A Practical BCC Crystal Plasticity Model Incorporating Grain Boundary Effects in Tantalum Oligocrystals

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17th U.S. National Congress on Theoretical & Applied Mechanics
June 18, 2014

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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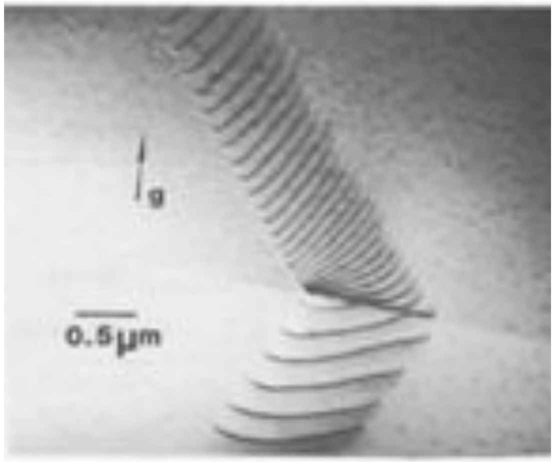
Outline

- **Introduction**
- **CP-FEM Simulations**
- **Grain Boundary Analysis**
- **Summary/ Future work**

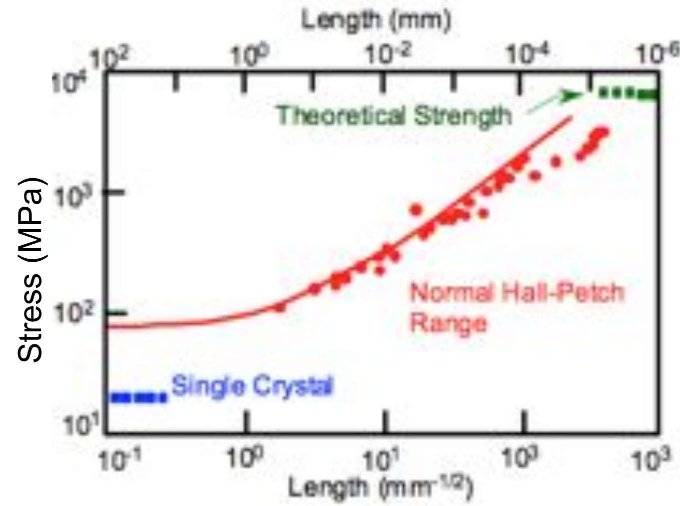
Introduction

Grain Boundary Effects



Dislocation pile-up and transmission
(Shen et al. 1998)

Intergranular fracture*

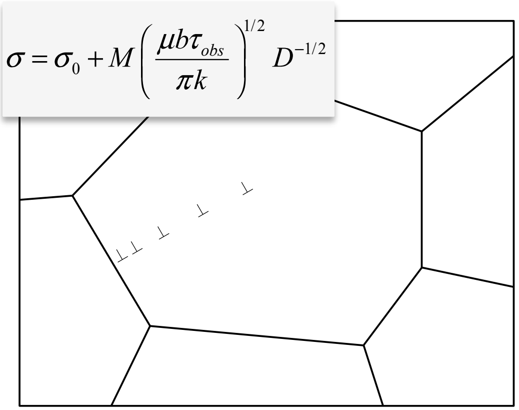


Hall-Petch plot for Fe
(Smith et al. 1995, Meyers and Chawla 1998)

Source: www.met-tech.com
Metallurgical Technologies, Inc.

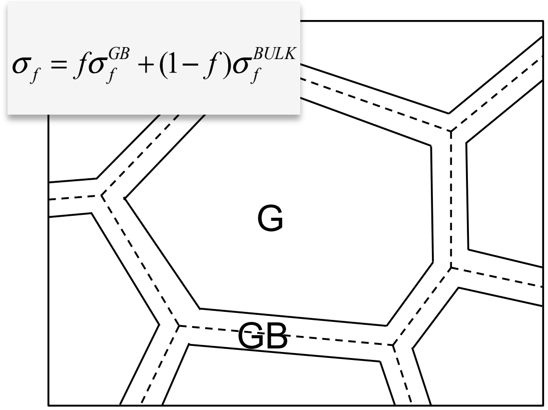
Length-scale aware models

$$\sigma = \sigma_0 + M\left(\frac{\mu b \tau_{obs}}{\pi k}\right)^{1/2} D^{-1/2}$$



