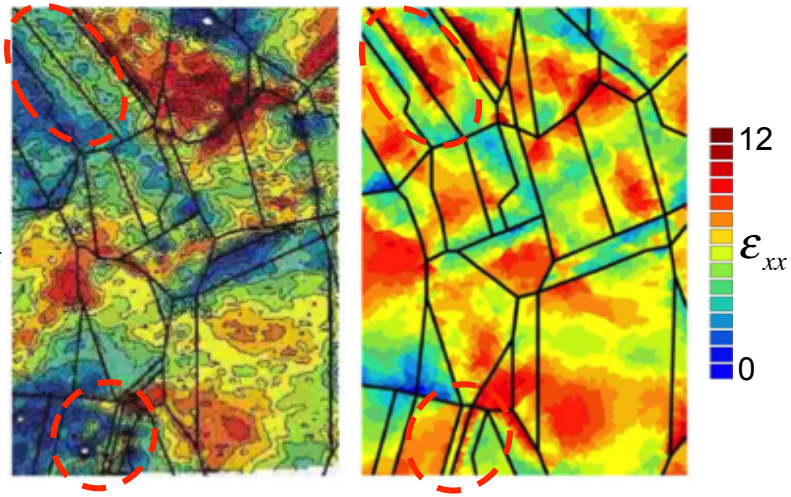
"Comparisons between the model and experiments"

Zr 702 polycrystal (Heripre et al, 2007)
(2.5 % strain)



Experiment Simulation

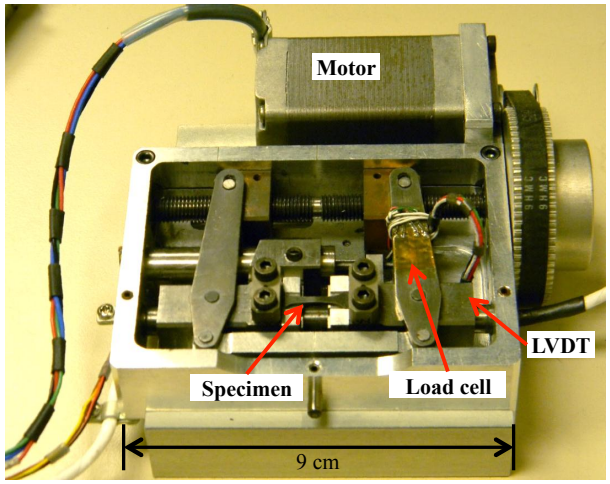
OFHC Cu polycrystal (Musienko et al, 2007)
(5 % strain)



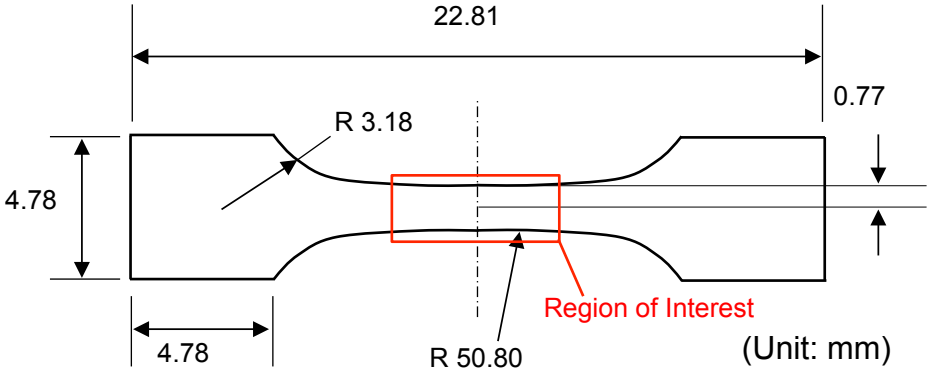
Experiment Simulation

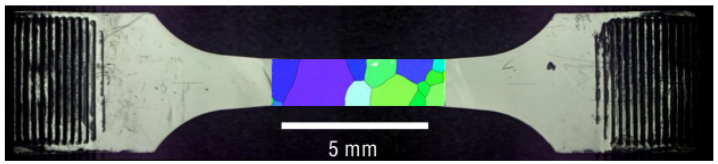
Limited success has been achieved in modeling polycrystal deformation behavior due to unknown subsurface grains

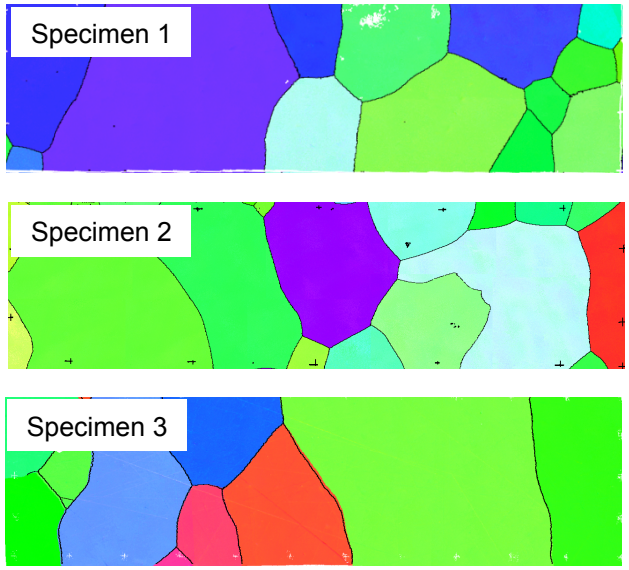
Experimental Setup



- Tantalum oligocrystals with mostly columnar 2D grain structure eliminate unknown subsurface grain morphology.
- *In-situ* load frame developed at Sandia
- HR-DIC (surface strain fields) and EBSD (crystal orientations) measurements at load inside SEM

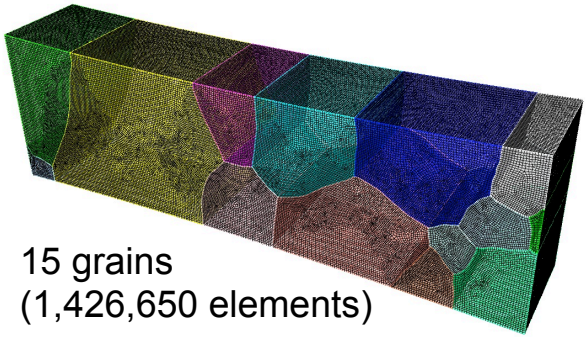






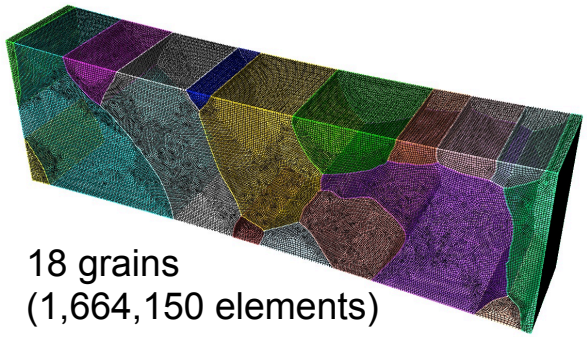
CP-FEM Simulations

- BCC CP-FEM model developed at Sandia (JAS3D)*
- 24 {110}<111> slip systems
- Rate dependent/ dislocation slip based: $\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha}\left(\frac{\tau^{\alpha}}{g^{\alpha}}\right)^{1/m}$
- Slip resistance: $g^{\alpha} = \min\left(\tau_{EI}^{*\alpha}, \tau_{LT}^{*\alpha}\right) + \tau_{obs}^{\alpha}$
- Strain hardening: $\tau_{obs}^{\alpha} = A\mu b\sqrt{\sum_{\beta=1}^{NS}\rho^{\beta}}$ $\qquad \dot{\rho}^{\alpha} = \left(\kappa_1\sqrt{\sum_{\beta=1}^{NS}\rho^{\beta}} - \kappa_2\rho^{\alpha}\right)\cdot\left|\dot{\gamma}^{\alpha}\right|$



