SAND2013-5906C

Finite Element Predictions of Grainscale Behavior in BCC Metals

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Sandia National Laboratories

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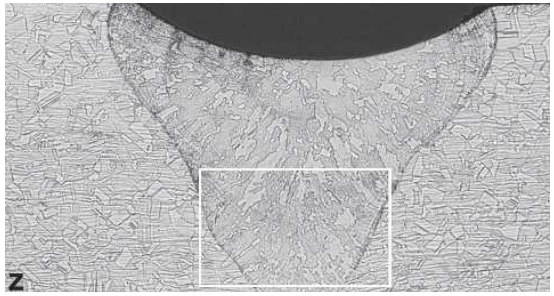
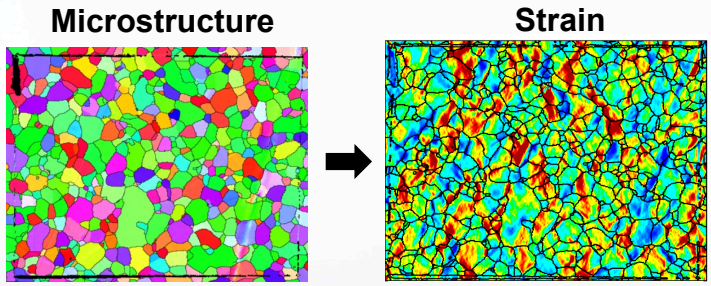
Can We Predict Grainscale Deformation Behavior?

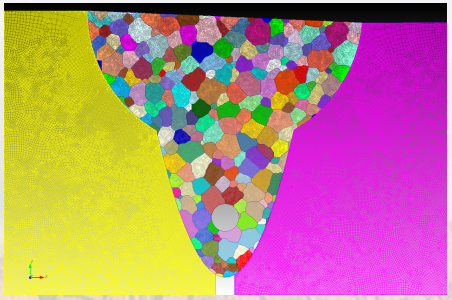
- Need the capability to model complex geometries with realistic microstructures.

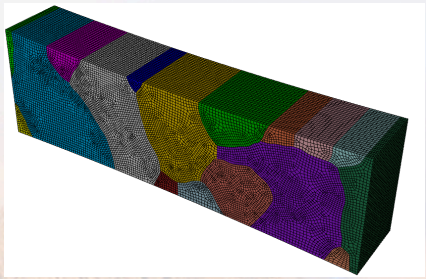


- Deformation in polycrystals involves the networks of grains



- Need expedient models grainscale deformation
  - Can we use current CPFEM models?
  - How well do they work?
  - What needs improvement?





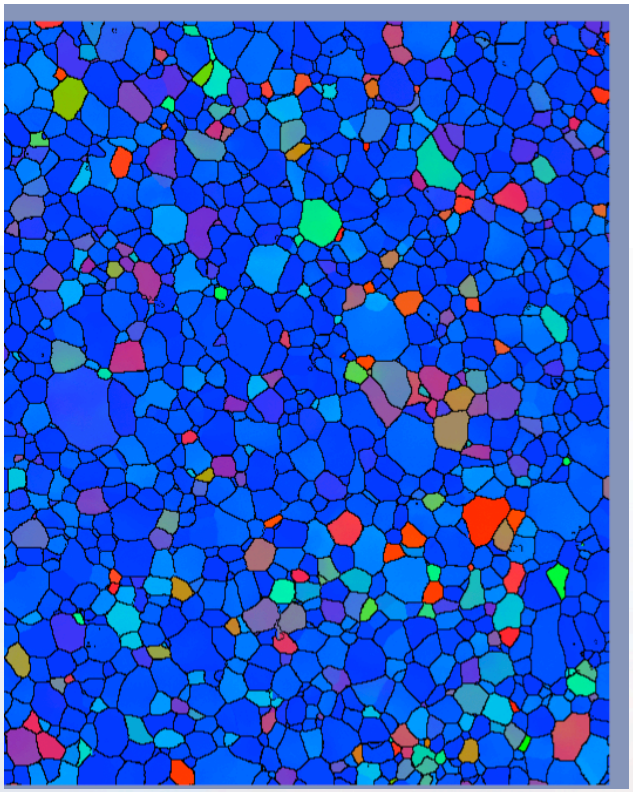
Finite Element Predictions of Grainscale Behavior in BCC Metals

- Previous work in validating CPFEM models
  - Crystal Rotations (EBSD)
  - Surface Strains (DIC)
- Our Ongoing Validation of BCC Tantalum CPFEM Models
  - Our CPFEM model and experiments
  - Surface Strain Comparisons
  - Texture Evolution and Crystal Rotations
  - Failure
- Model Sensitivity
  - Mesh Sensitivity
  - Sensitivity to Initial Orientations
  - Sensitivity to Slip Planes

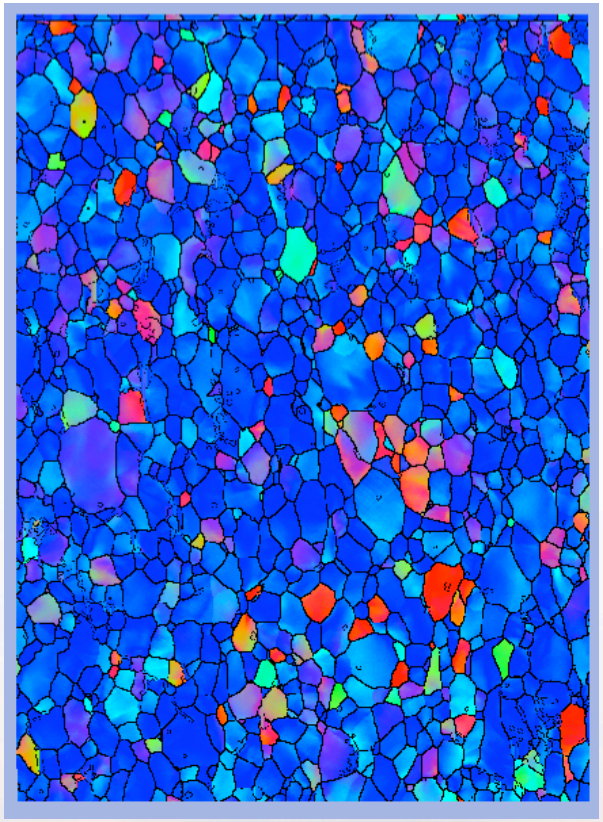
Previous Validation Attempts Using EBSD & DIC

(A limited sampling…)

EBSD of Interstitial-Free Steel Polycrystals

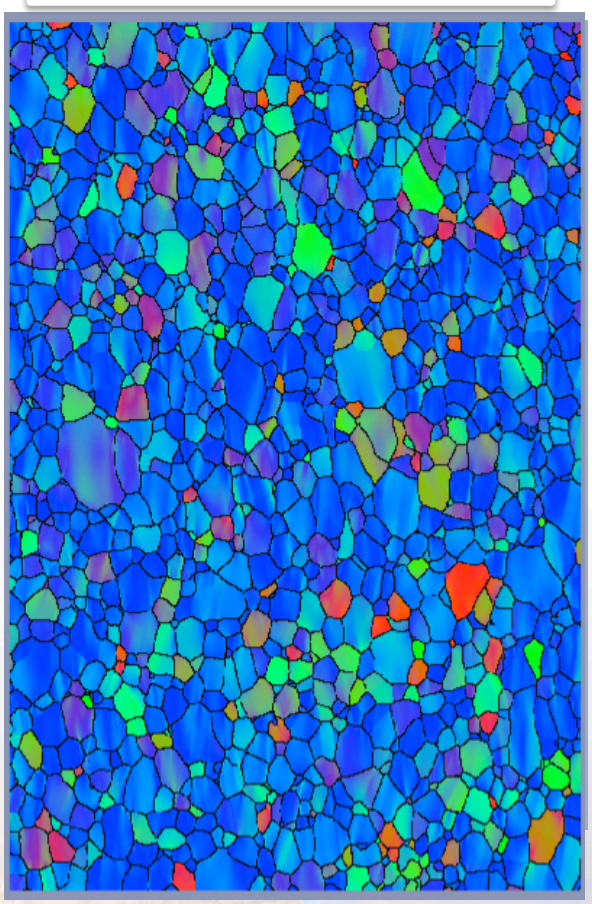


Experiment, 0% Strain



Experiment, 12% Strain

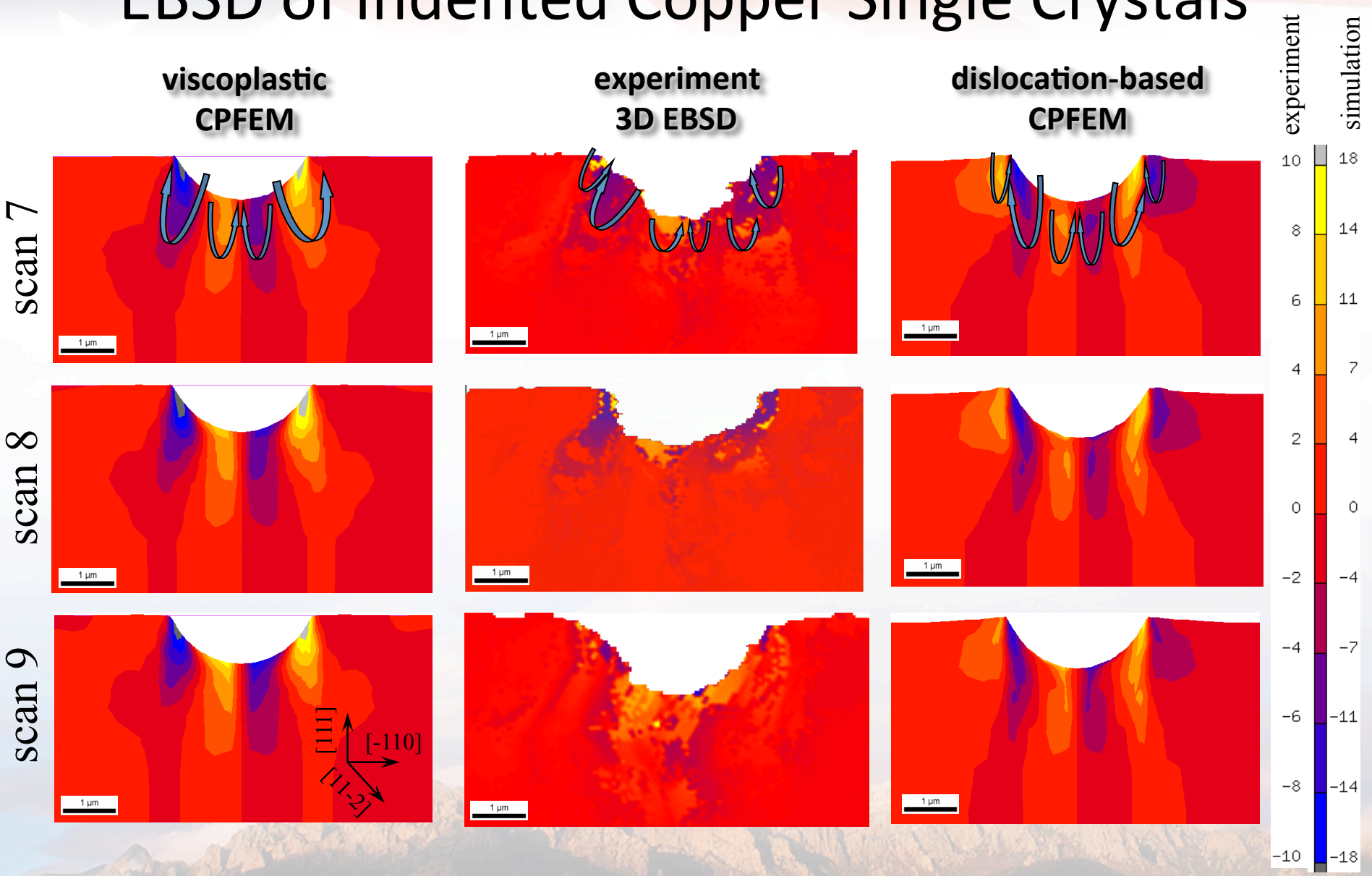
{110+112} only, surface layer



Simulation, 12% Strain

Courtesy of Tony Rollett.

EBSD of Indented Copper Single Crystals



Courtesy of Dierk Raabe.

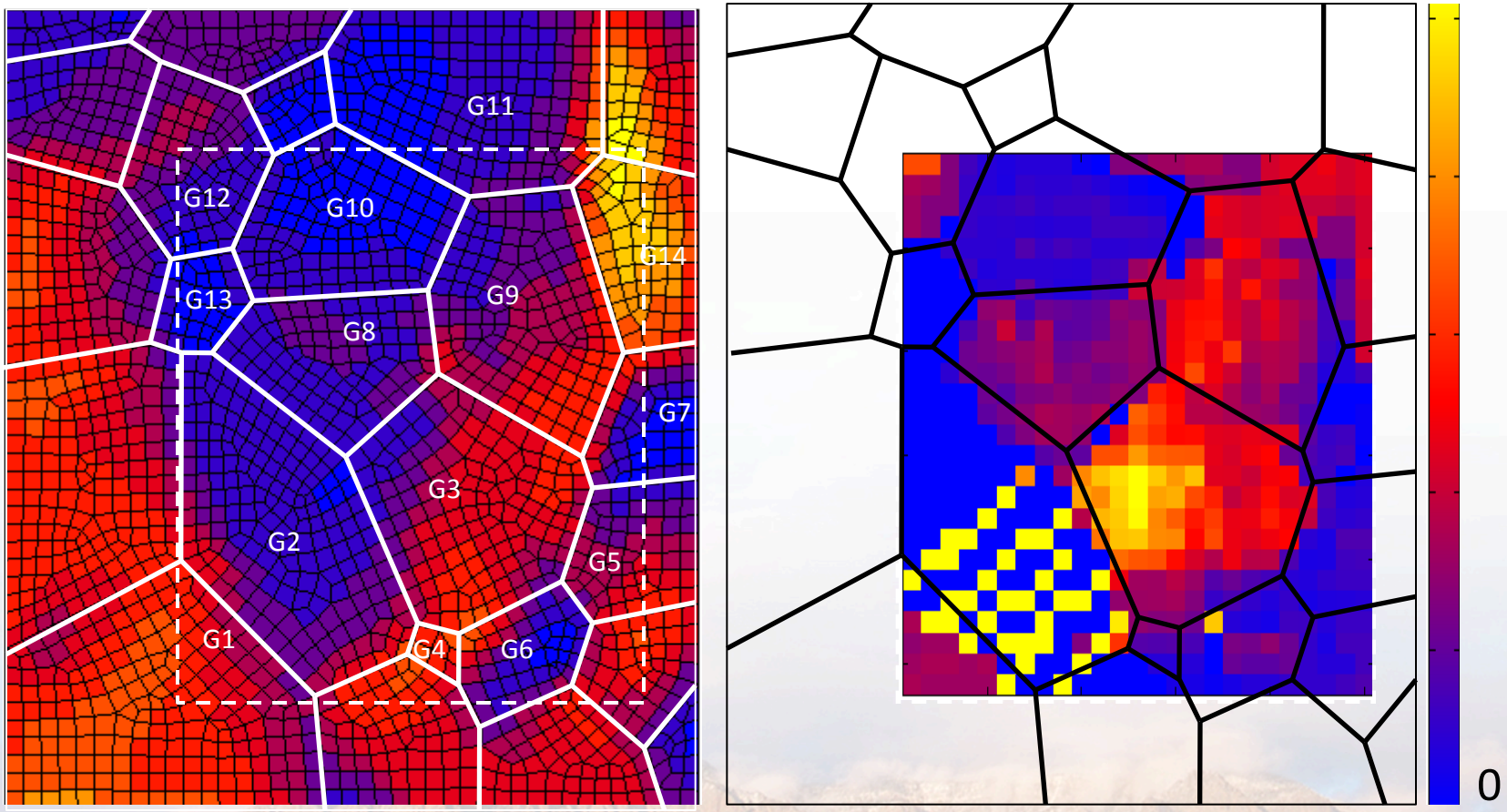
N. Zaafarani, D. Raabe, R.N. Singh, F. Roters, S. Zaefferer, *Acta Mater.* **54** (2006) 1707.