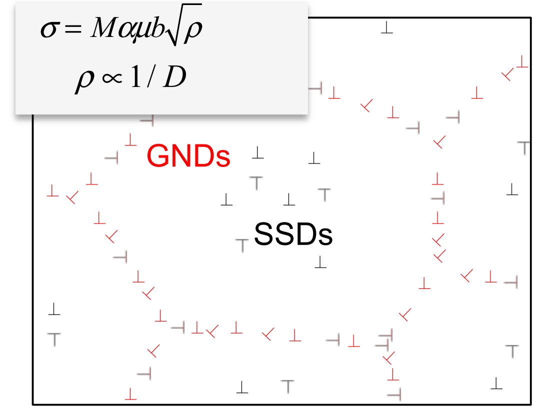
Dislocation pileup model
[Hall, 1951; Petch, 1953]

$$\sigma_f = f\sigma_f^{GB} + (1-f)\sigma_f^{BULK}$$

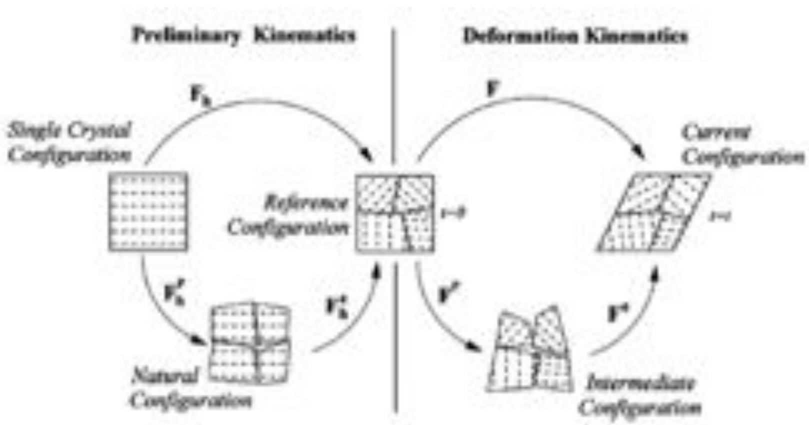


Composite model
[Kocks, 1970; Meyers, 1982]

$$\sigma = M\alpha\mu b\sqrt{\rho}$$
$$\rho \propto 1/D$$

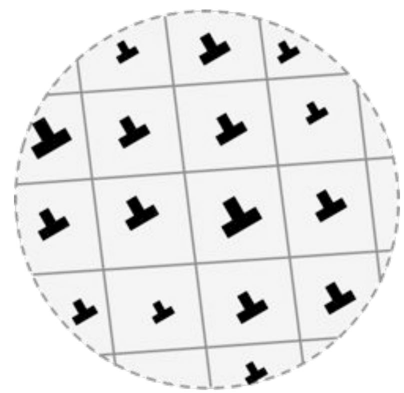


Work hardening model
[Conrad, 1961; Li. 1963]



Sandia's NLCP model
[Counts et al, 2007, 2008]

kernel-based, non-local "integration" of D**F** with augmented kinematics.



SuperDislocation model

dislocation "lumping," dislocation transfer, and dislocation / GB back-stress.

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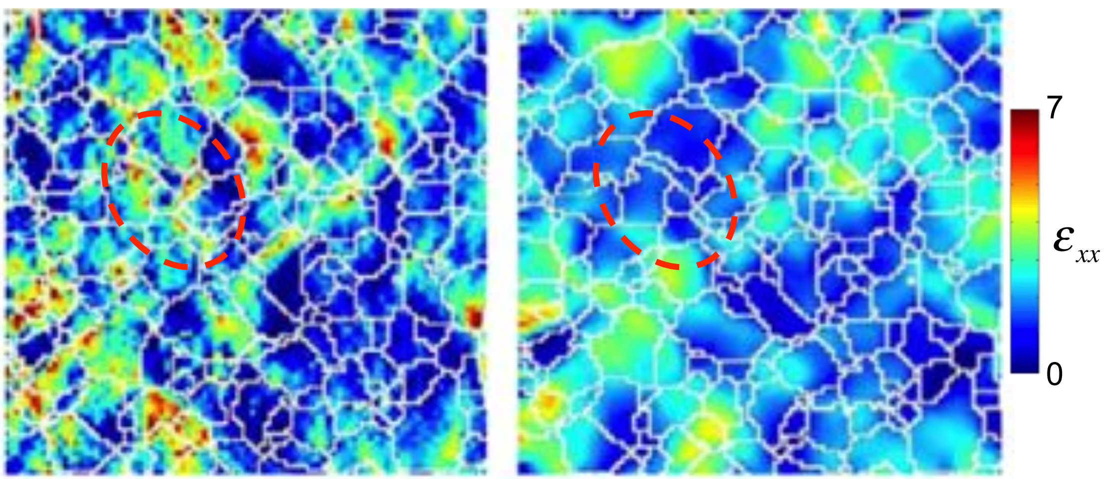
Previous work on sim-exp. comparison