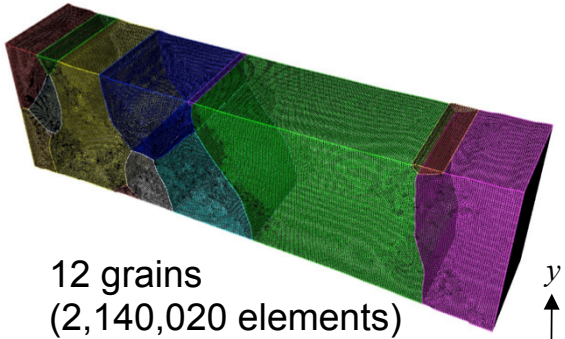
15 grains
(1,426,650 elements)

Specimen 1



18 grains
(1,664,150 elements)

Specimen 2

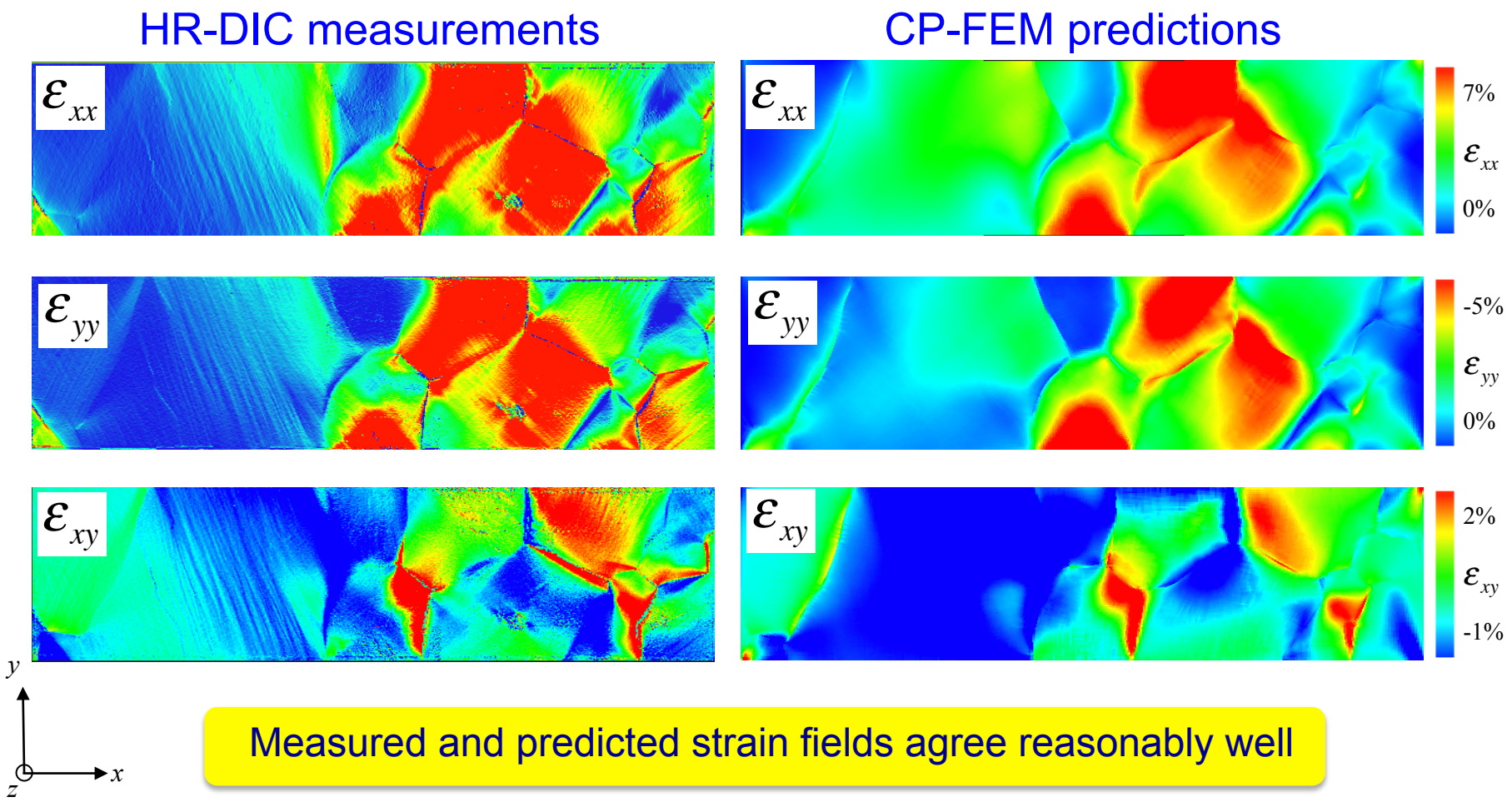


12 grains
(2,140,020 elements)

Specimen 3

*Lim et al., *Int. J. Plasticity* (2014)

Surface Strain Field Predictions: Specimen 1

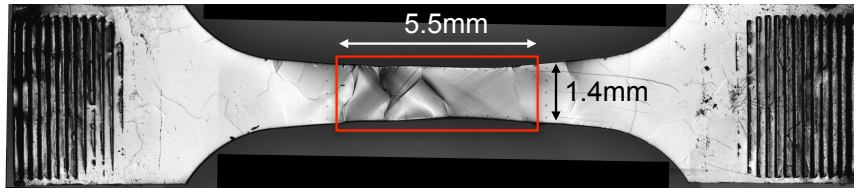


Measured and predicted strain fields agree reasonably well

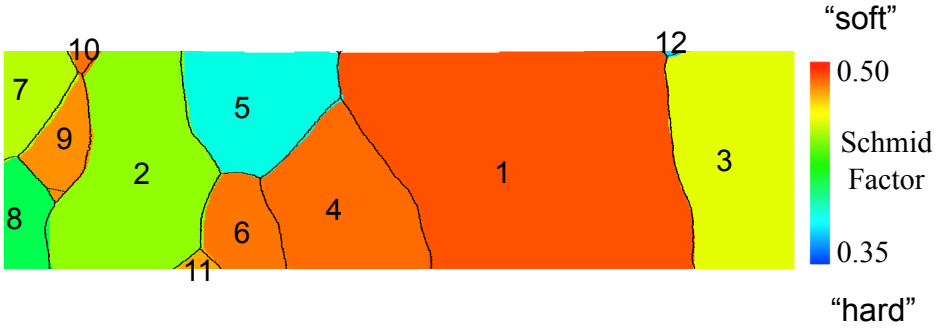
Applied strain = 4.3%

Surface Strain Field Predictions: Specimen 3

Deformed specimen



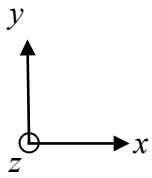
Max. Schmid factor



Measured strain fields (HR-DIC)

Predicted strain fields (CP-FEM)