Strain Mapping in a Titanium Polycrystal

Total shear after 1.5% applied strain:

Simulation

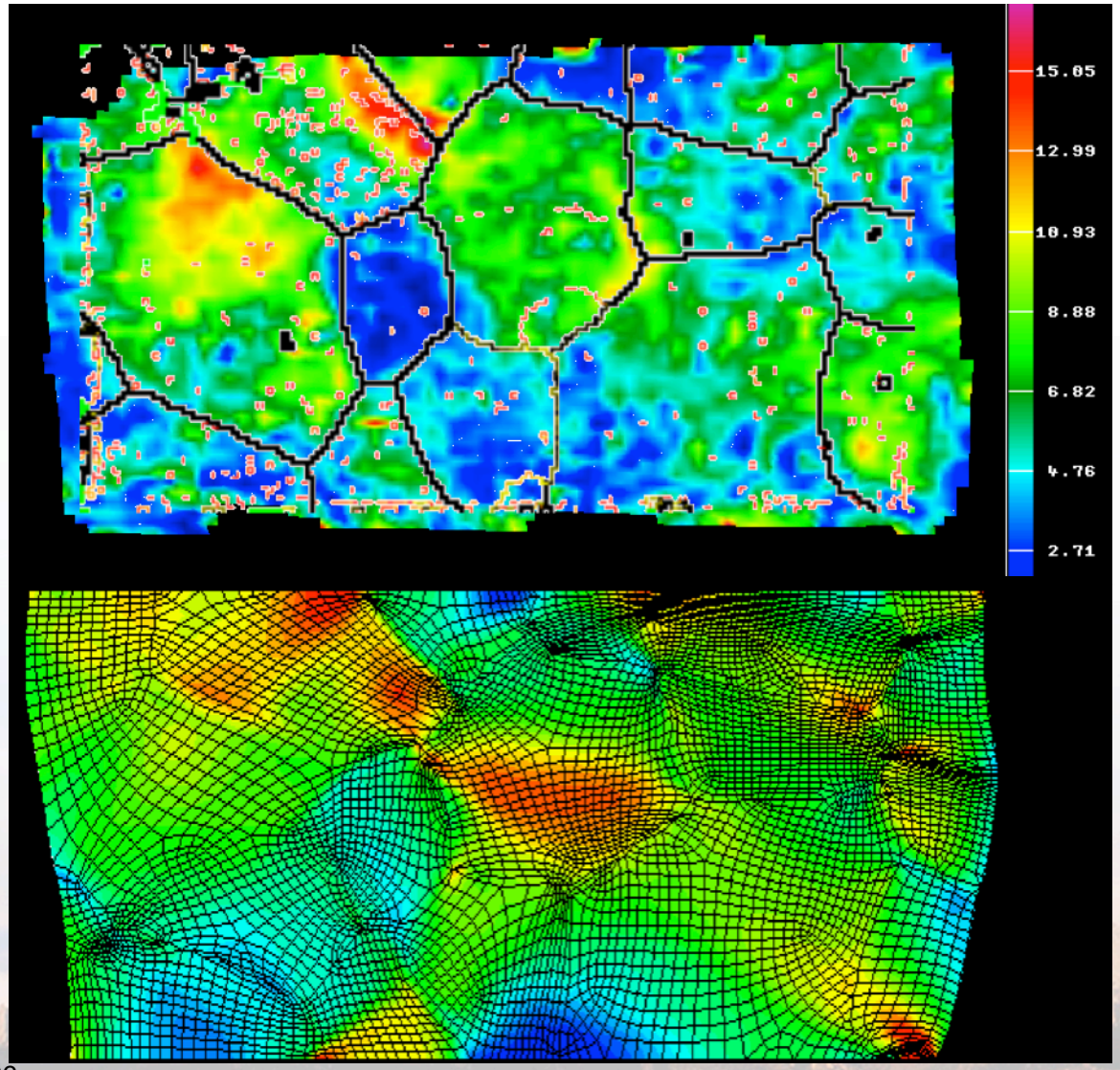
Experiment



Courtesy of Marty Crimp and Tom Bieler.

Y. Yang, L. Wang, T.R. Bieler, P. Eisenlohr, M.A. Crimp, *Met. Trans. A* **42A** (2011) 636.

Strains in an Al Oligocrystal



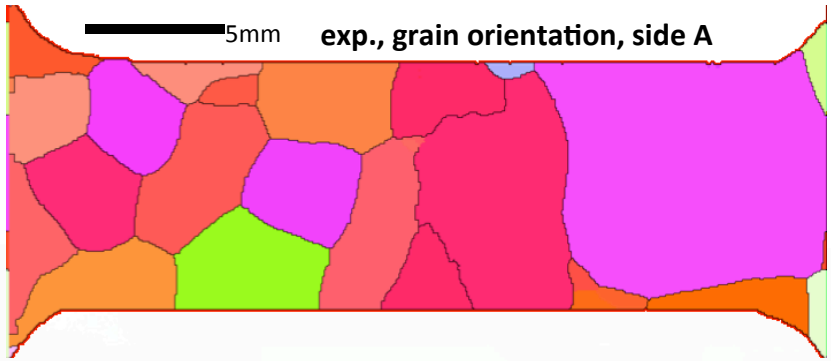
Experiment
(DIC, EBSD)
Mises strain

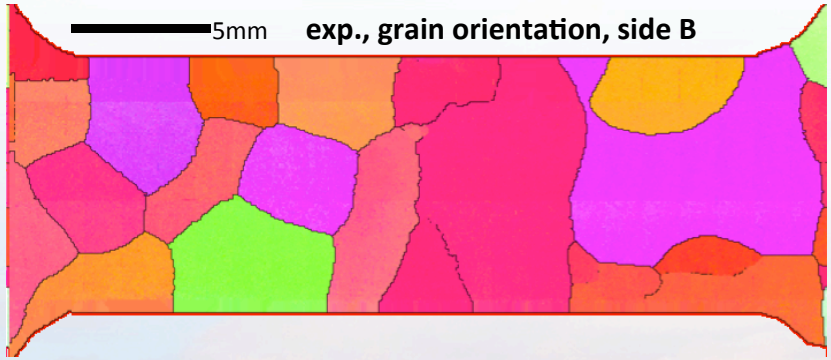
Simulation
(Viscoplastic
CP-FEM)
Mises strain

Courtesy of Dierk Raabe.

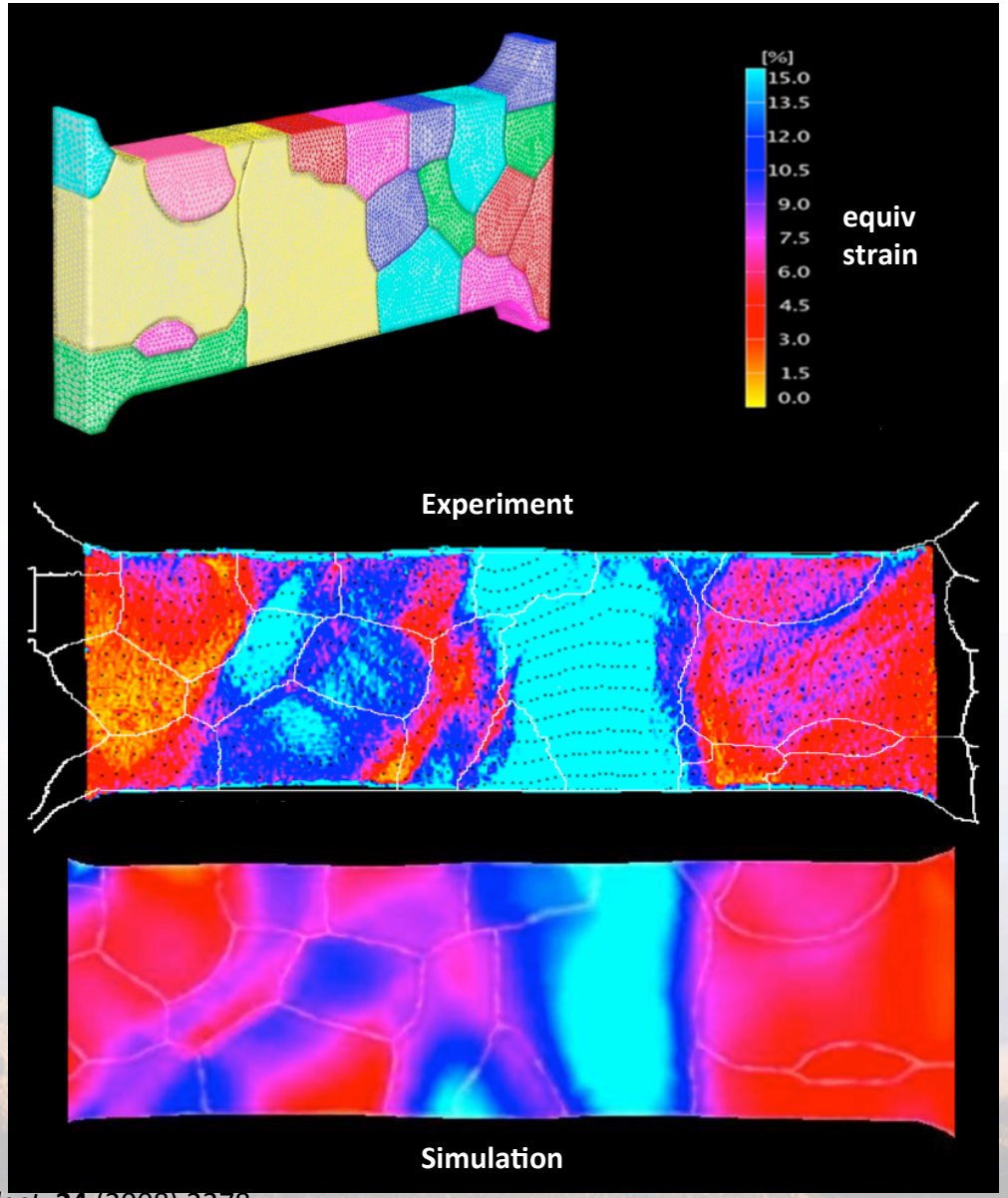
D. Ma, F. Roters, D. Raabe, *Acta Mater.* **54** (2006) 2169 and 2181.

Strains in another Al Oligocrystal





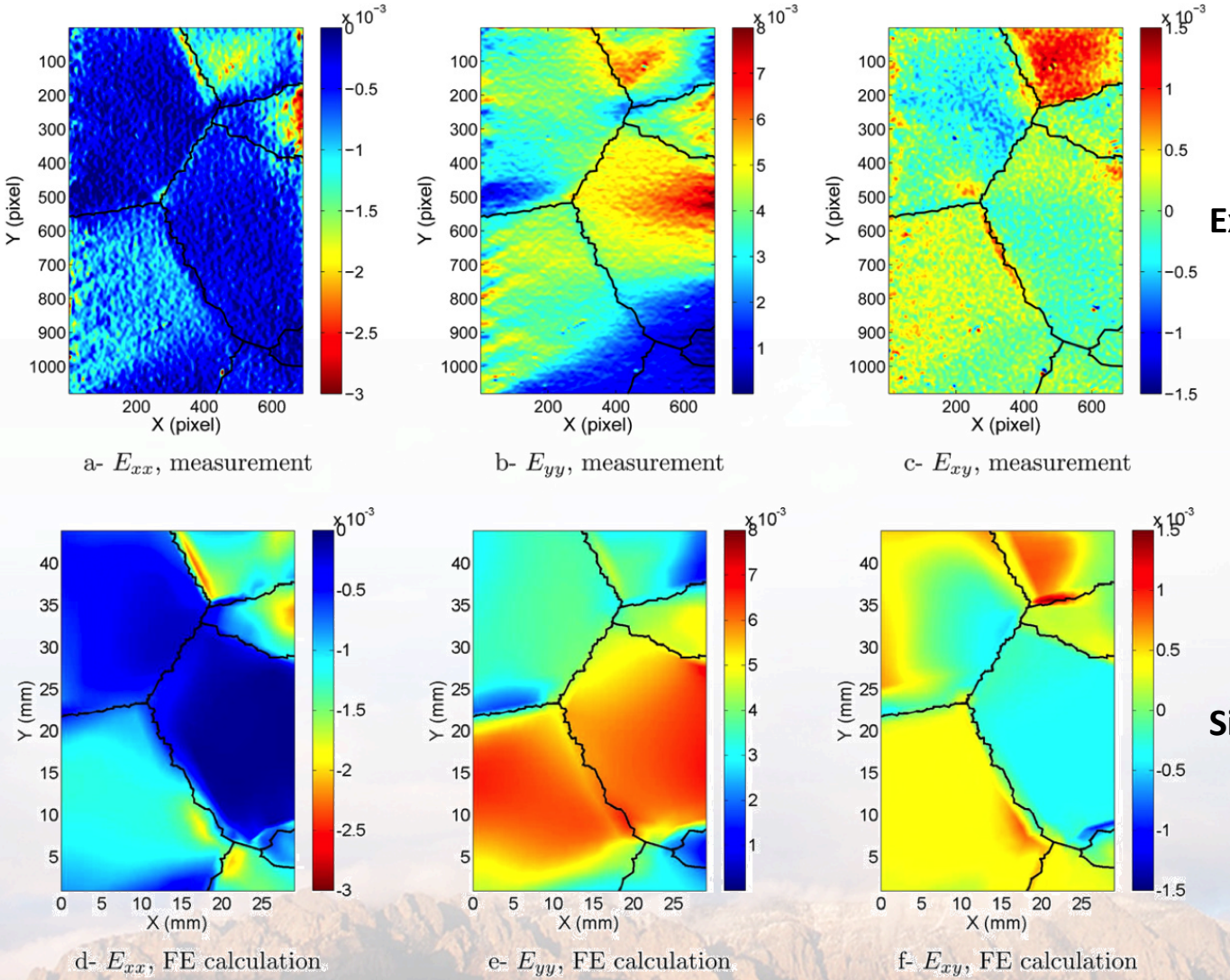
21mm X 8mm X 1mm



Courtesy of Dierk Raabe.