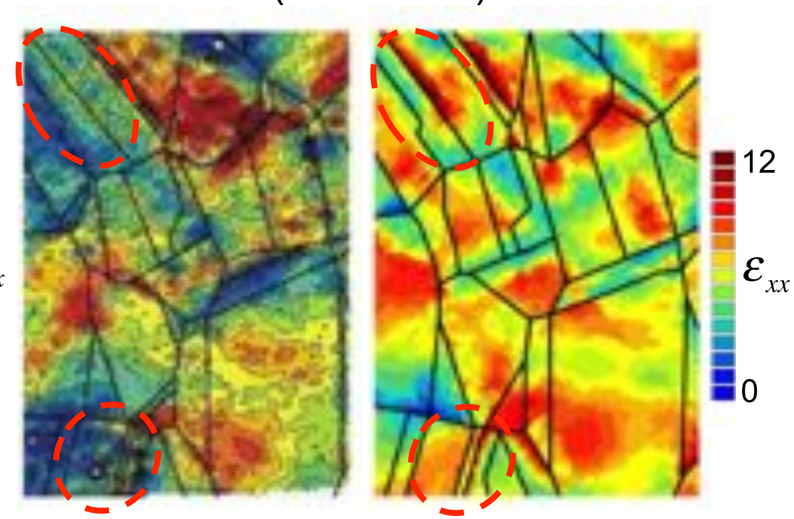
Limited success has been achieved in modeling polycrystal deformation behavior due to unknown subsurface grains