Applied strain = 0 %

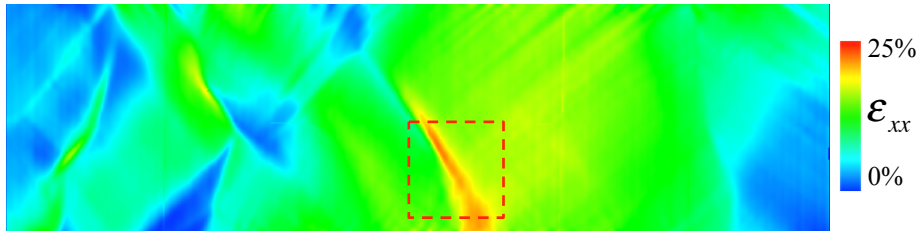


Measured and predicted strain fields agree reasonably well

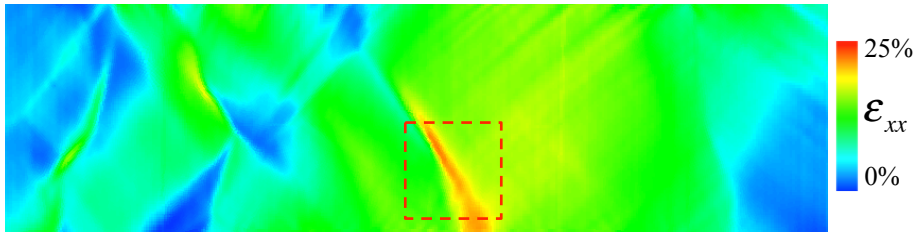
Rescaling of DIC Data: Specimen 3

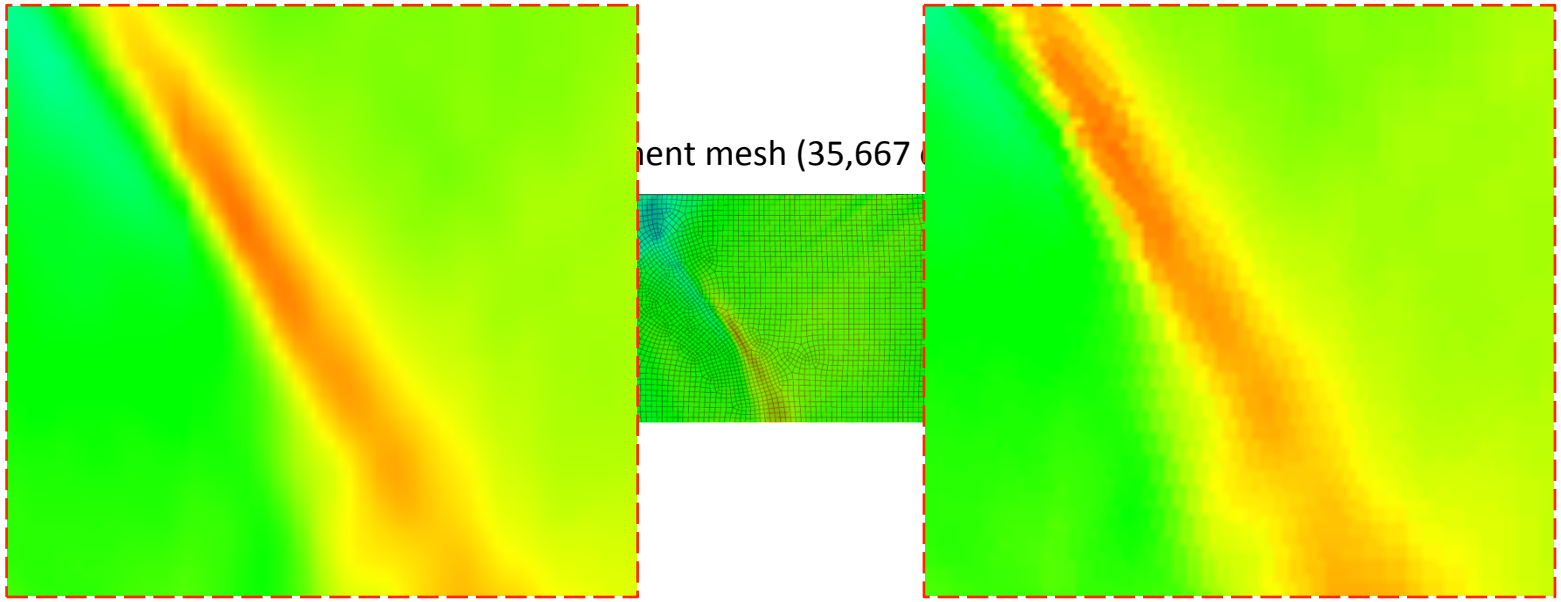
Projection of raw HR-DIC data onto the finite element mesh

Full DIC data (781,015 data points)



Reduced DIC data (35,667 data points)





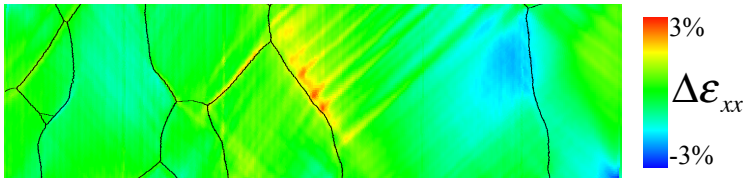
Quantitative Sim.-Exp. Comparisons

Deviation between measured and simulated ε_{xx}

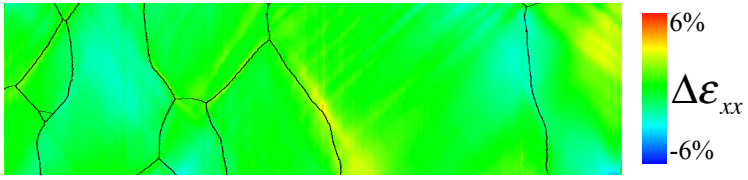
$$\Delta\varepsilon = \varepsilon^{DIC} - \varepsilon^{sim}$$ (per element basis)