Z. Zhao, M. Ramesh, D. Raabe, A.M. Cuitino, R. Radovitzky, *Int. J. Plast.* **24** (2008) 2278.

Strains in yet another Al Oligocrystal



a- E_{xx}, measurement

b- E_{yy}, measurement

c- E_{xy}, measurement

Experiment

Simulation

d- E_{xx}, FE calculation

e- E_{yy}, FE calculation

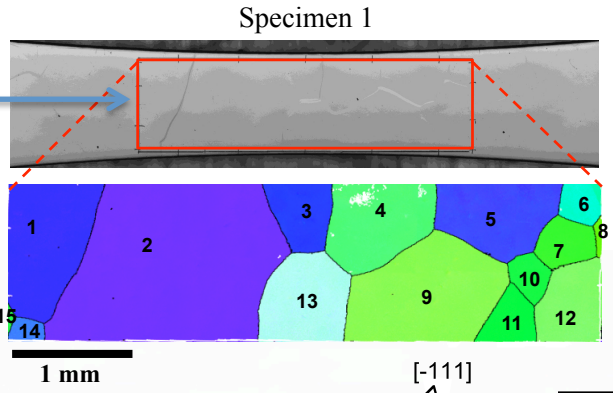
f- E_{xy}, FE calculation

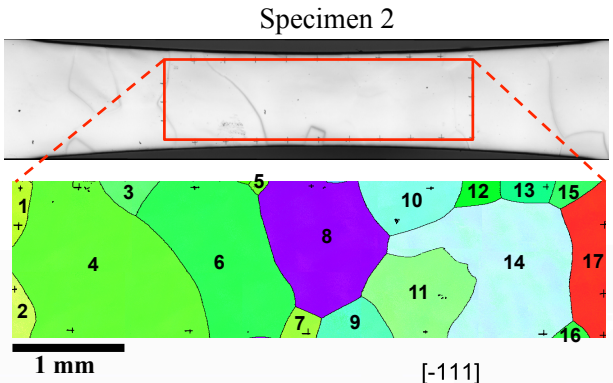
C. Badulescu, M. Grédiac, H. Haddadi, J.-D. Mathias, X. Balandraud, H.-S. Tran, *Mech. Mater.* **43** (2011) 36.

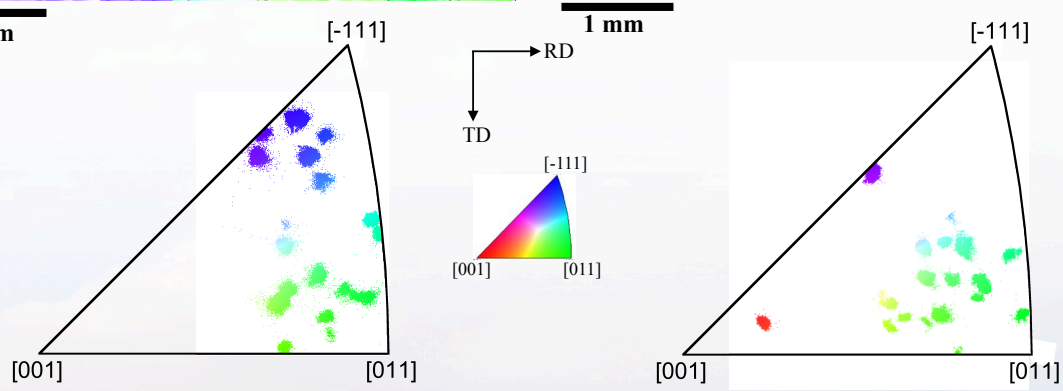
Validation of BCC Tantalum CPFEM Models

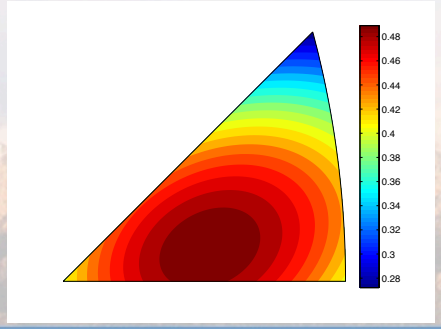
Oligocrystals

Area Of Interest









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BCC CPFEM Formulation

Slip rate: $\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \left(\frac{\tau^{\alpha}}{g^{\alpha}} \right)^{1/m}$ (Hutchinson, 1976)

Slip resistance: $g^{\alpha} = \max\left(\tau_{\mathrm{cr}}^{\alpha} - \tau_{\mathrm{ns}}^{\alpha}, 0\right) + \tau_{\mathrm{obs}}^{\alpha}$ (Weinberger, 2012)

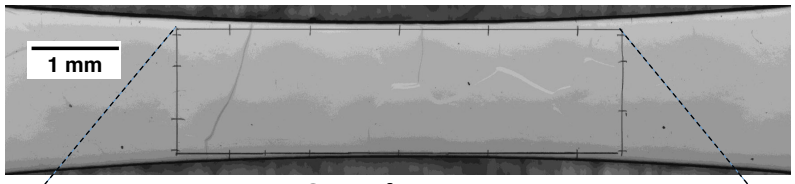
$\tau_{\mathrm{obs}}^{\alpha}$: Obstacle stress

$\tau_{\mathrm{cr}}^{\alpha} - \tau_{\mathrm{ns}}^{\alpha}$: Lattice friction

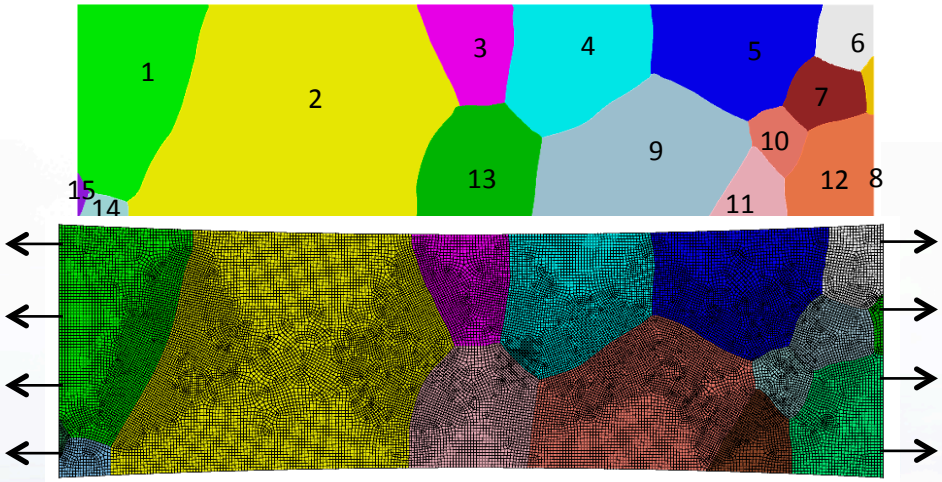
Obstacle stress: $\tau_{\mathrm{obs}}^{\alpha} = \alpha \mu \mathrm{b} \sqrt{\sum_{\beta=1}^{NS} \rho^{\beta}}$ (Taylor, 1934)

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

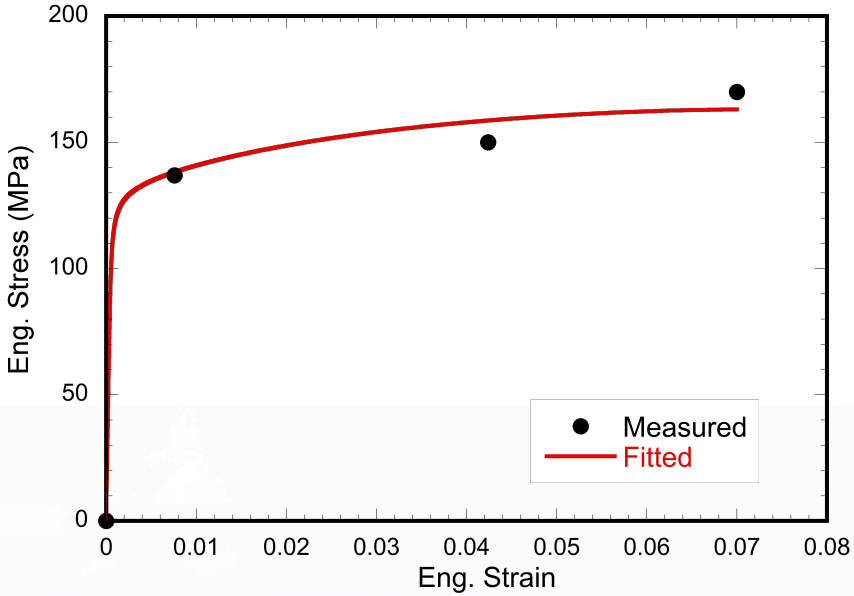
Tantalum Oligocrystal 1



Specimen



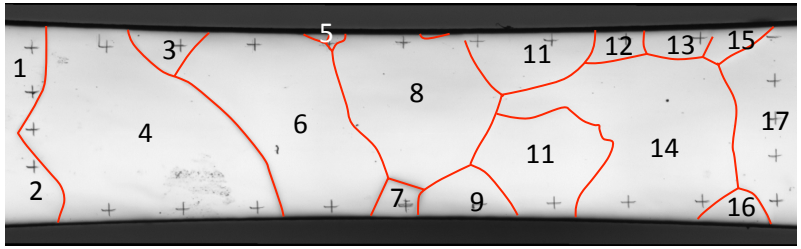
Finite Element Mesh



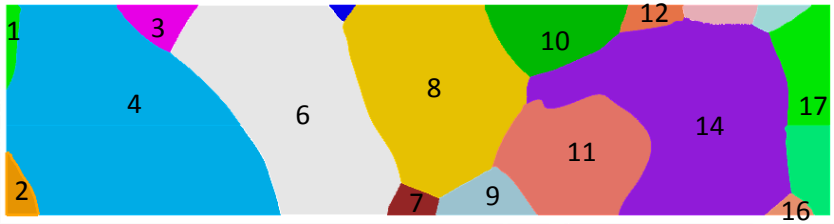
$$\overline{\tau} = 28\,MPa$$

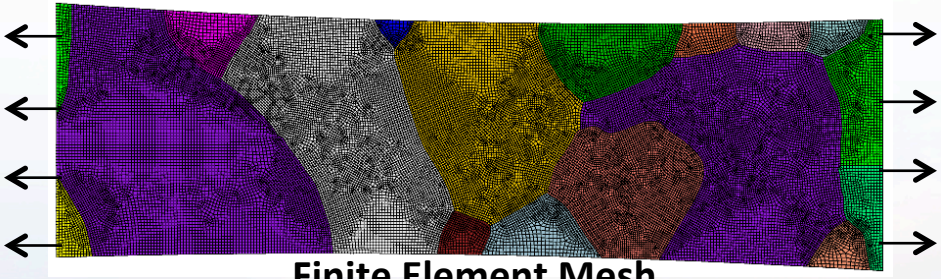
Elastic constants (GPa)			Hardening coefficients	
C_{11}	C_{12}	C_{44}	k_1 (m^{-1})	k_2
267	161	82.5	1.4×10^6	14

Tantalum Oligocrystal 2

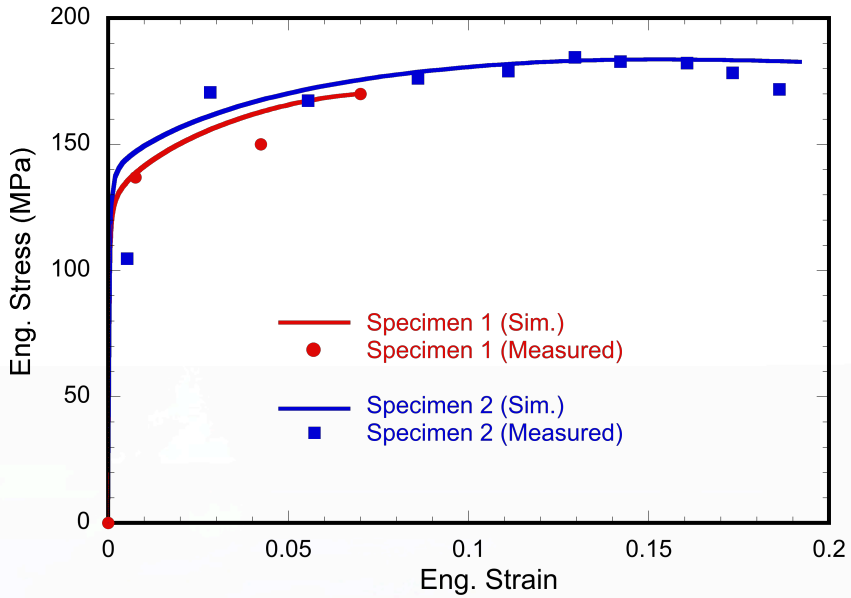


Specimen





Finite Element Mesh



$$\bar{\tau} = 37\ MPa$$

Elastic constants (GPa)			Hardening coefficients	
C_{11}	C_{12}	C_{44}	k_1 (m^{-1})	k_2
267	161	82.5	1.4×10^6	14

(Same as for Oligocrystal #1)

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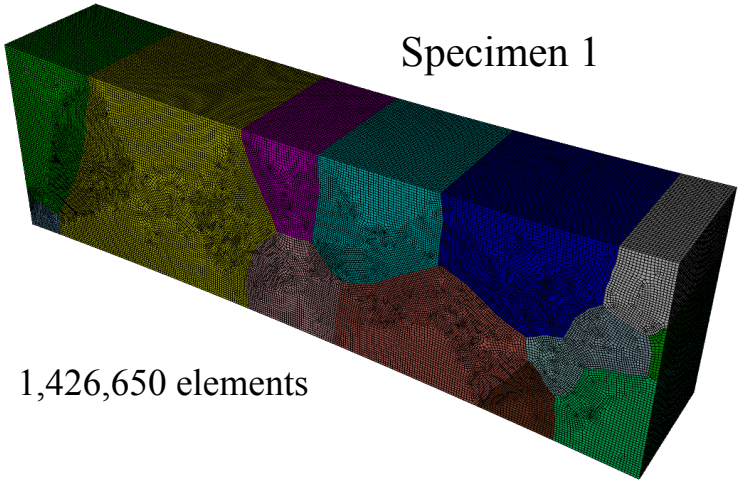
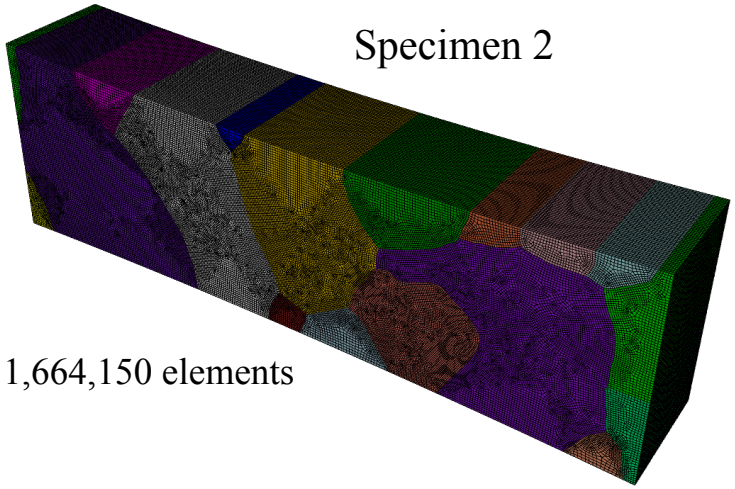
Columnarity