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



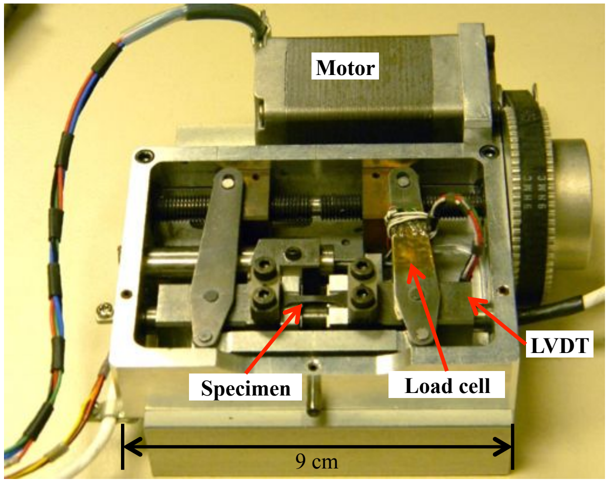
Experiment   Simulation

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

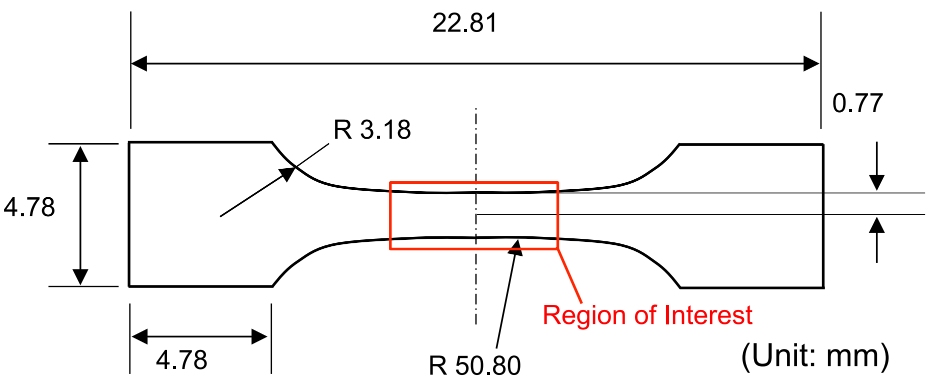


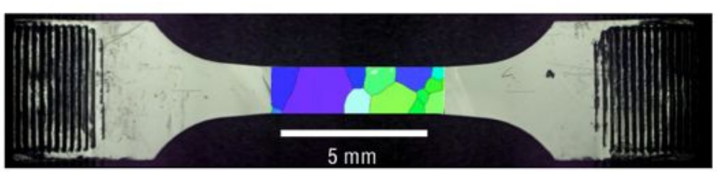
Experiment   Simulation

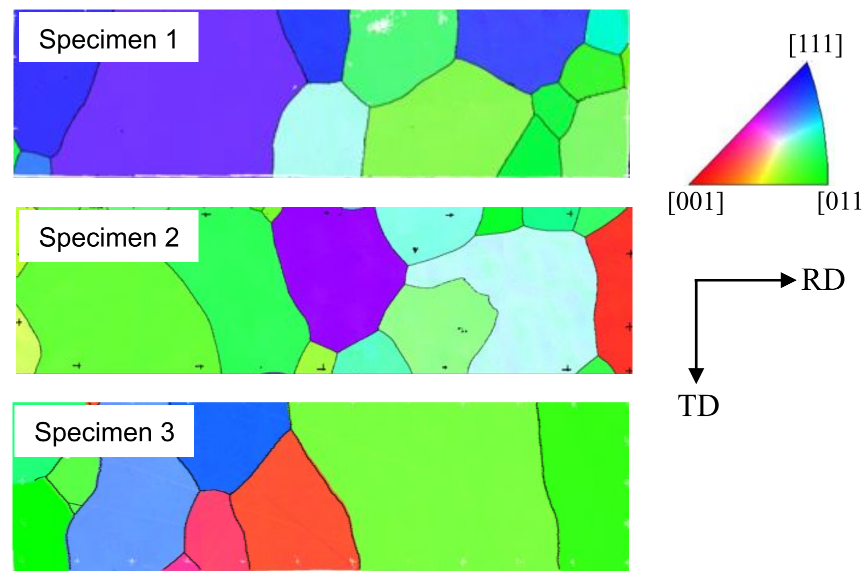
Experimental setup



- 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

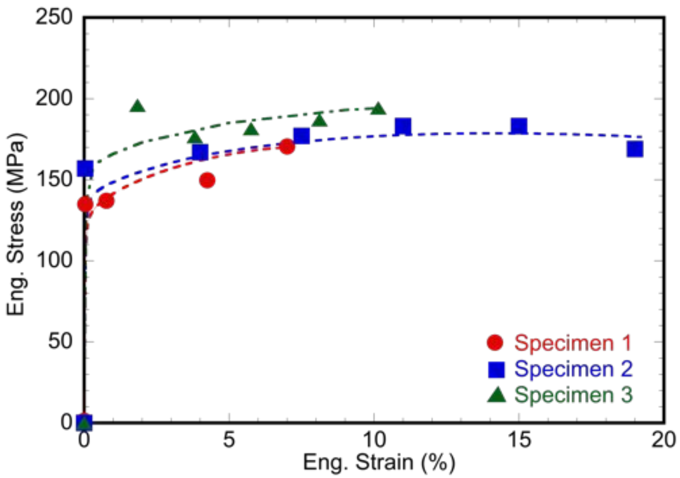


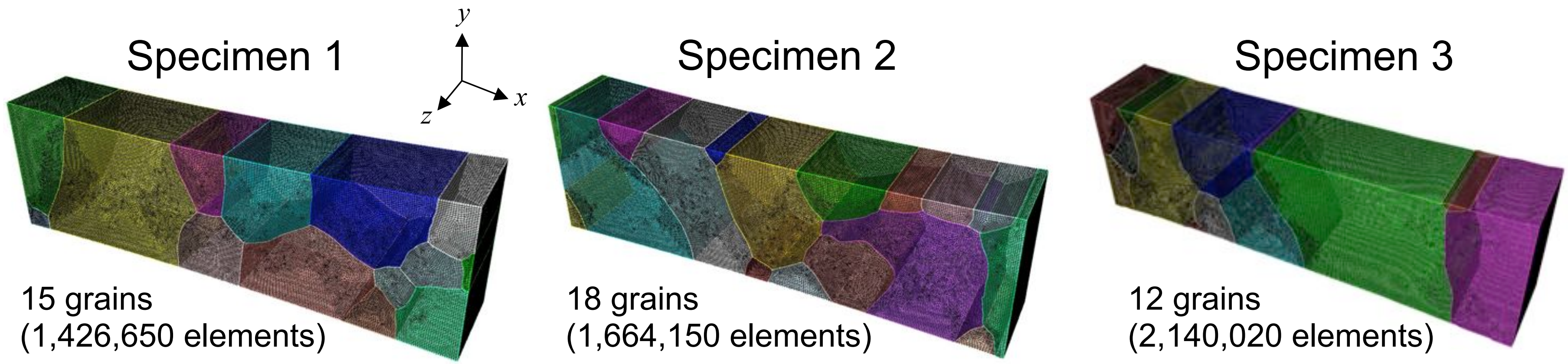




CP-FEM simulations

- 24 {110}<111> slip systems
- Slip rate: $\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \left(\frac{\tau^{\alpha}}{g^{\alpha}} \right)^{1/m}$
- Slip resistance: $g^{\alpha} = \min\left(\tau_{EI}^{*\alpha}, \tau_{LT}^{*\alpha}\right) + \tau_{obs}^{\alpha}$
- Obstacle stress: $\tau_{obs}^{\alpha} = A\mu b \sqrt{\sum_{\beta=1}^{NS} \rho^{\beta}}$ $\qquad \dot{\rho}^{\alpha} = \left(\kappa_1 \sqrt{\sum_{\beta=1}^{NS} \rho^{\beta}} - \kappa_2 \rho^{\alpha} \right) \cdot \left| \dot{\gamma}^{\alpha} \right|$