Applied strain

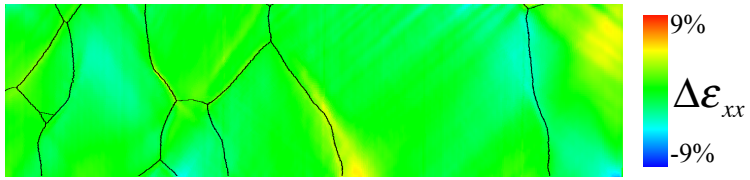
$\varepsilon_a = 0.02$



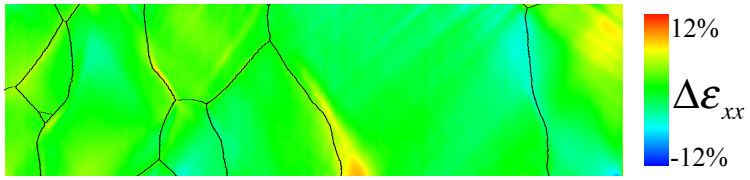
$\varepsilon_a = 0.04$



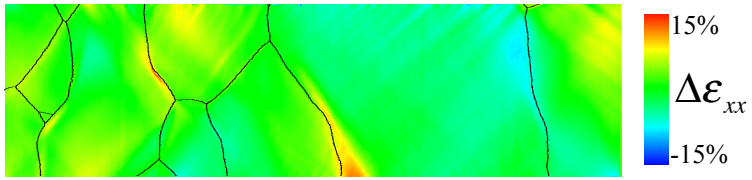
$\varepsilon_a = 0.06$



$\varepsilon_a = 0.08$



$\varepsilon_a = 0.10$



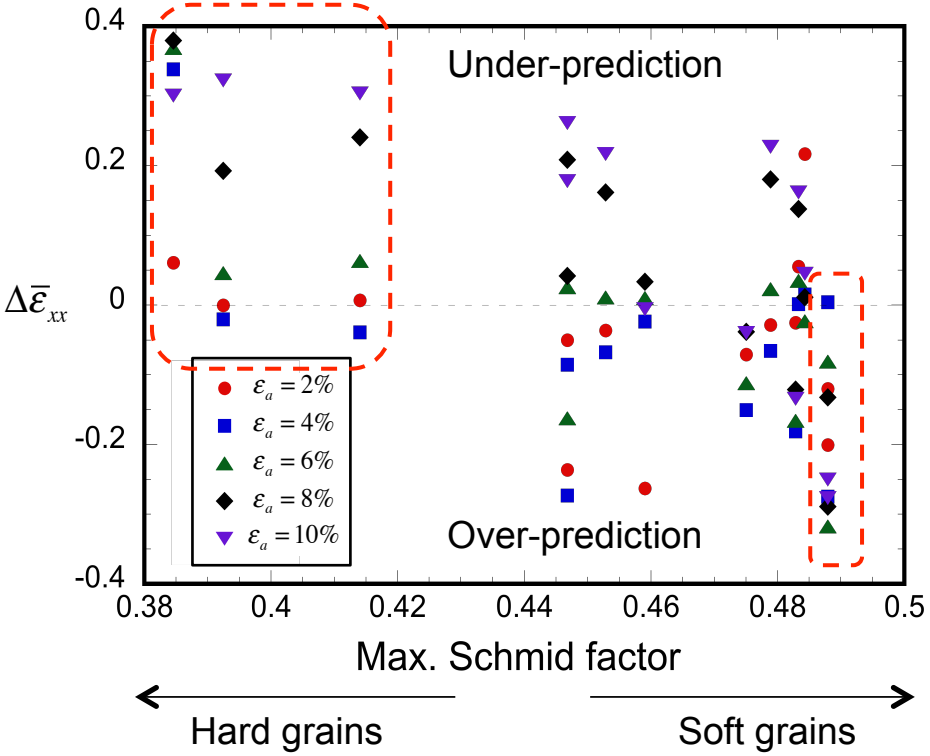
$$\Delta\varepsilon^{avg} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\varepsilon_i^{DIC} - \varepsilon_i^{sim}\right)^2}$$

Applied strain	$\Delta\varepsilon_{xx}^{avg}$	$\Delta\varepsilon_{yy}^{avg}$	$\Delta\varepsilon_{xy}^{avg}$
0.02	0.007	0.006	0.003
0.04	0.010	0.010	0.007
0.06	0.014	0.012	0.010
0.08	0.021	0.014	0.014
0.10	0.034	0.018	0.016

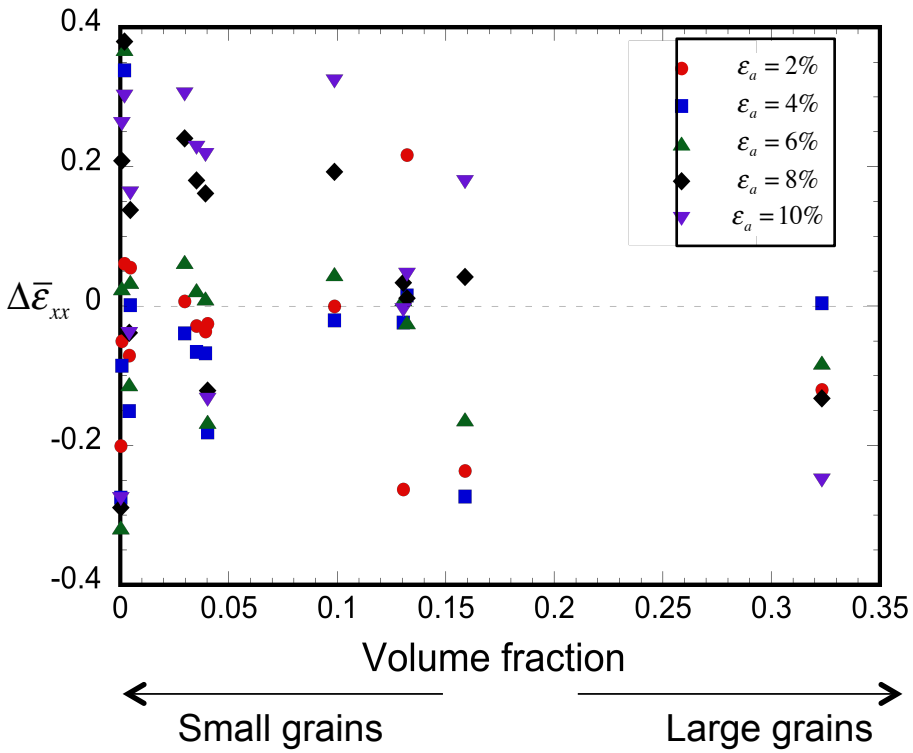
Effects of Crystal Orientations and Grain Sizes

$$\Delta\bar{\varepsilon}_{xx} = \frac{\varepsilon_{xx}^{DIC} - \varepsilon_{xx}^{sim}}{\varepsilon_a} \quad \text{(per grain basis)}$$