Specimen 1

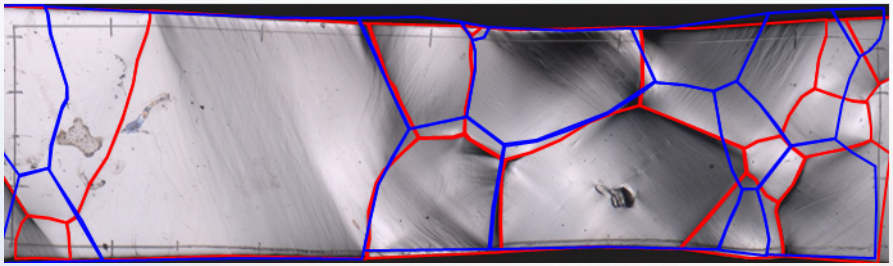


1,426,650 elements

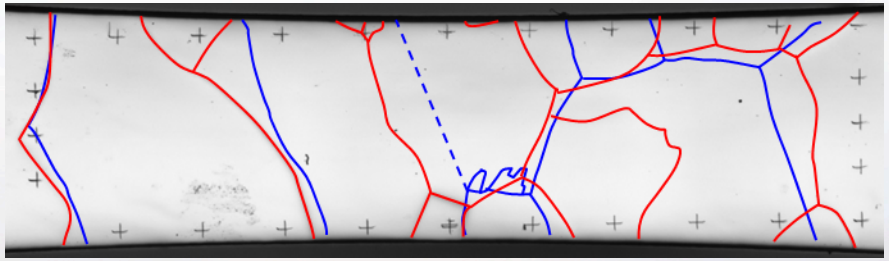
Specimen 2



1,664,150 elements



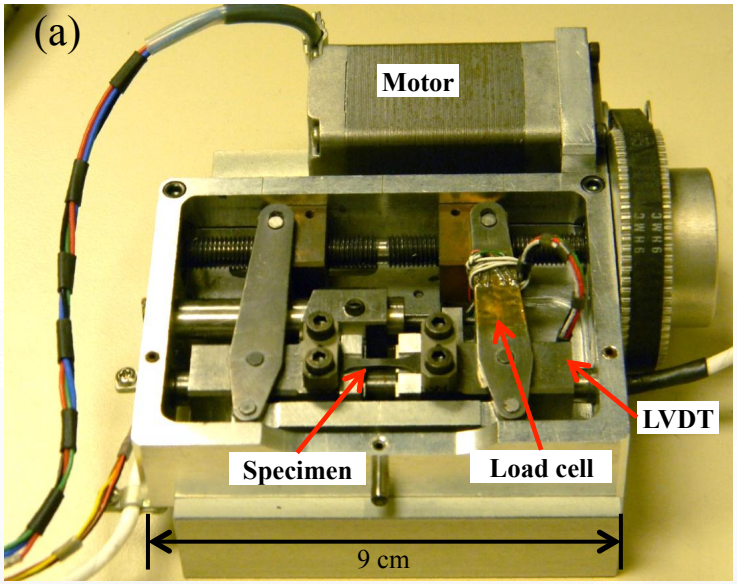
Grain boundary (Front)

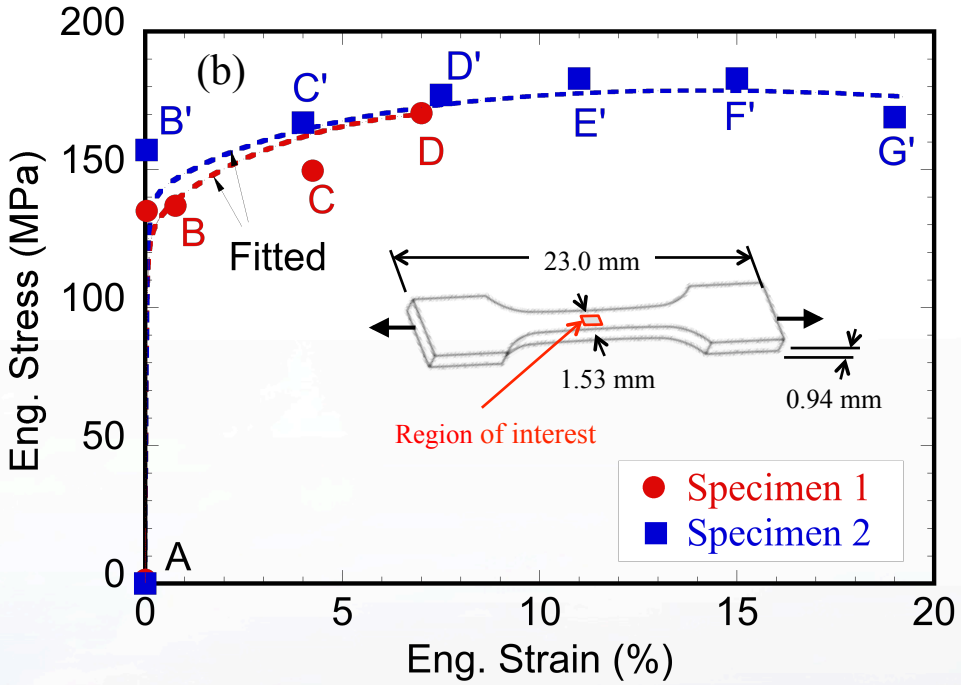


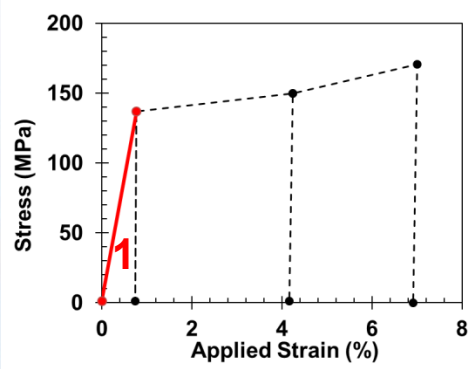
Grain boundary (Back)