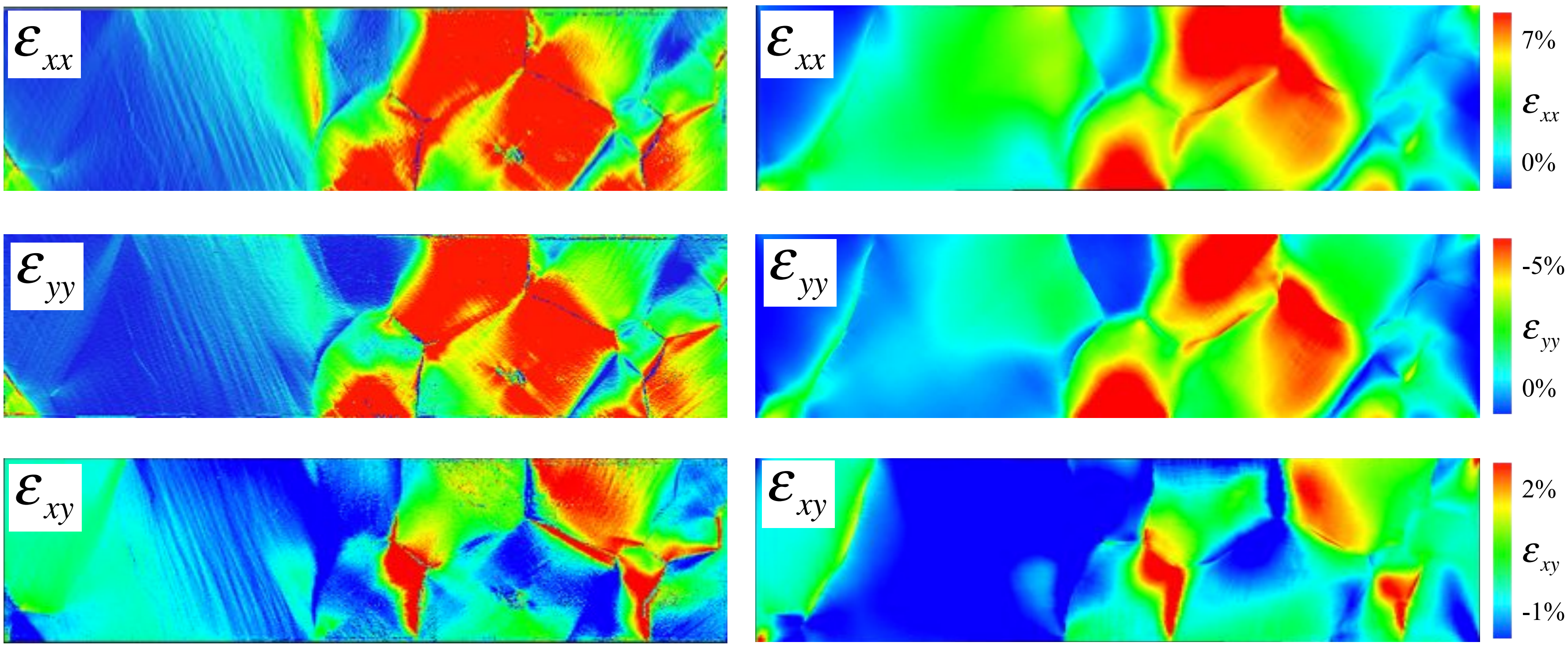




Strain field predictions: specimen 1

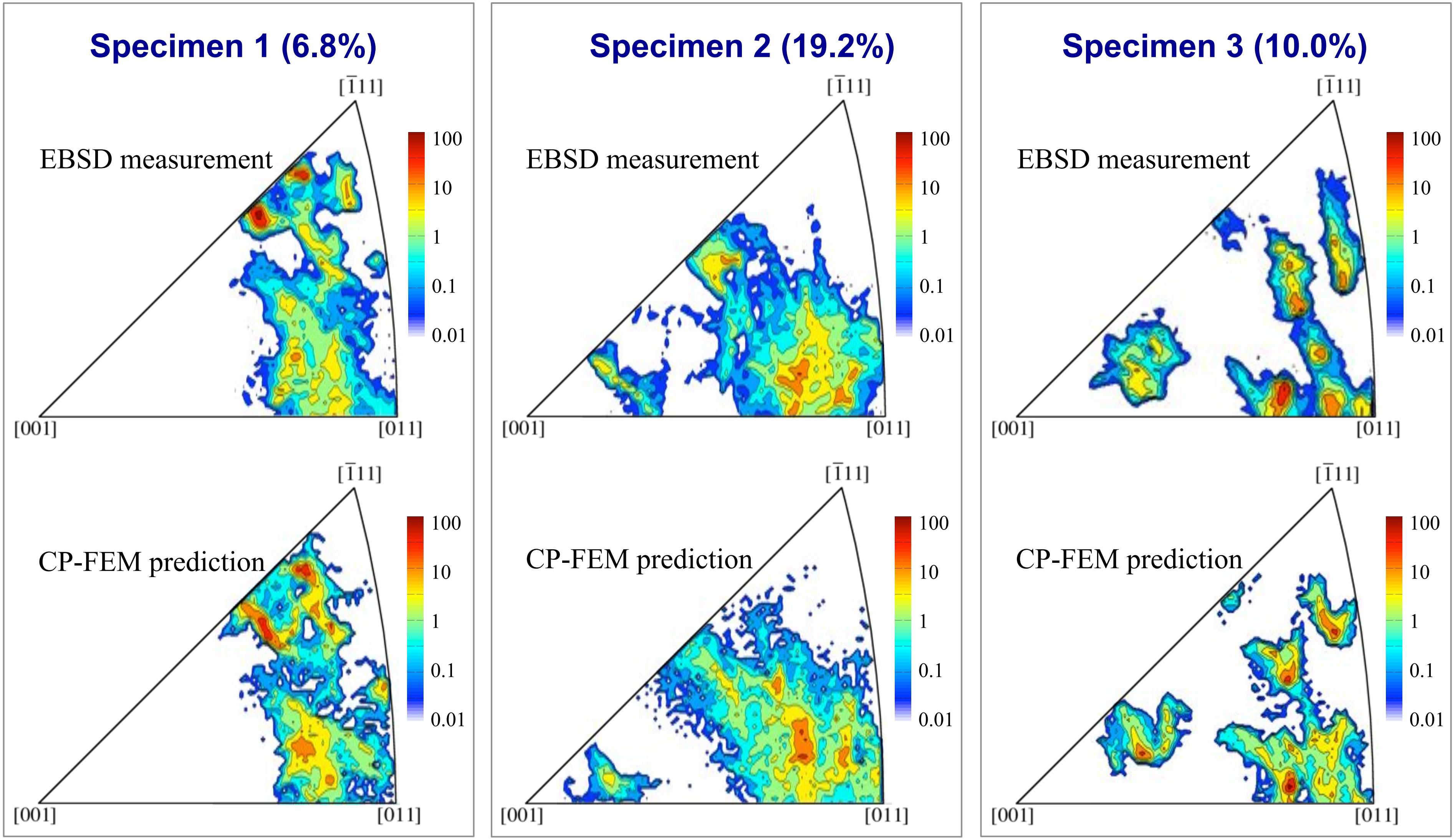
HR-DIC measurements

CP-FEM predictions



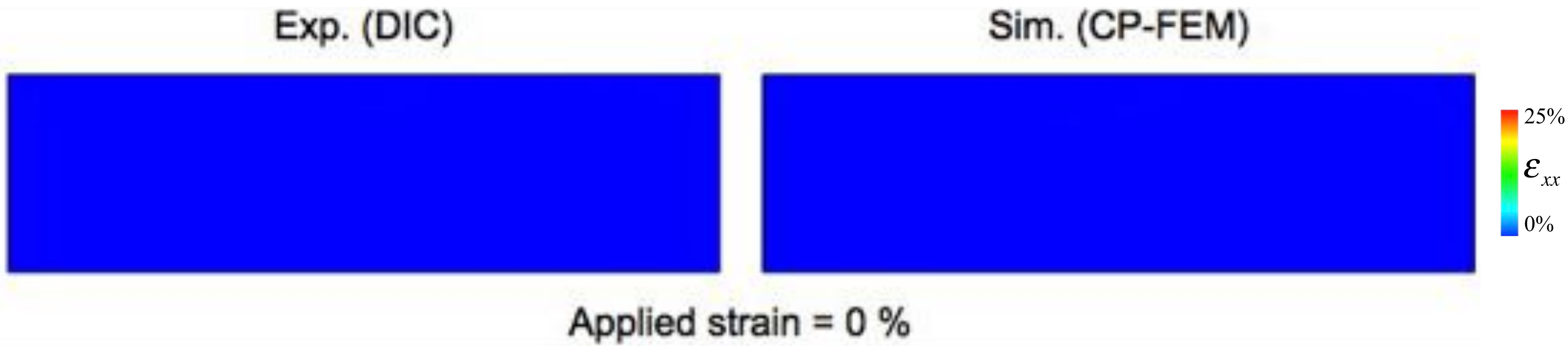