Effects of max. Schmid factor

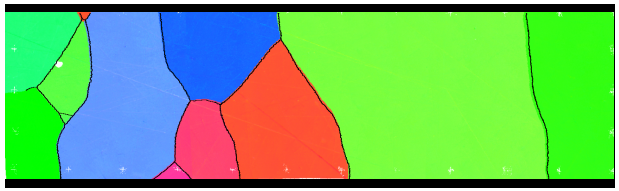


Effects of volume fraction

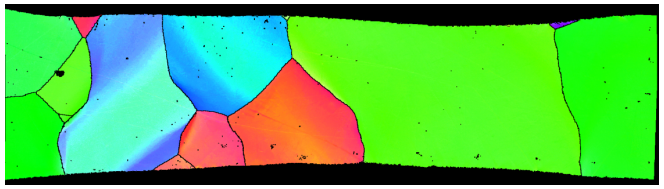


CP-FEM predictions are less successful for grains in extreme orientations

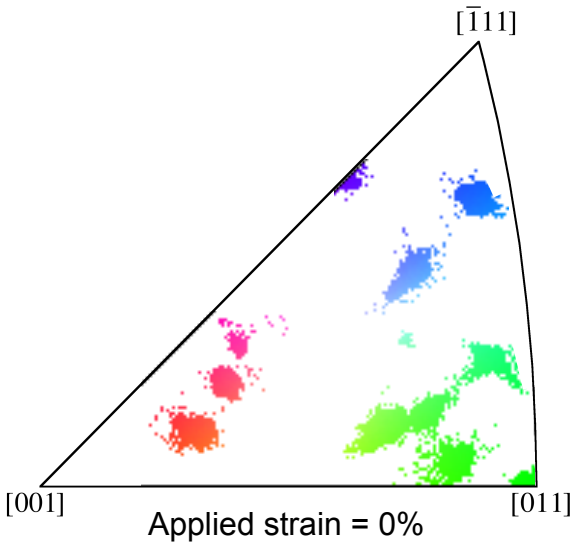
Crystal Rotations: IPFs in RD



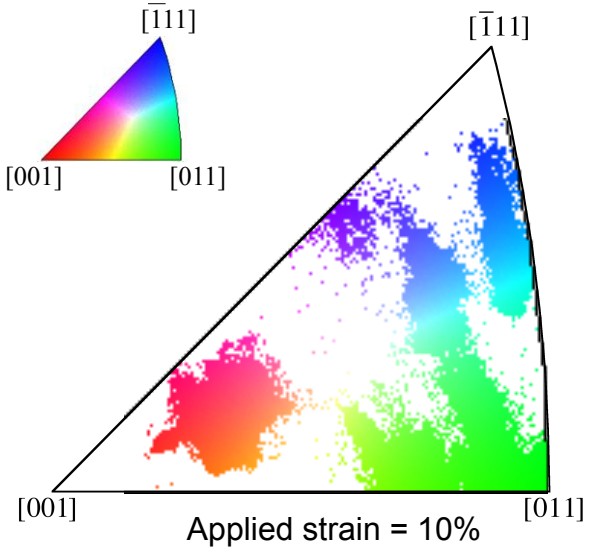
Applied strain = 0%



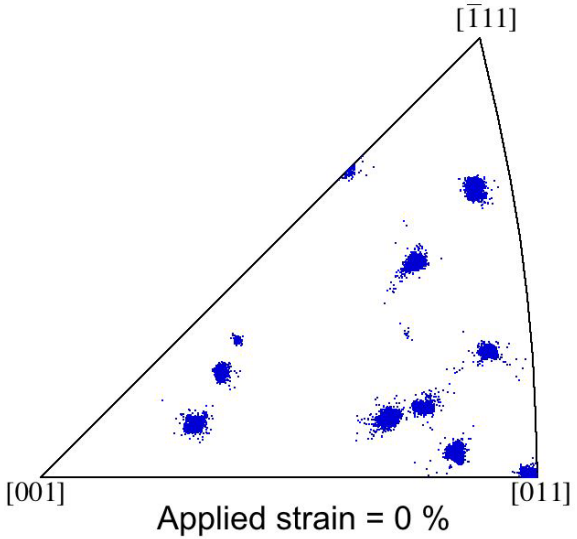
Applied strain = 10%



Applied strain = 0%



Applied strain = 10%



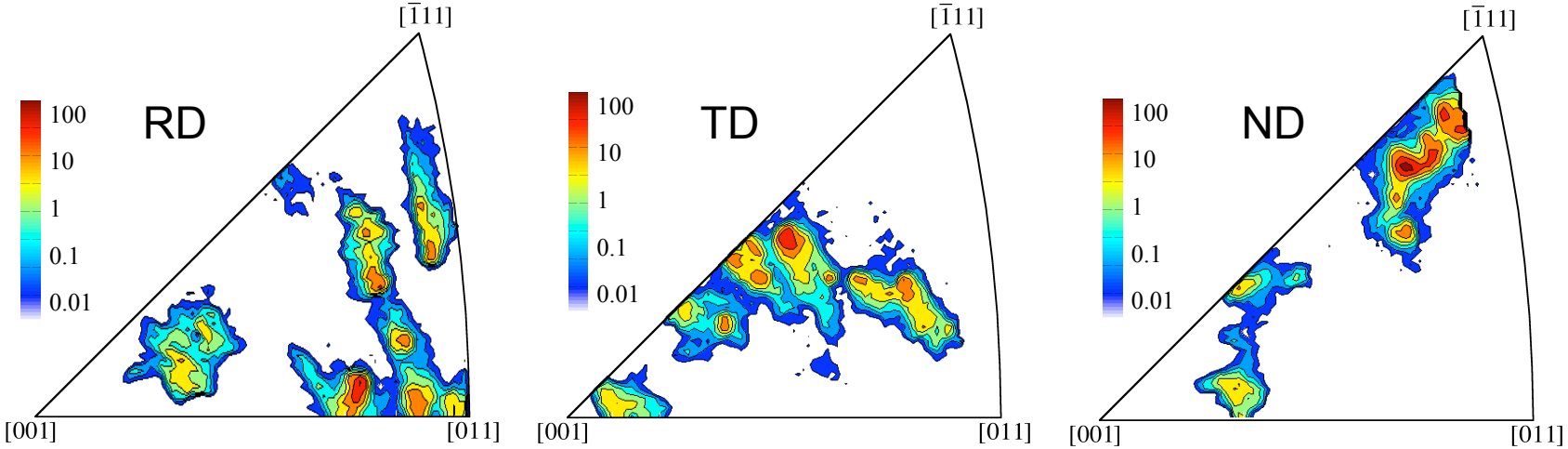
Applied strain = 0 %

EBSD measurement

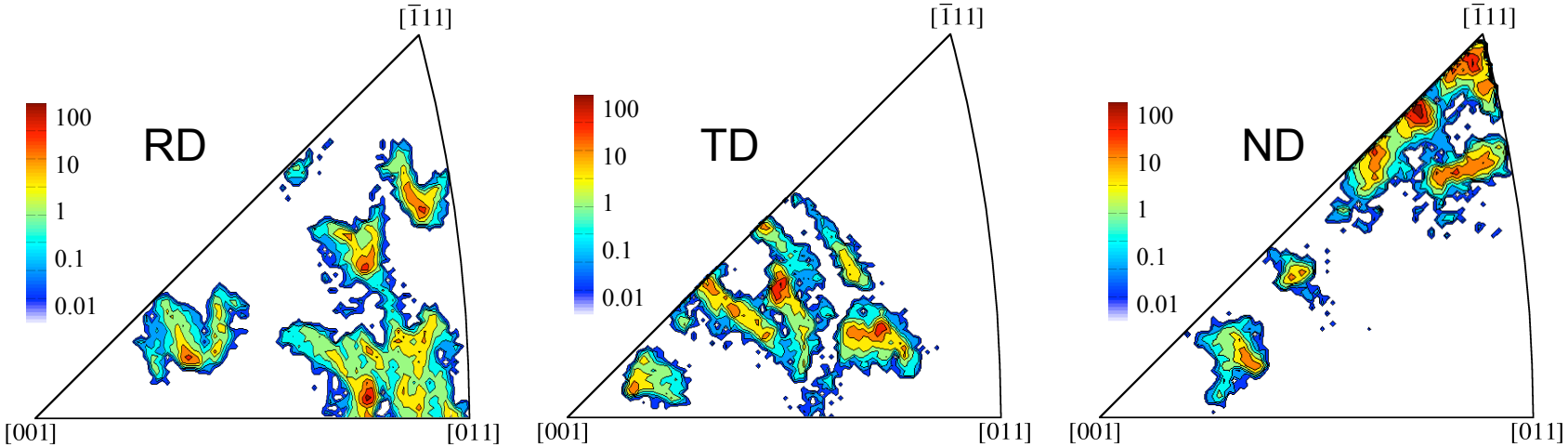
CP-FEM prediction

IPF contour plots indicate good agreement between model and experiment.

Deformed Texture Predictions



EBSD measurements



CP-FEM predictions

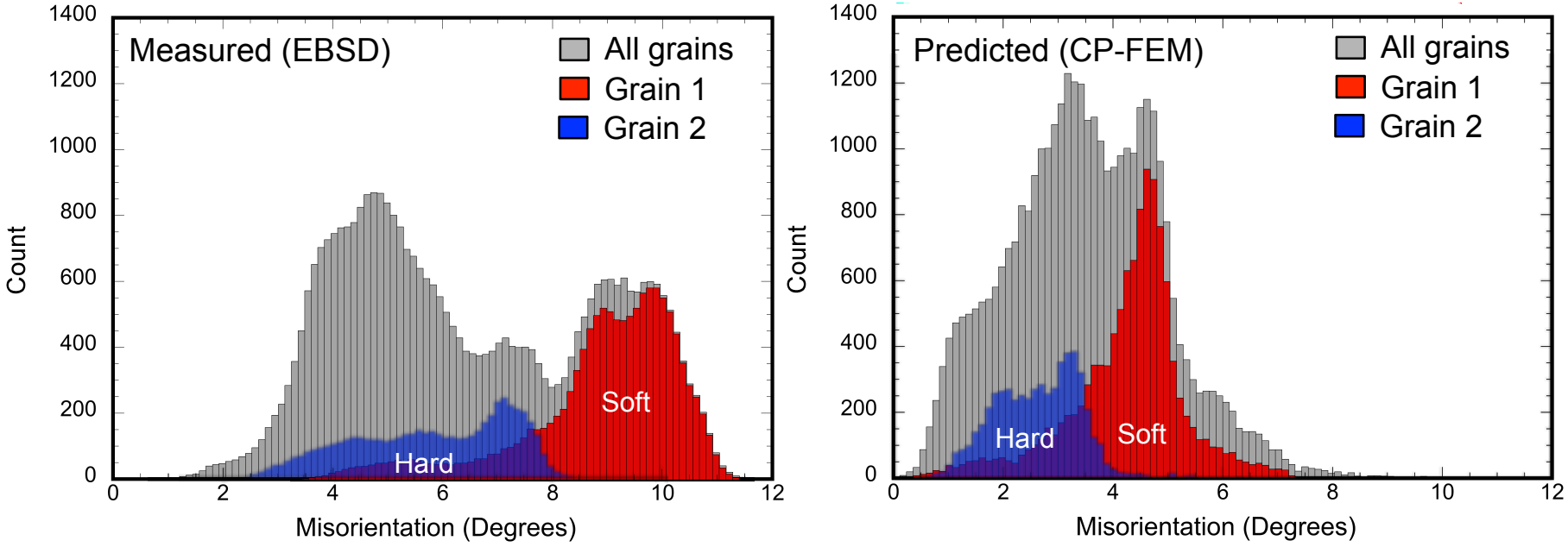
IPF contour plots indicate good agreement between model and experiment.