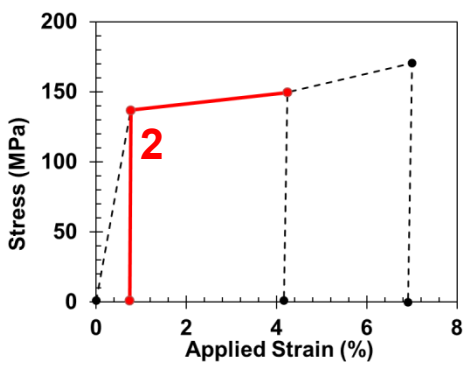
1 mm

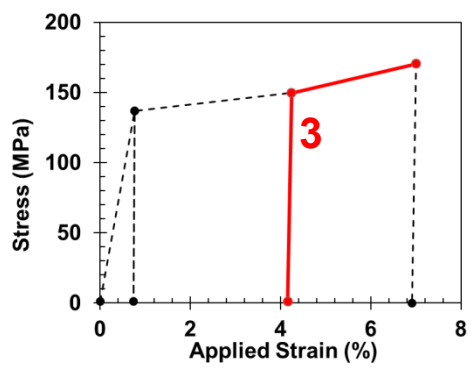
Loading of Specimens and EBSD

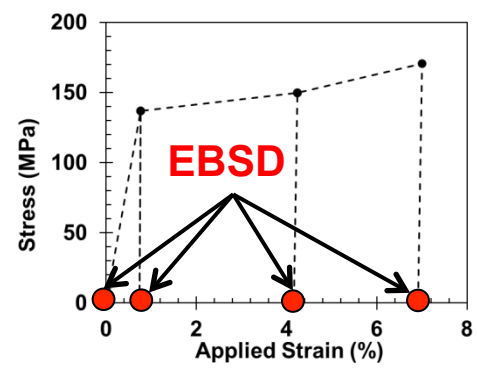




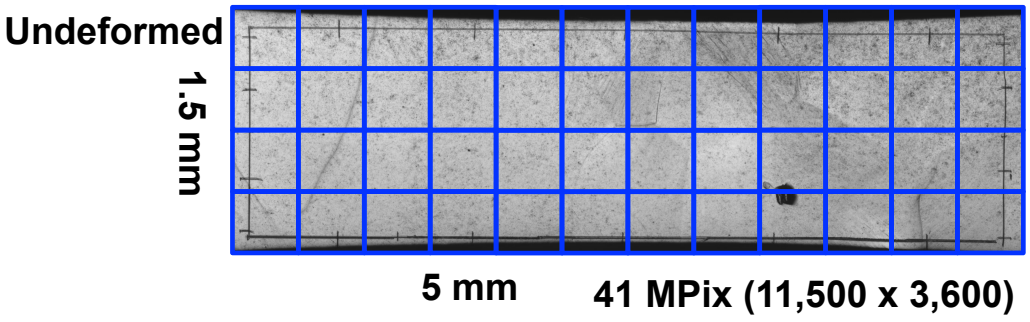


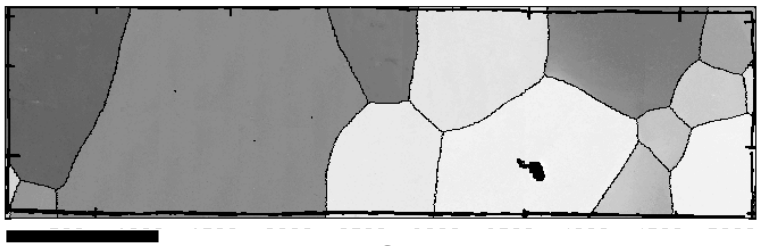


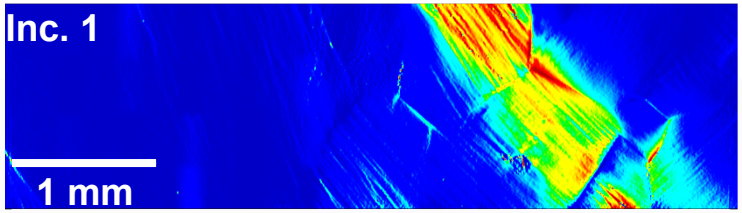


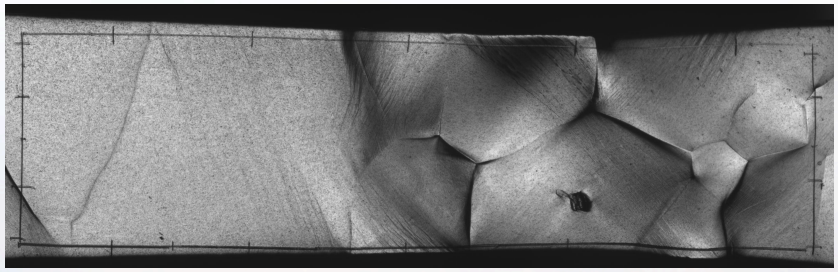


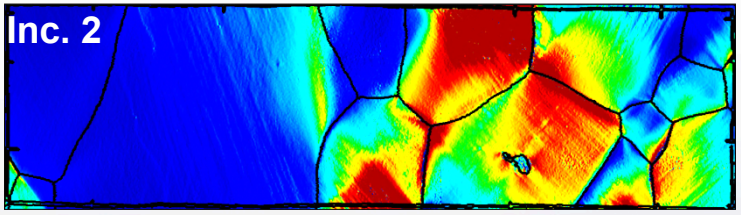
Digital Image Correlation

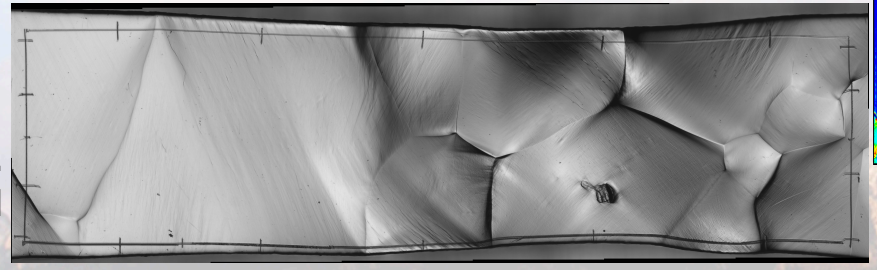


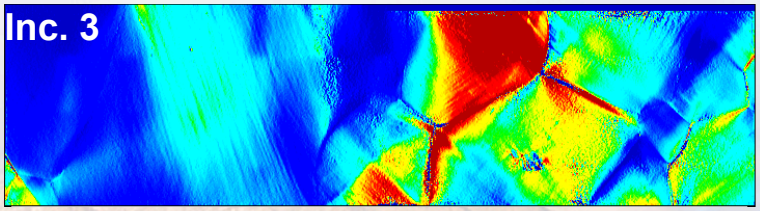






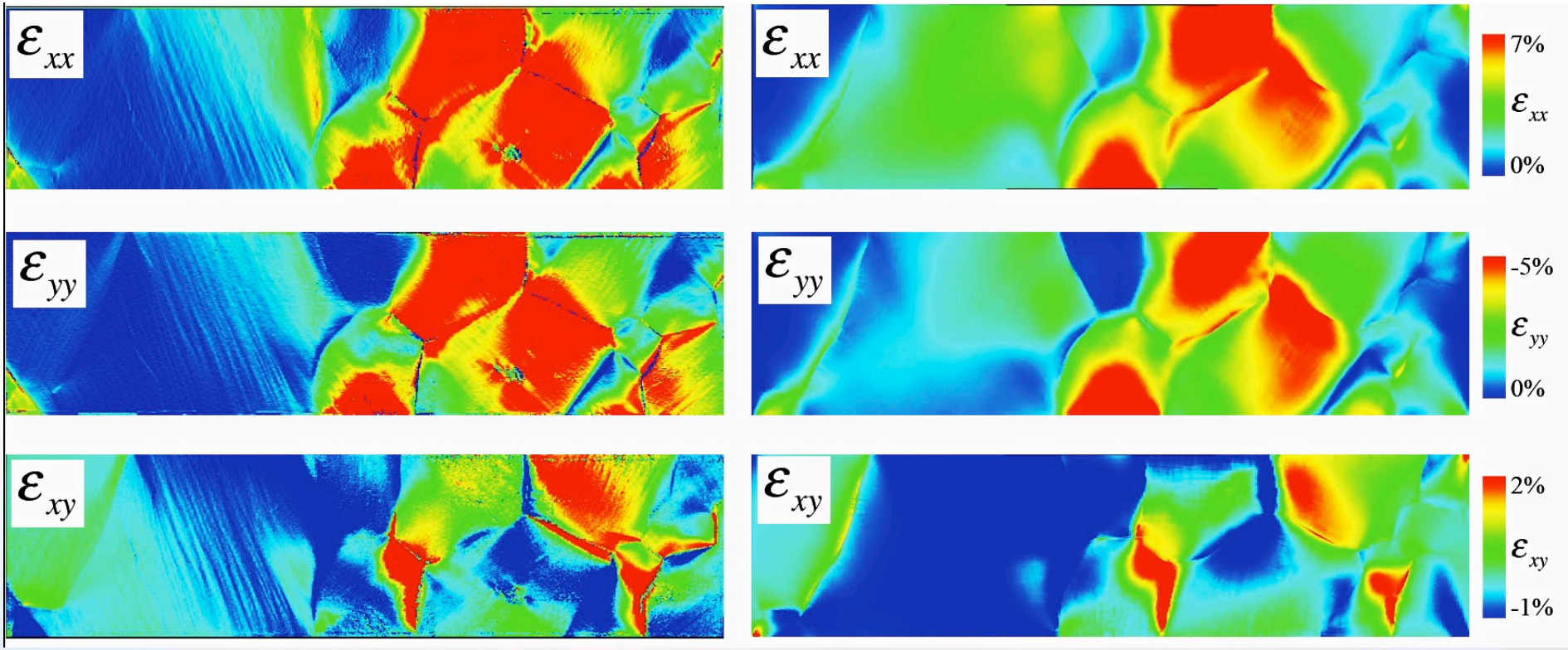




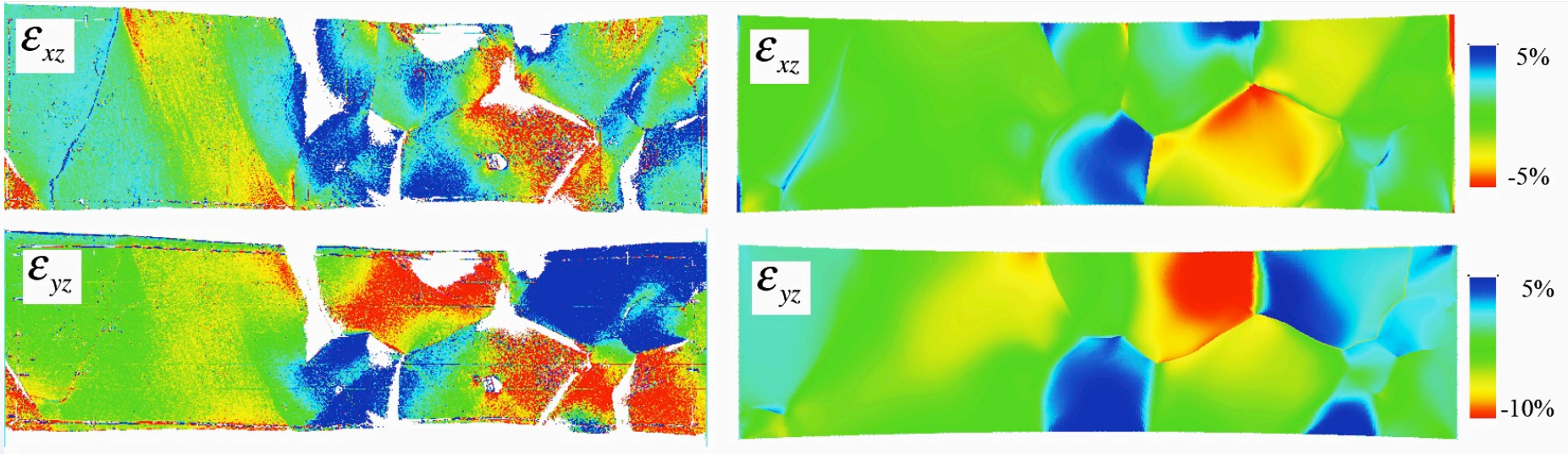


Carroll J.D., Clark B.G., Buchheit T.E., Boyce B.L., Weinberger C.R., Mater. Sci. Eng. A (2013)

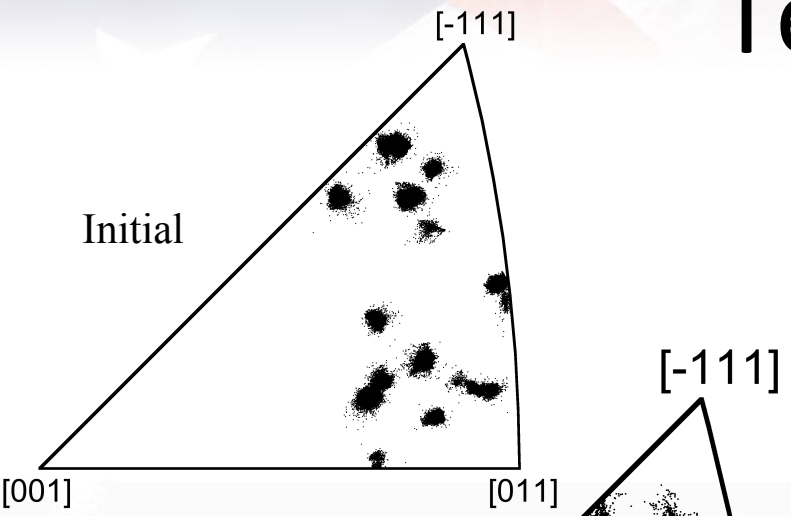
Predicted In-Plane Strains

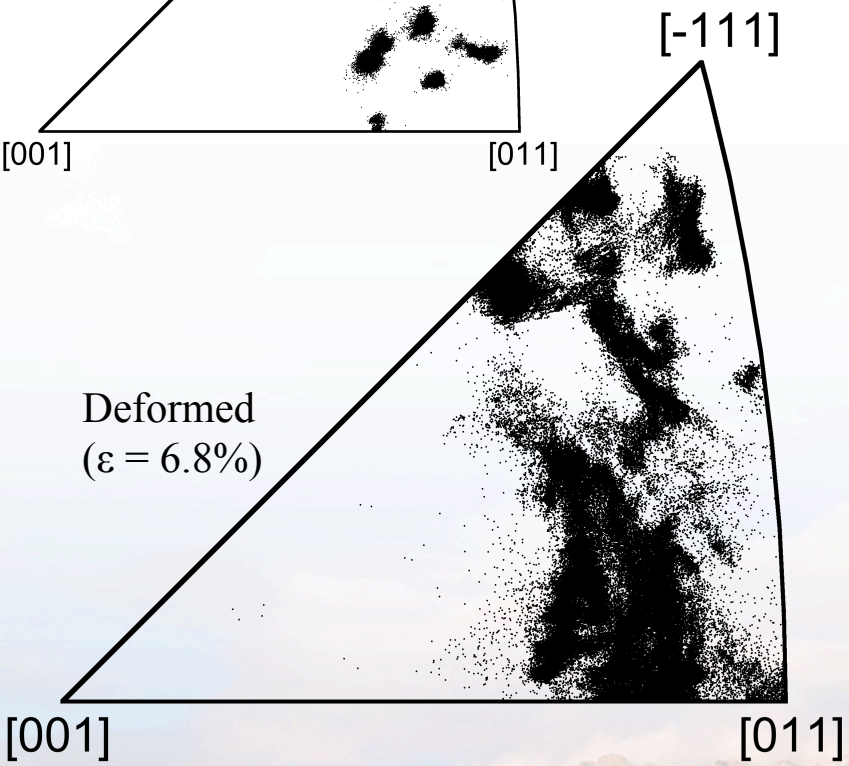


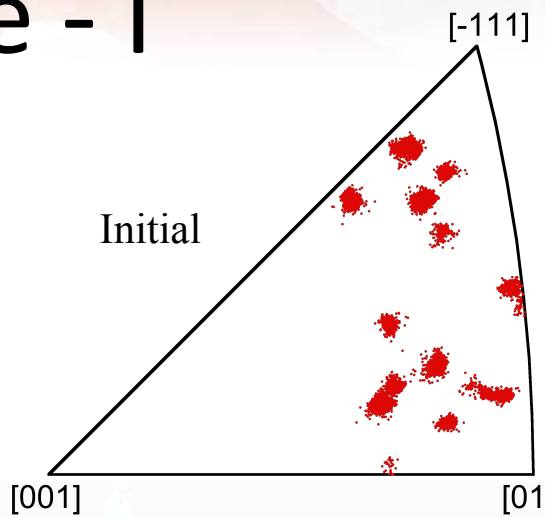
Out-Of-Plane Strains

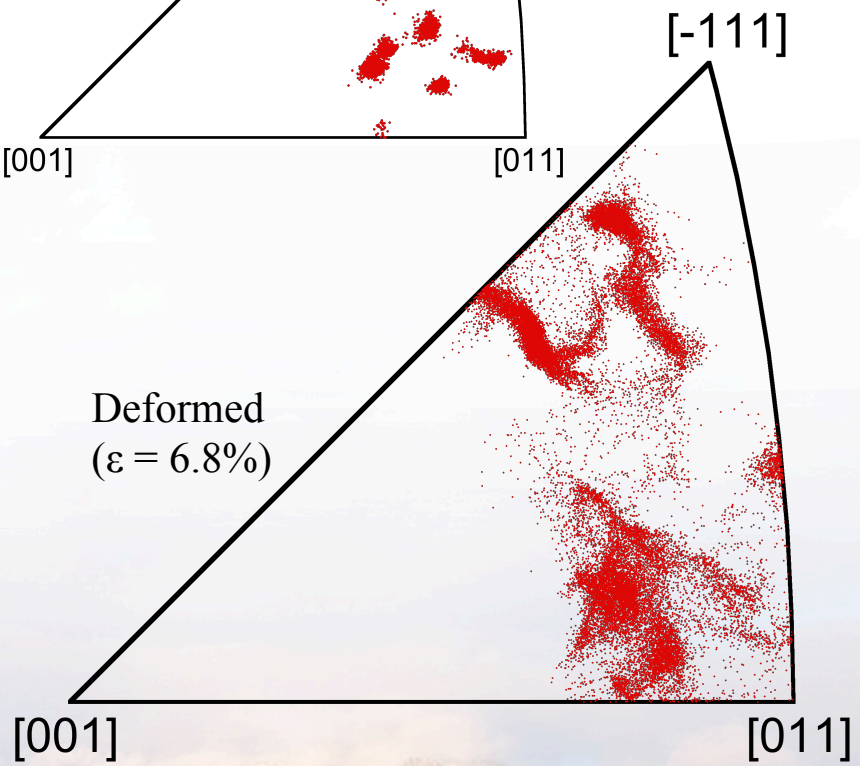


Texture - I

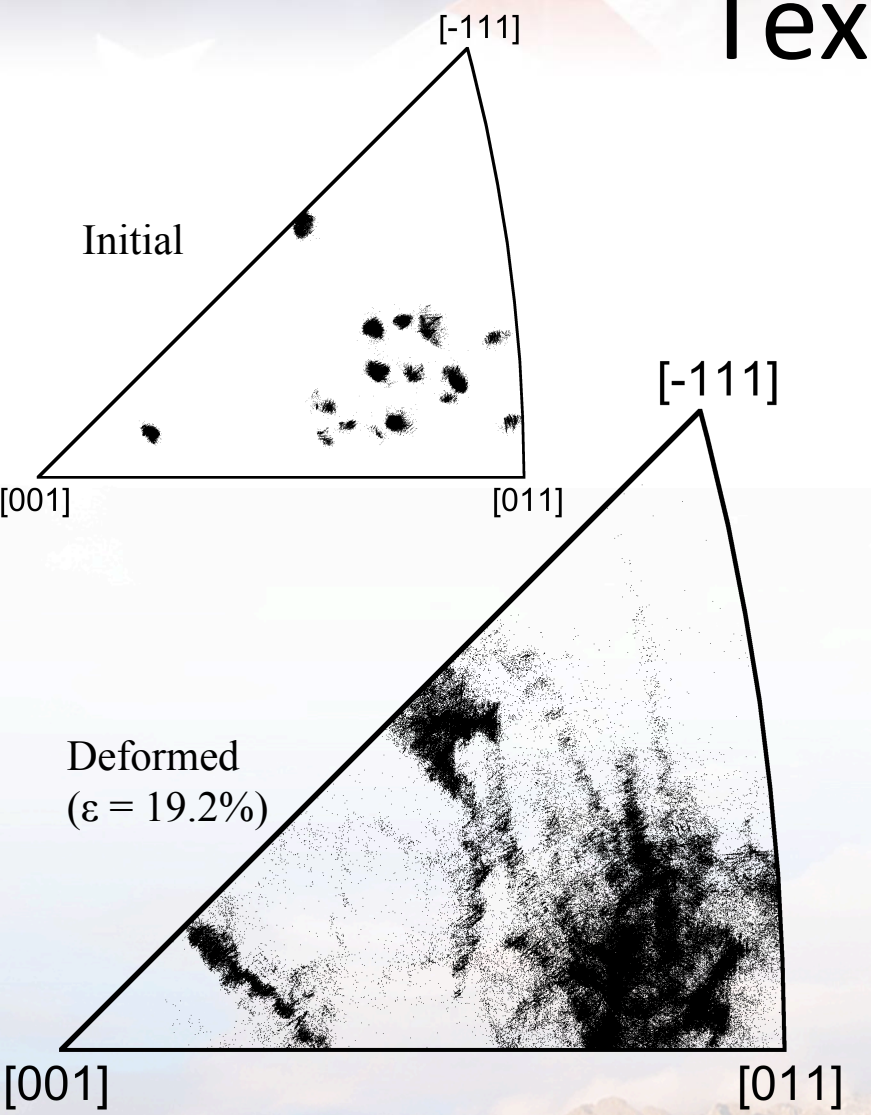

[-111]
Initial
[001]
[011]

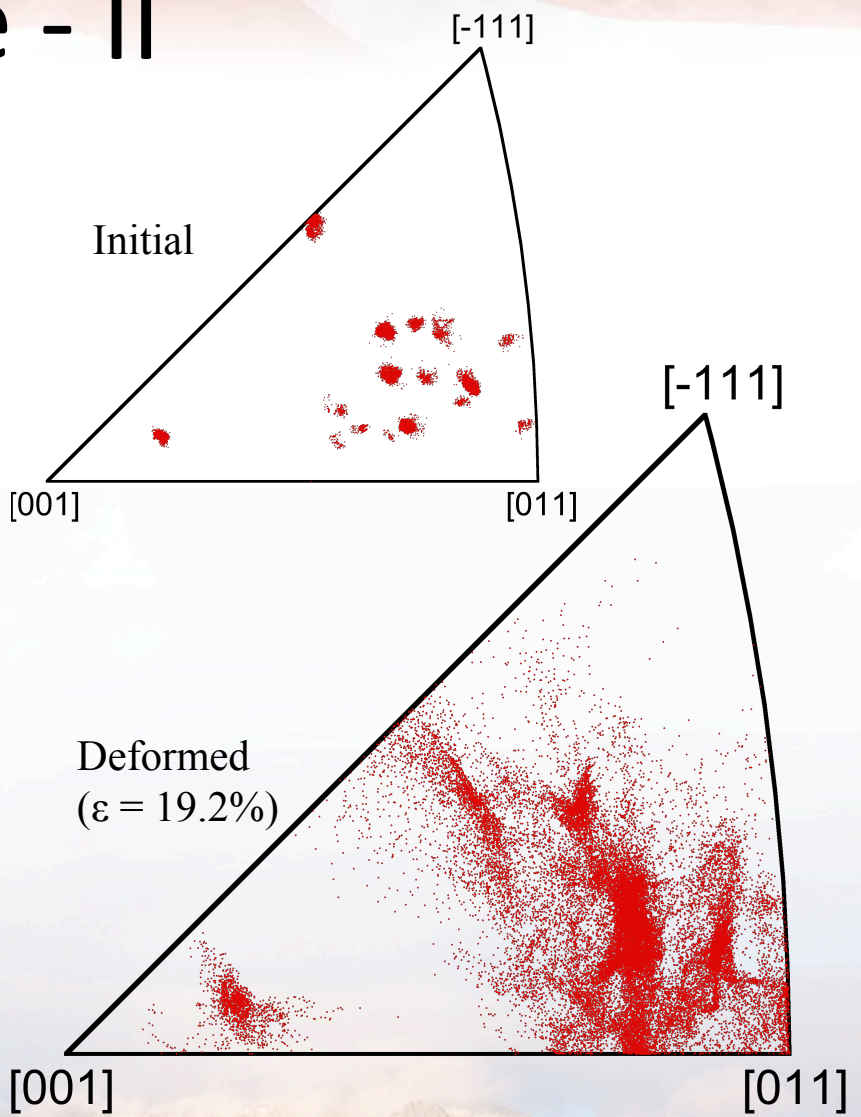

[-111]
Deformed
(ε = 6.8%)
[001]
[011]