Crystal Rotations: Misorientation

$$\theta = \cos^{-1}\left[\frac{1}{2}\left(\Delta g_{11}^{AB} + \Delta g_{22}^{AB} + \Delta g_{33}^{AB} - 1\right)\right] \qquad \Delta g^{AB} = g^{B}\left(g^{A}\right)^{-1}$$

g : rotation matrix

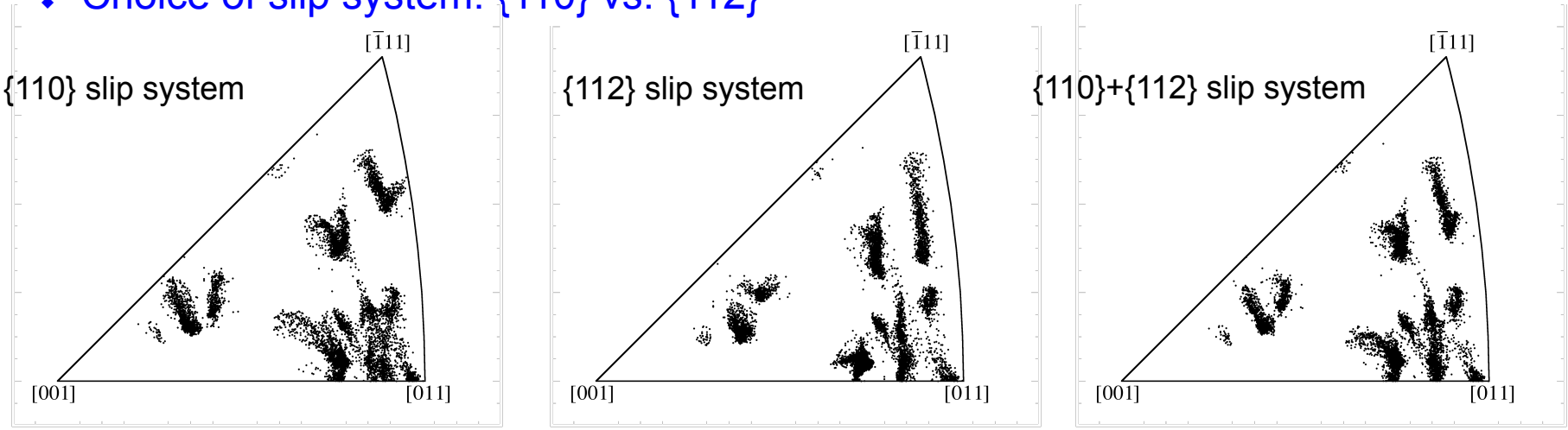
Misorientation angles (at 10% deformation) relative to the initial orientation



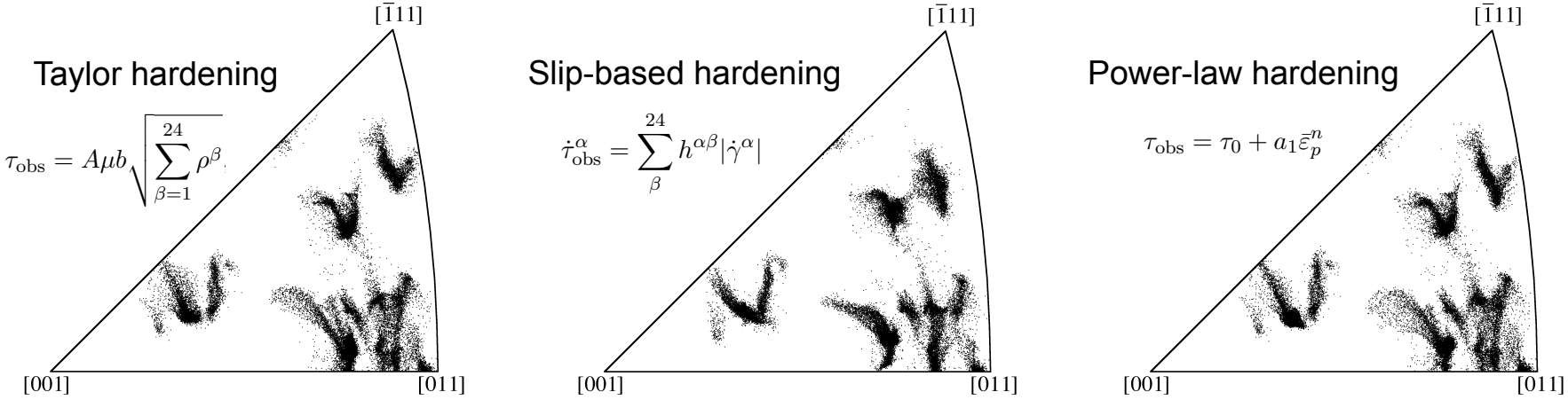
CP-FEM model under-predicted measured crystal rotation

Other Constitutive Effects

❖ Choice of slip system: {110} vs. {112}

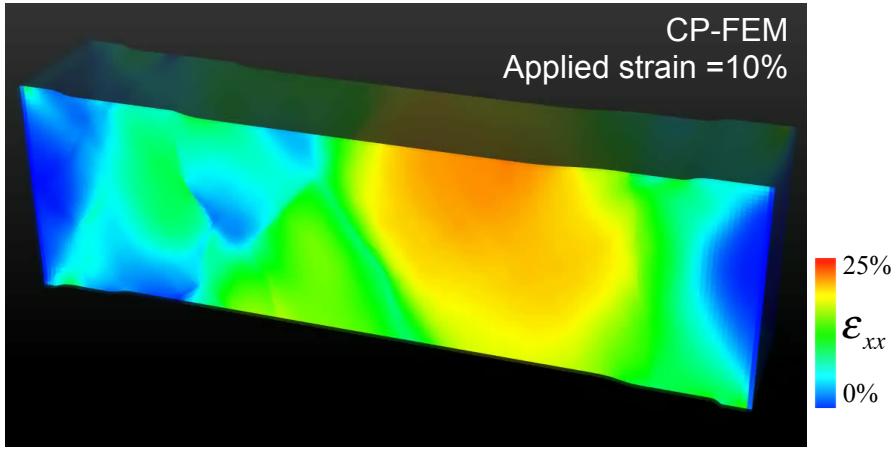


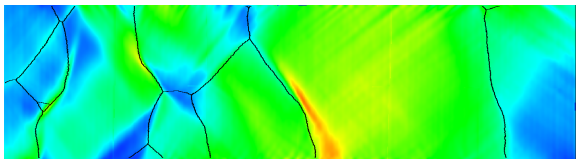
❖ Effects of different hardening laws



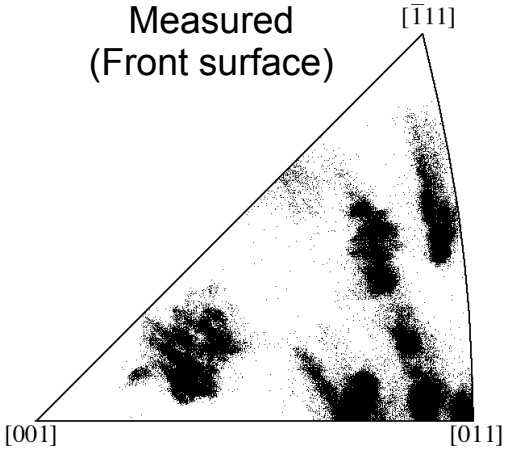
Choice of slip system and hardening law has relatively small effect

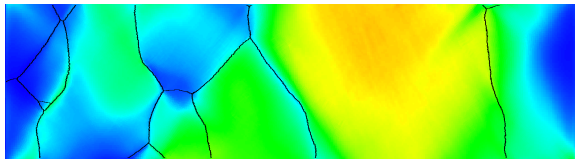
3D Effects



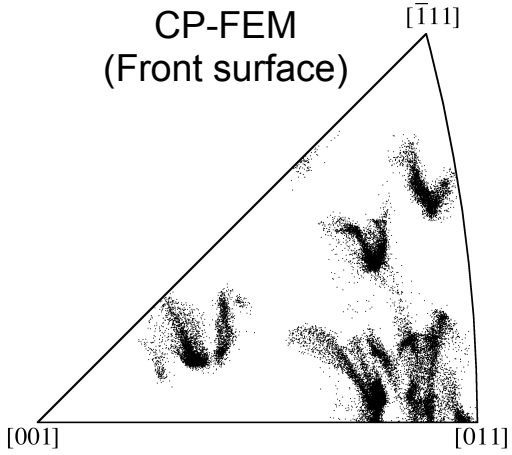


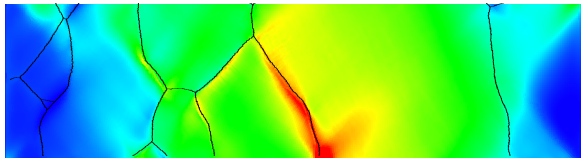
Measured
(Front surface)



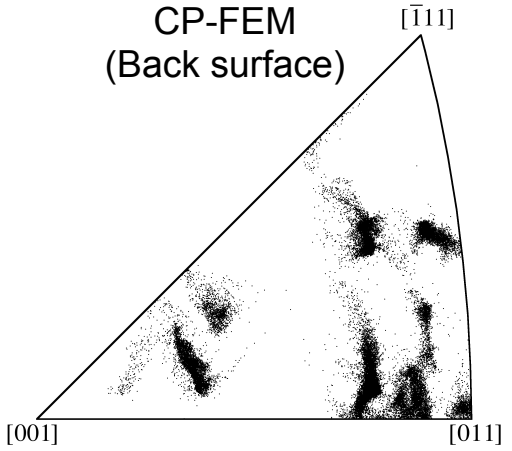


CP-FEM
(Front surface)





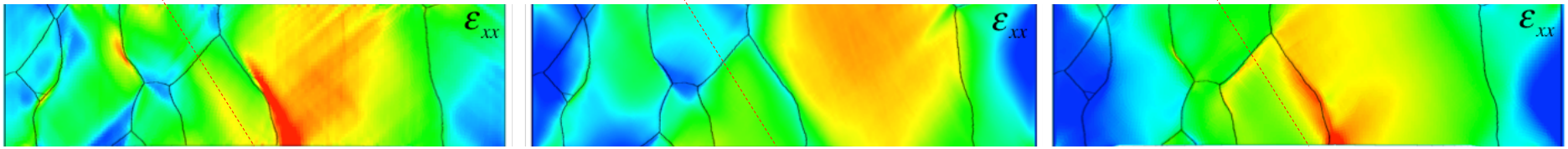
CP-FEM
(Back surface)

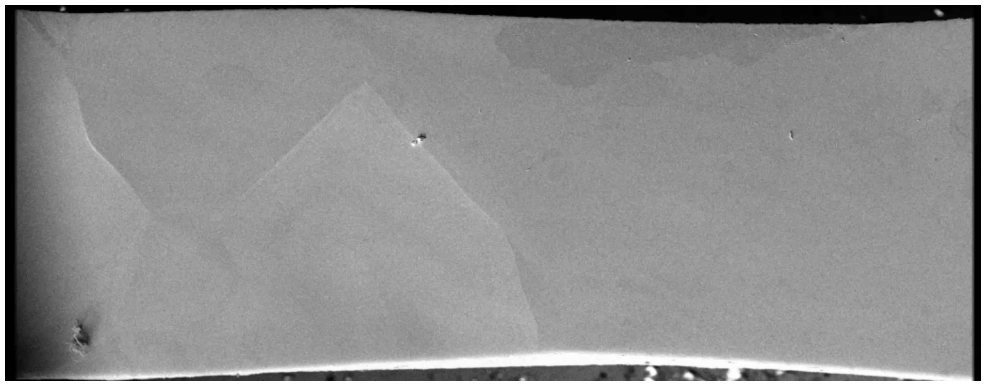


Full 3D model is required to accurately model columnar structured specimens.

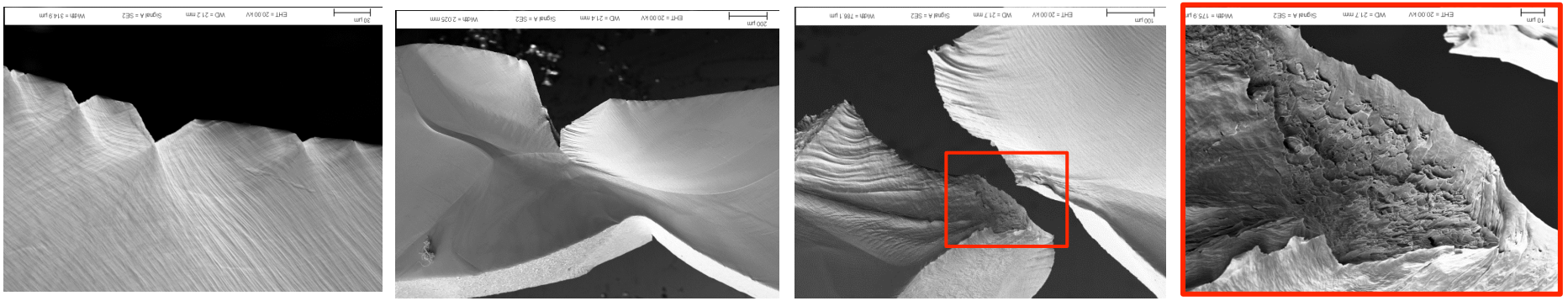
Limitations: Fracture

Experiment (front) | Model (front) | Model (back)





Selected images from various points in the fracture process.



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Summary

Conclusions

- First quantitative comparison between CP-FEM simulations and experimental measurements
- Model predictions of strain fields showed good agreement with HR-DIC measurements (~ 3% deviation at 10% applied strain).
- Model predictions of crystal rotations showed good agreement with EBSD measurements. Larger deviations at extreme crystal orientations.