[-111]
Initial
[001]
[011]

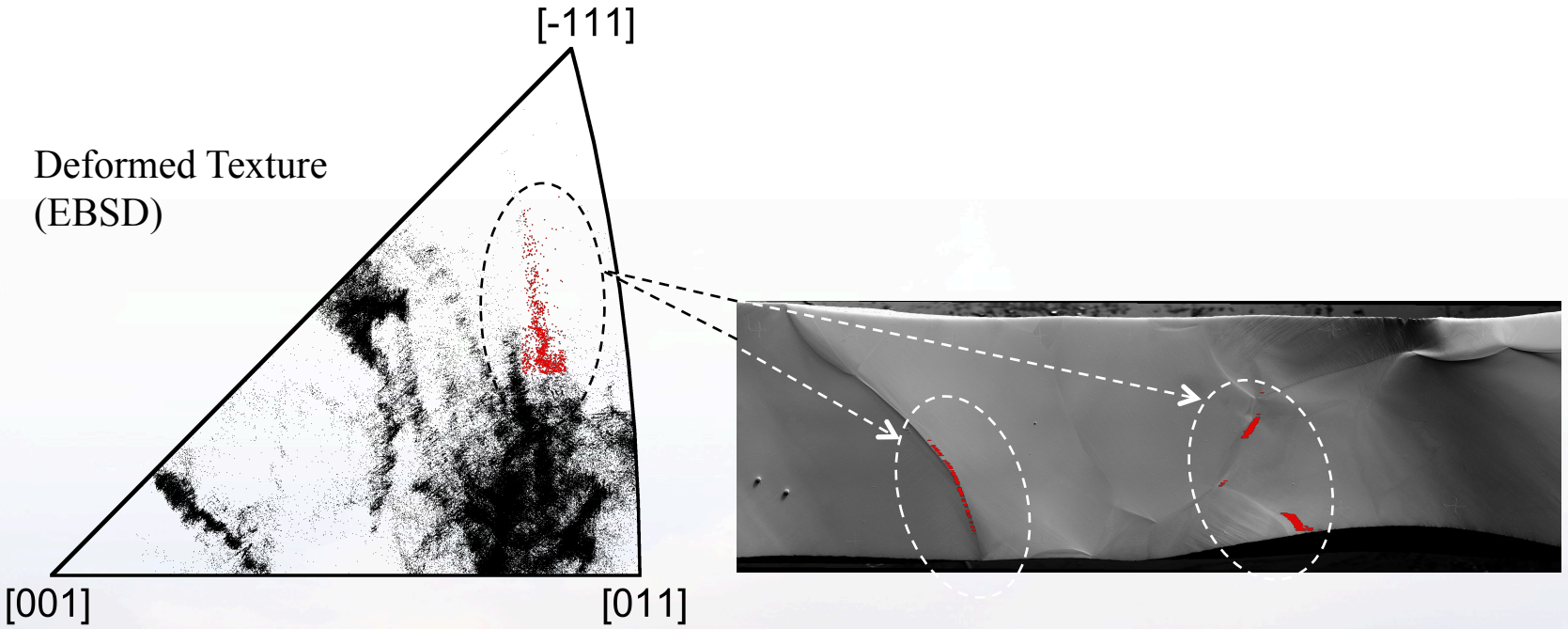

[-111]
Deformed
(ε = 6.8%)
[001]
[011]

Texture - II

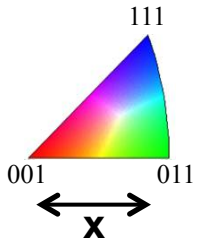

[-111]
Initial
[001]
[011]
[-111]
Deformed
(ε = 19.2%)
[001]
[011]

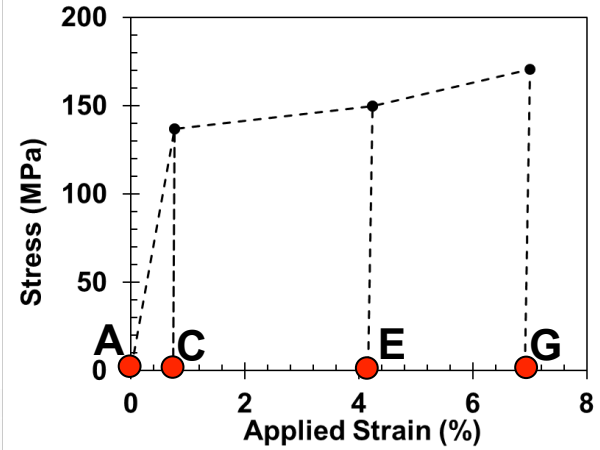

[-111]
Initial
[001]
[011]
[-111]
Deformed
(ε = 19.2%)
[001]
[011]

Texture Issues Occur Near GBs



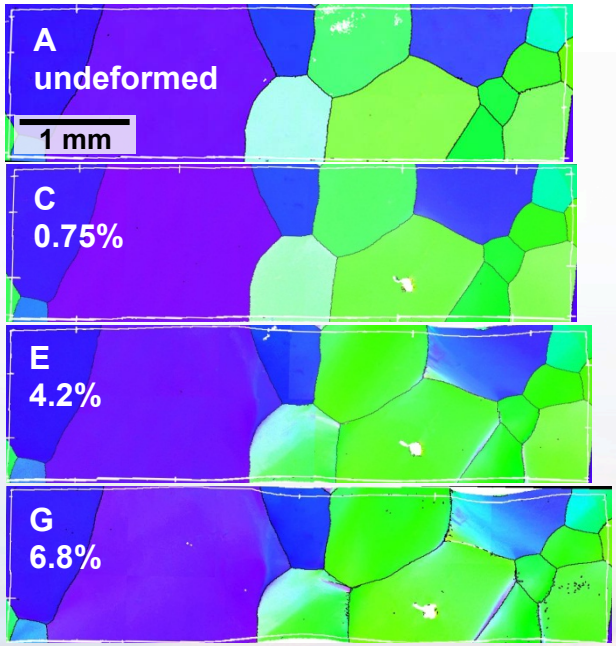
Misorientation

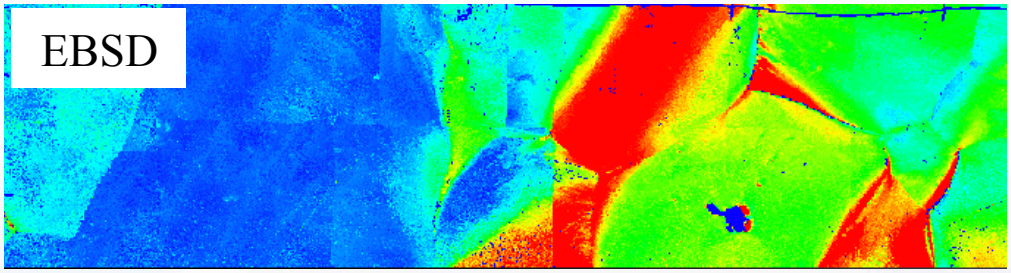


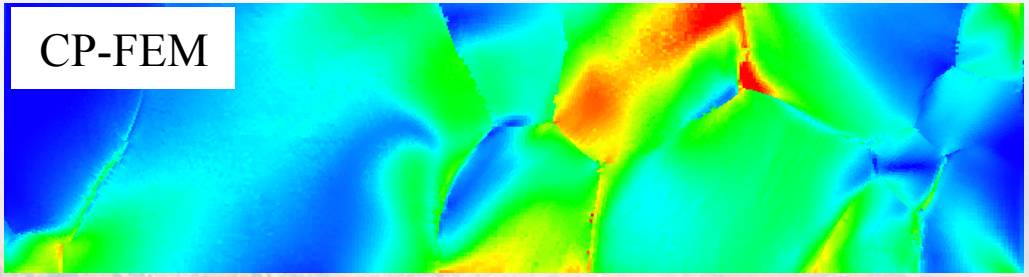


$$\Delta g_{AB} = g_B g_A^{-1}$$

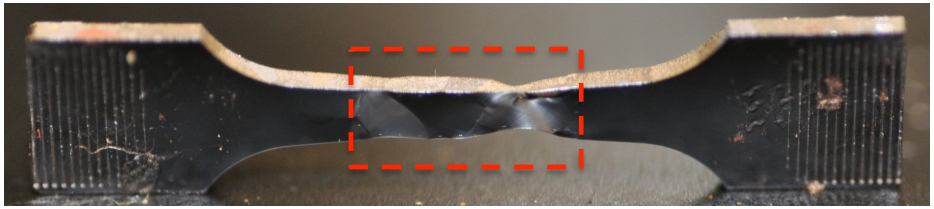
$$\cos\theta = \frac{1}{2}(\Delta g_{11} + \Delta g_{22} + \Delta g_{33} - 1)$$

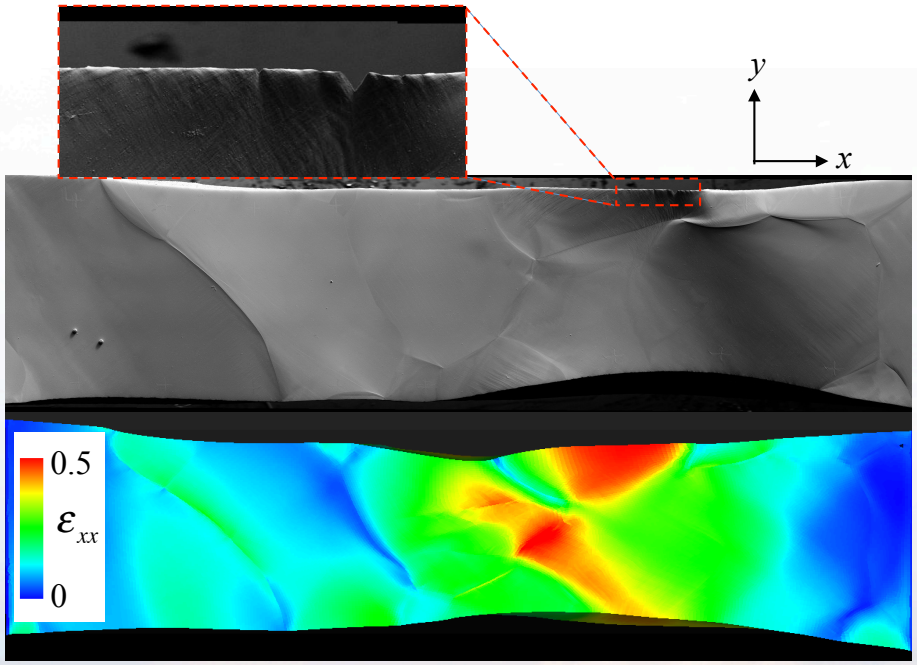


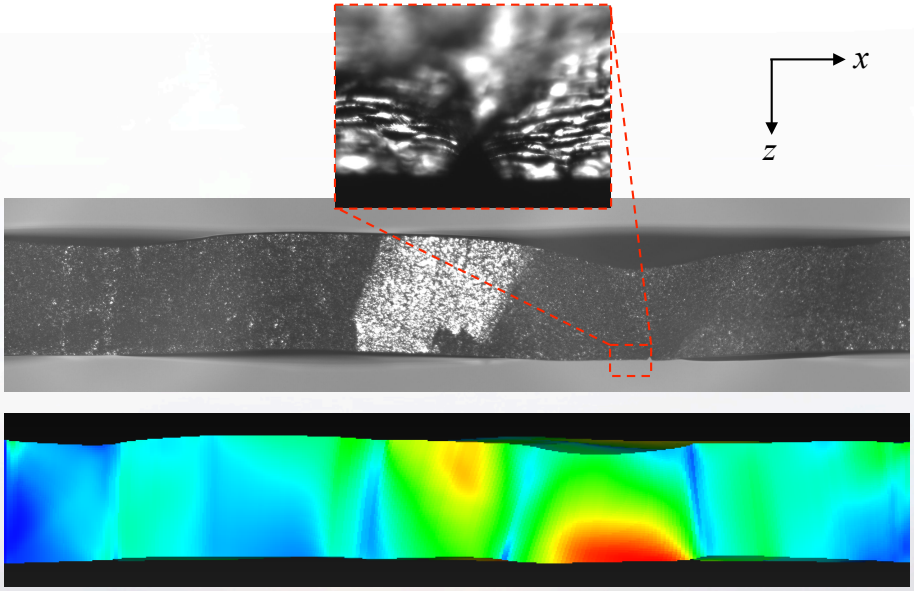




Failure Predictions



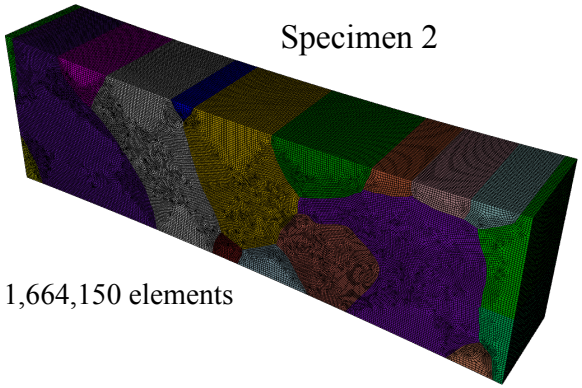


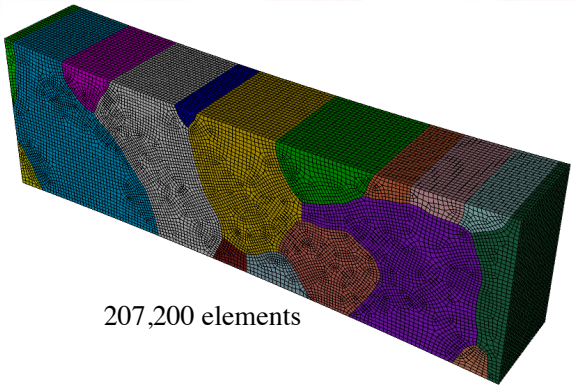


Model Sensitivity

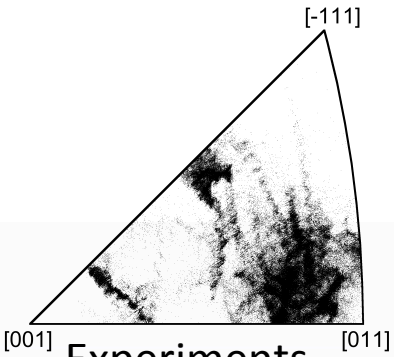
- Sensitivity of Mesh
- Sensitivity of Orientation Choices
- Sensitivity of Slip plane Choice

Mesh



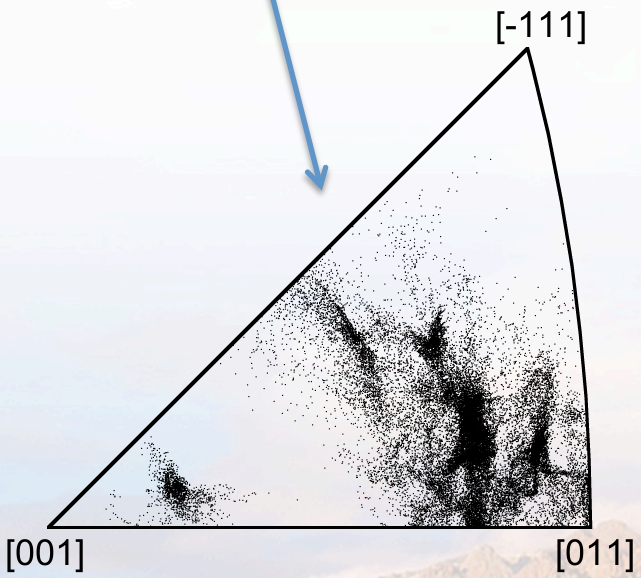


Fine Mesh (Running)



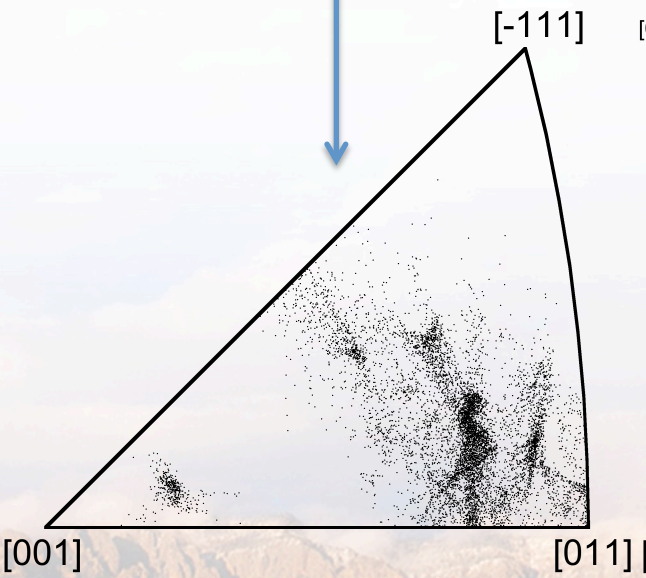
Experiments

Medium Mesh

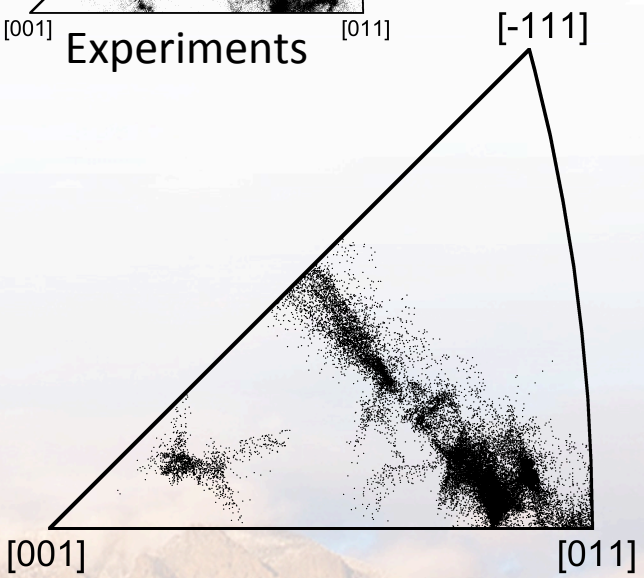


(a) 33,283 × 50 elements

Coarse Mesh

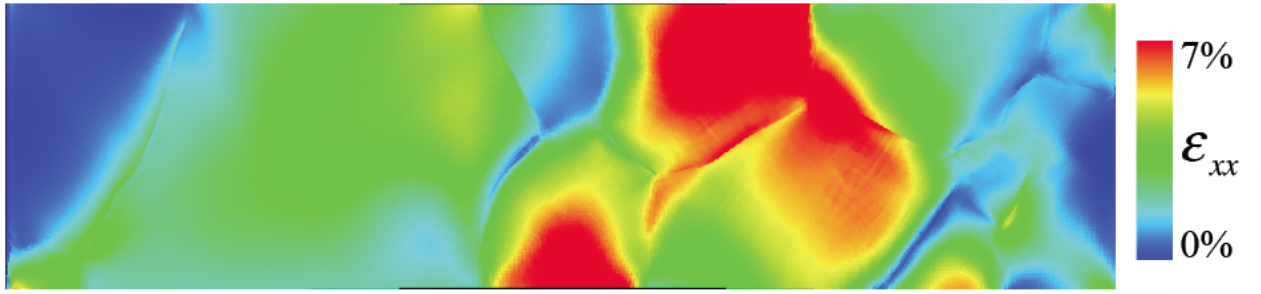


(b) 8,288 × 25 elements

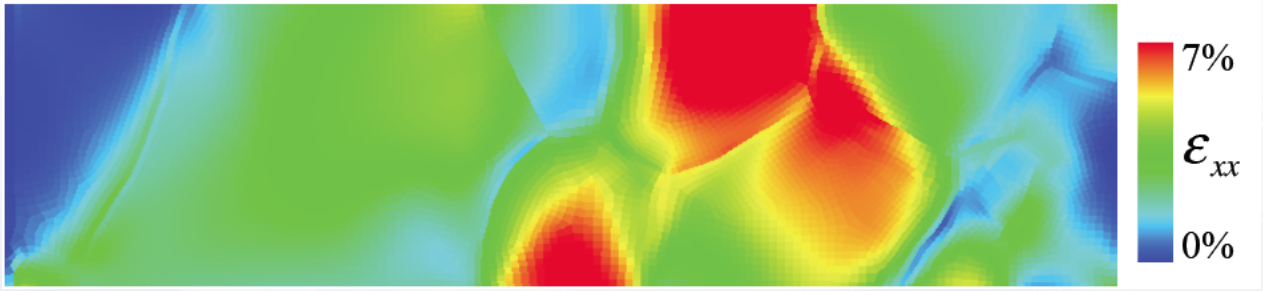


(c) 33,283 × 1 elements

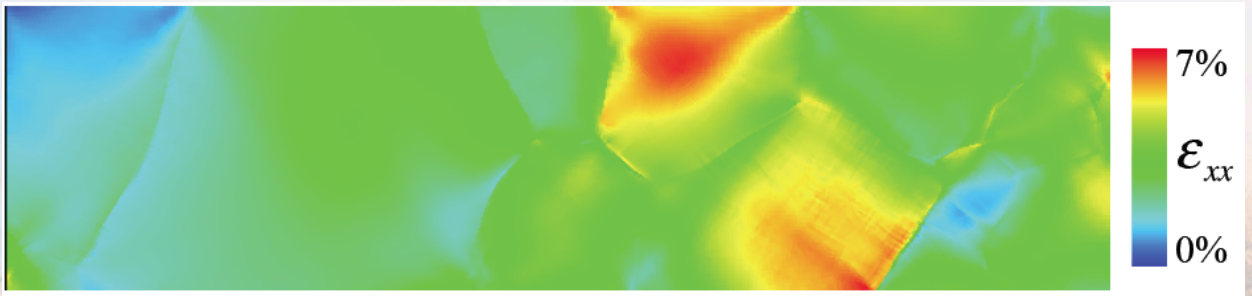
Mesh - Strain Predictions



Medium Mesh

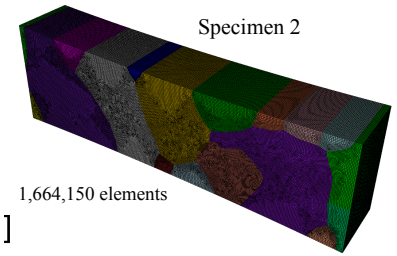


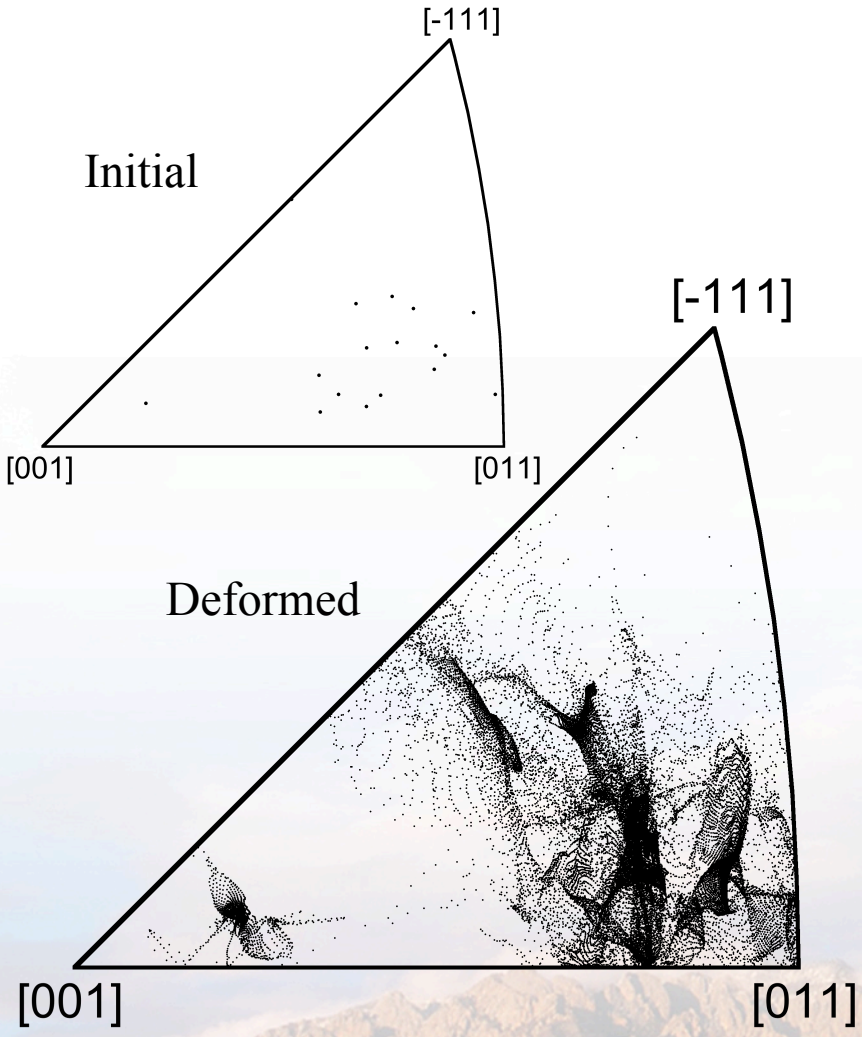
Coarse Mesh



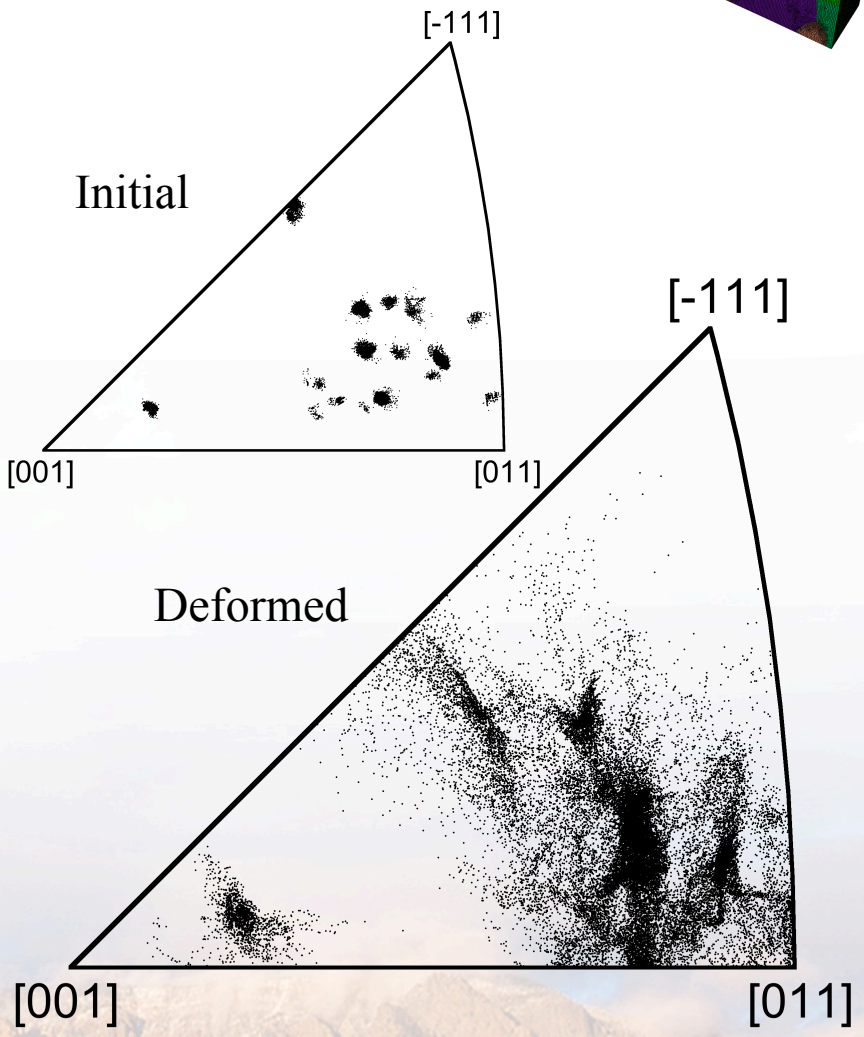
Medium Mesh
1 element through thickness

Initial Orientations



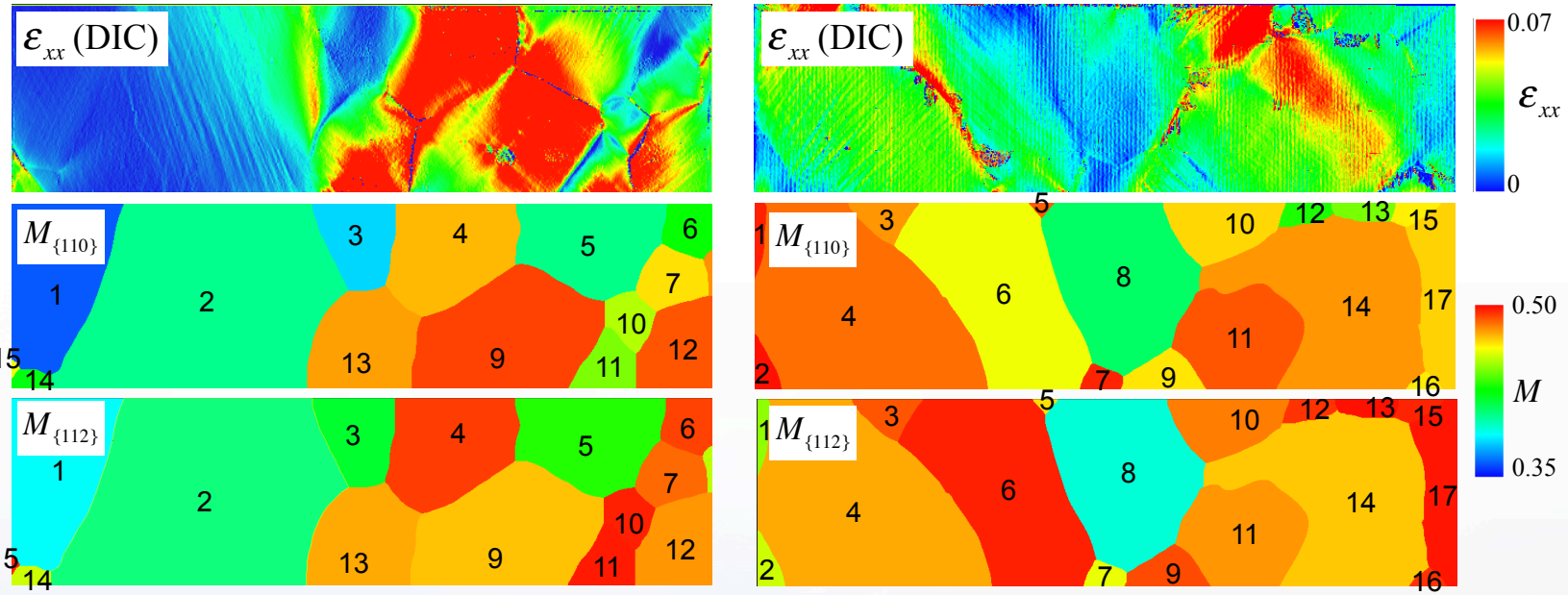


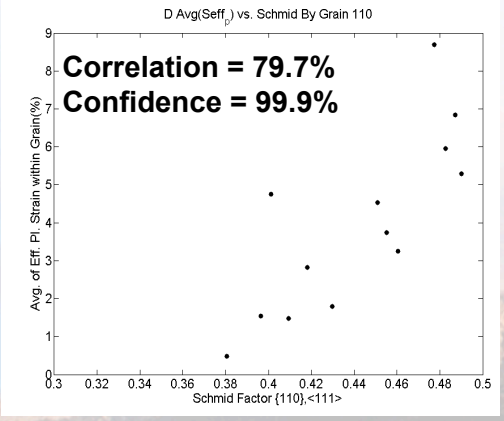
(a) Orientation per grain

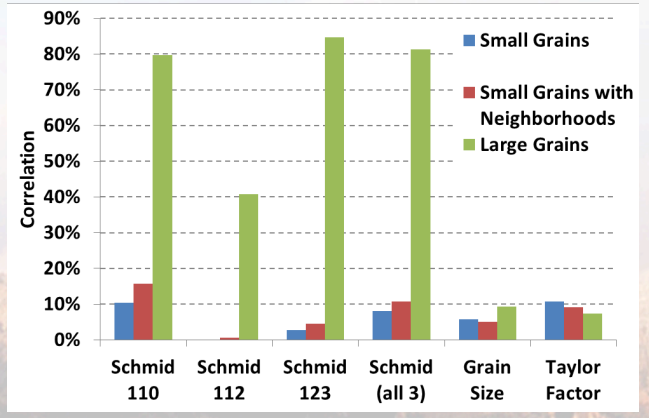


(b) Orientation per element

Slip Planes

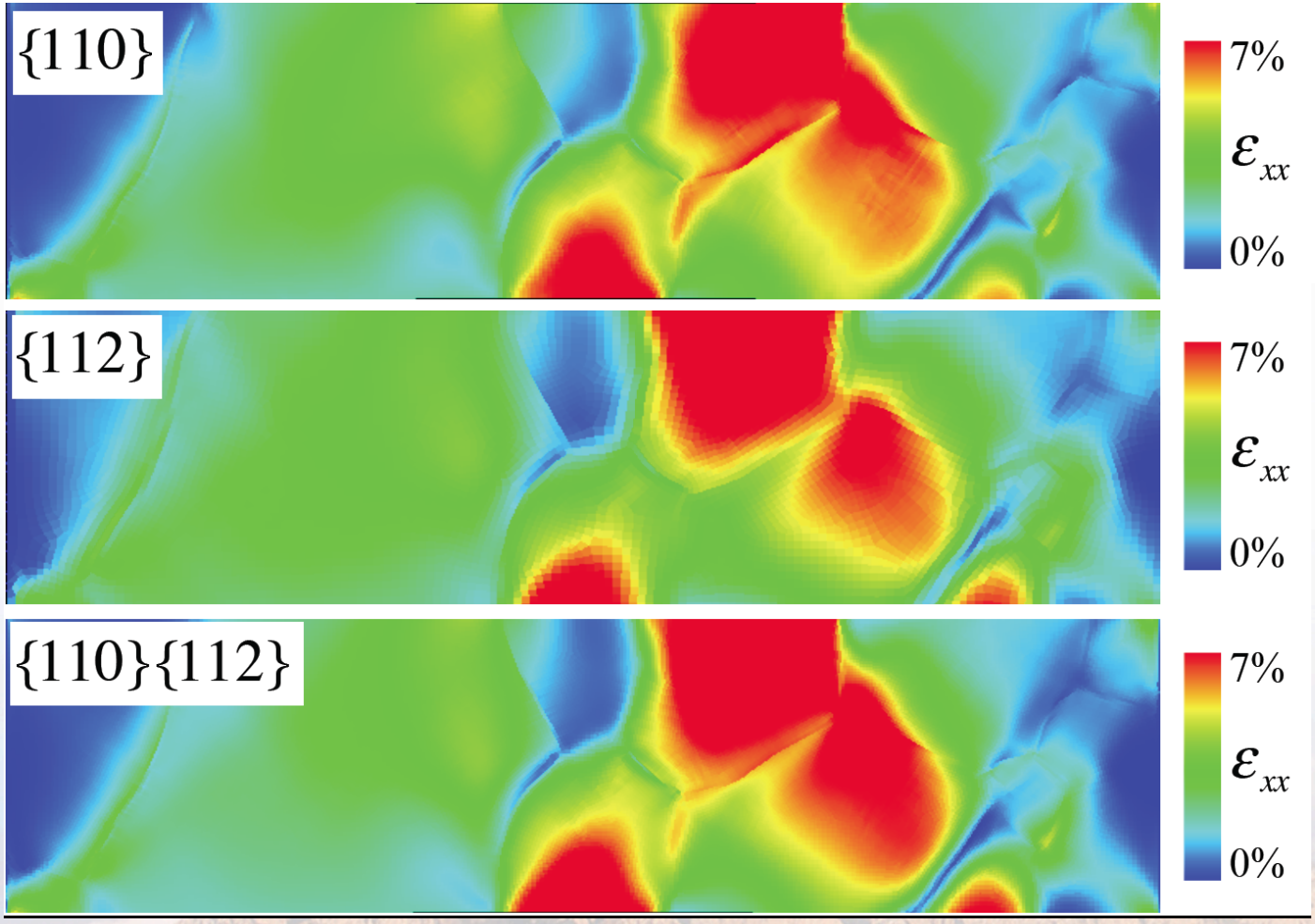




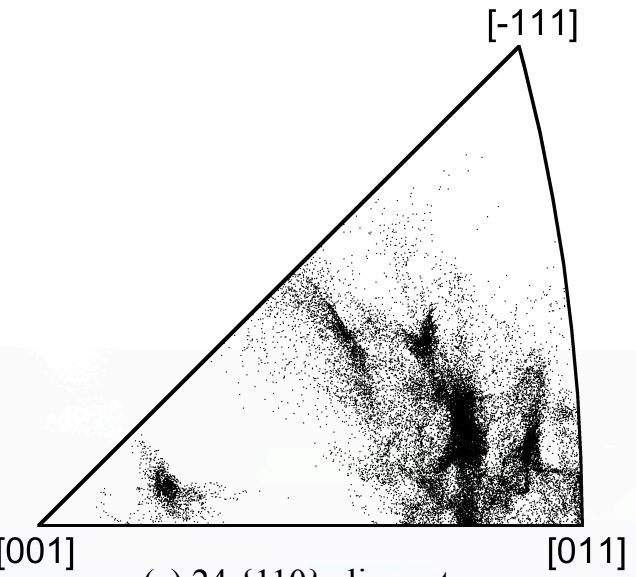


Carroll J.D., Clark B.G., Buchheit T.E., Boyce B.L., Weinberger C.R., Mater. Sci. Eng. A (2013)

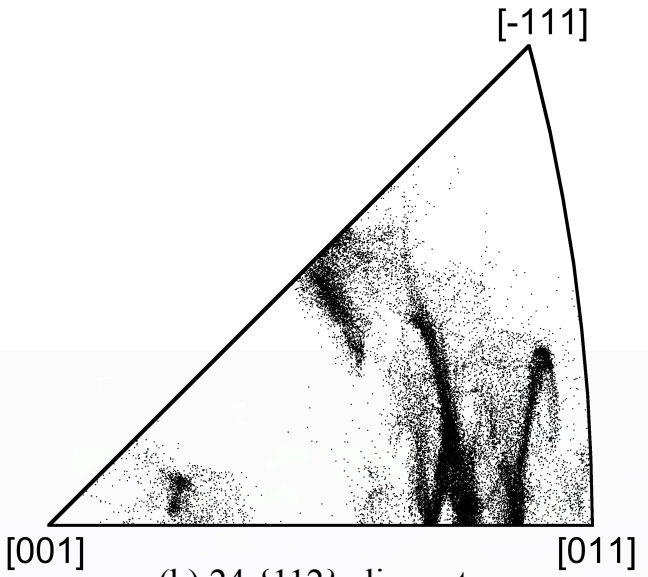