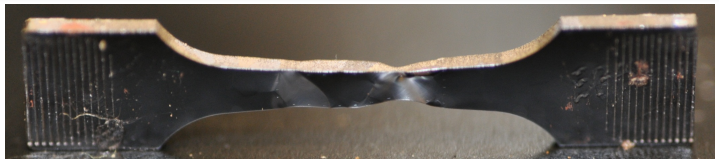
Future Work

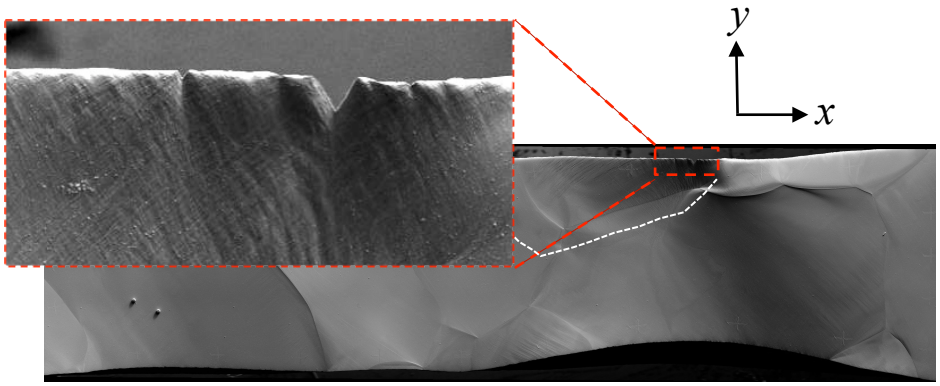
- More sophisticated treatment of grain boundary and dislocation – grain boundary interactions
- Damage/ Fracture modeling

THANK YOU !

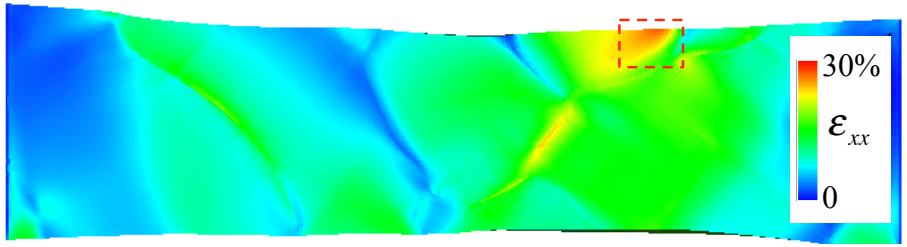
Email: hnlim@sandia.gov

Failure Predictions: Specimen 2



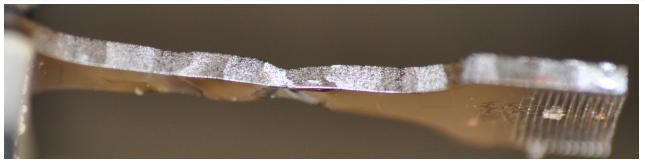


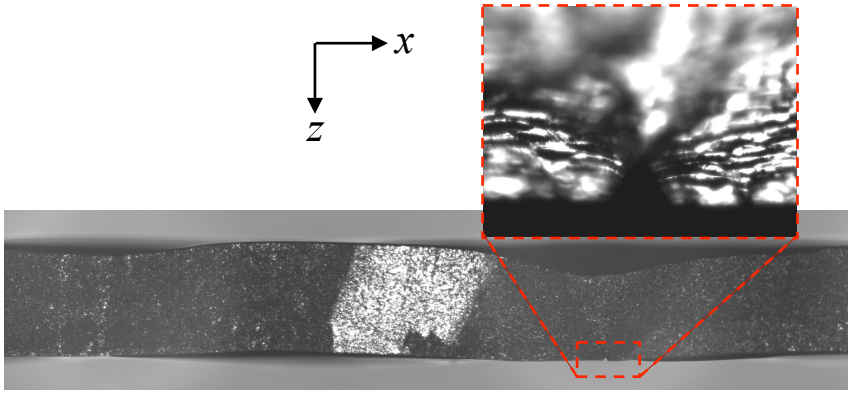
Surface image (19.2%)



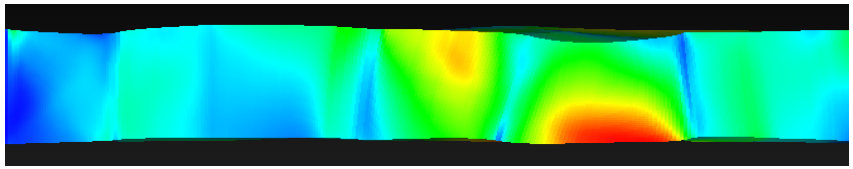
Simulated ε_{xx}

Side view





Surface image (19.2%)



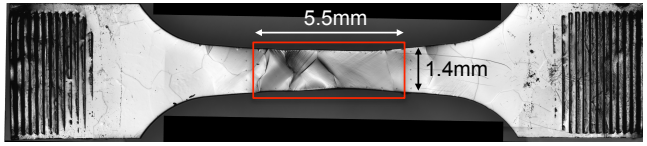
Simulated ε_{xx}

Top view

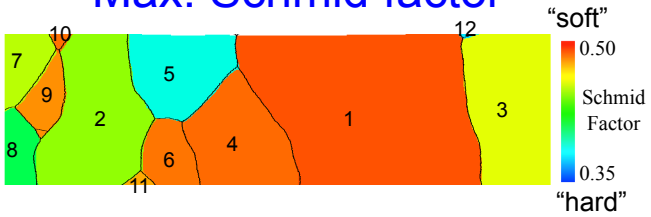
Failure location agrees with the location of the highest ε_{xx} from the simulation

Surface Strain Field Predictions: Specimen 3

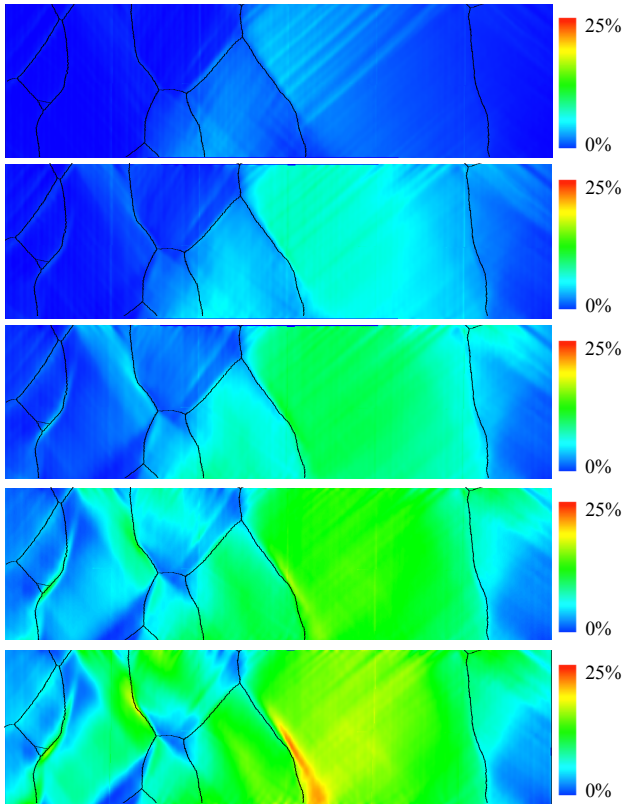
Deformed specimen



Max. Schmid factor



Measured strain fields (HR-DIC)



$\varepsilon_a = 2\%$

$\varepsilon_a = 4\%$

$\varepsilon_a = 6\%$

$\varepsilon_a = 8\%$

$\varepsilon_a = 10\%$

Predicted strain fields (CP-FEM)