Slip Planes – Strain Distributions



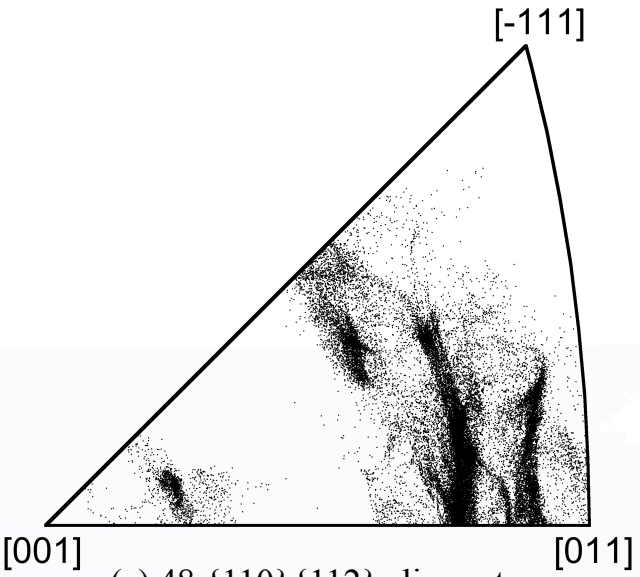
Texture Evolution



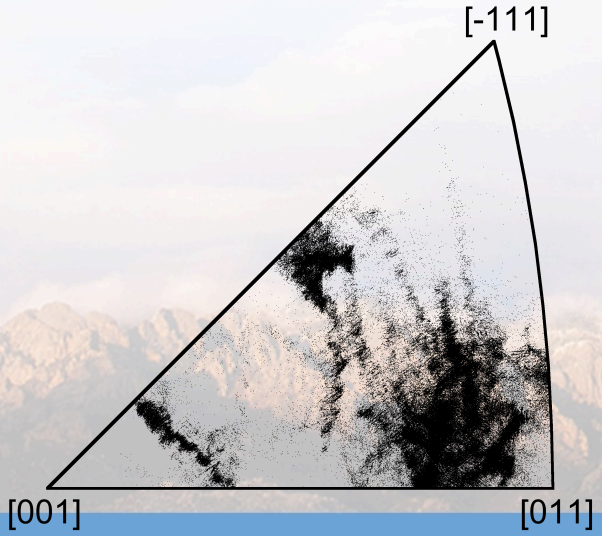
(a) 24 {110} slip systems



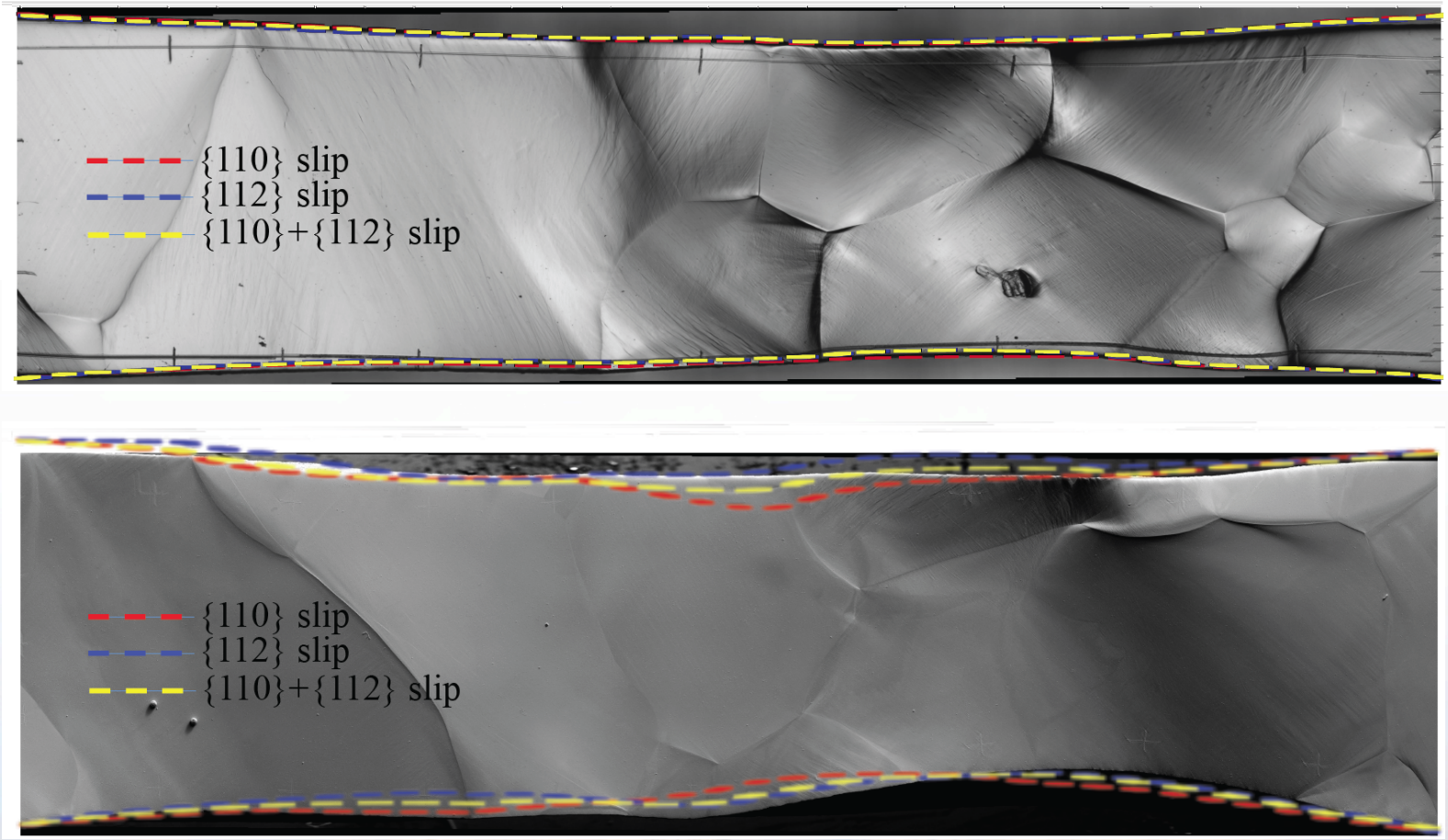
(b) 24 {112} slip systems



(c) 48 {110}{112} slip systems



Deformed Shapes



Conclusions

- Numerous studies indicate good qualitative agreement – the "trends" are correct – but the quantitative details are often missing.
- CPFEM simulations appear to predict grain-scale strains accurately (relatively)
  - Relatively insensitive to mesh size & slip planes
  - Does depend on through thickness
- CPFEM simulations predict texture evolution moderately well
  - Missing some details
  - More mesh sensitive than strains
- Sub-grain deformations depend on many factors. Thus the details of deformation depend on the details of the experimentation and simulation.
- What level of agreement / validation can we reasonably expect from models of this class?
- More work is needed to "dot i's and cross t's."