Measured and predicted strain fields agree reasonably well.

Texture predictions

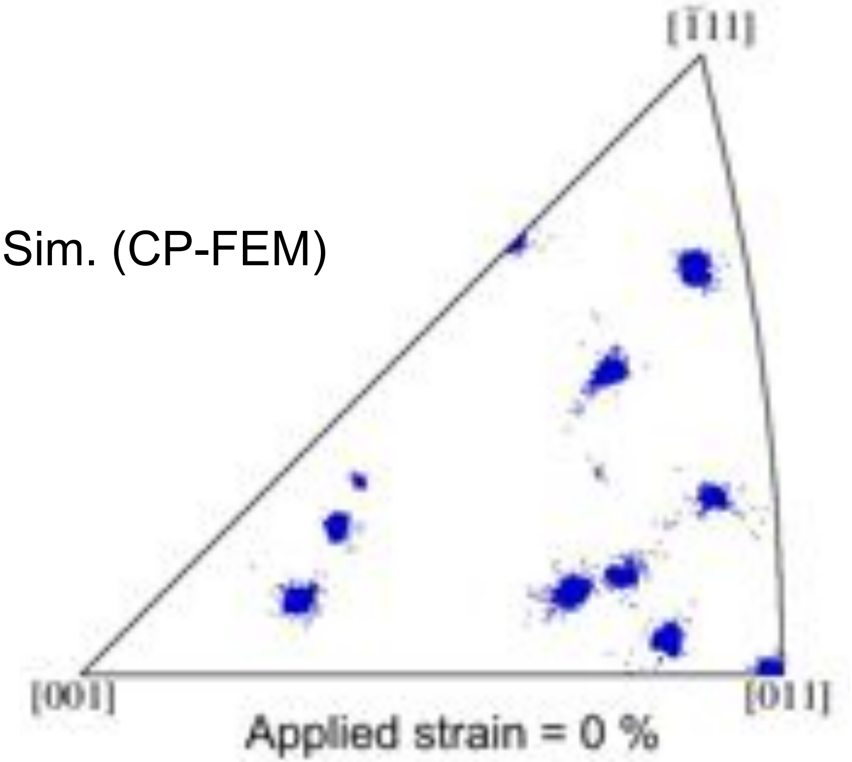


IPF contour plots indicate very good agreement between model and experiment.

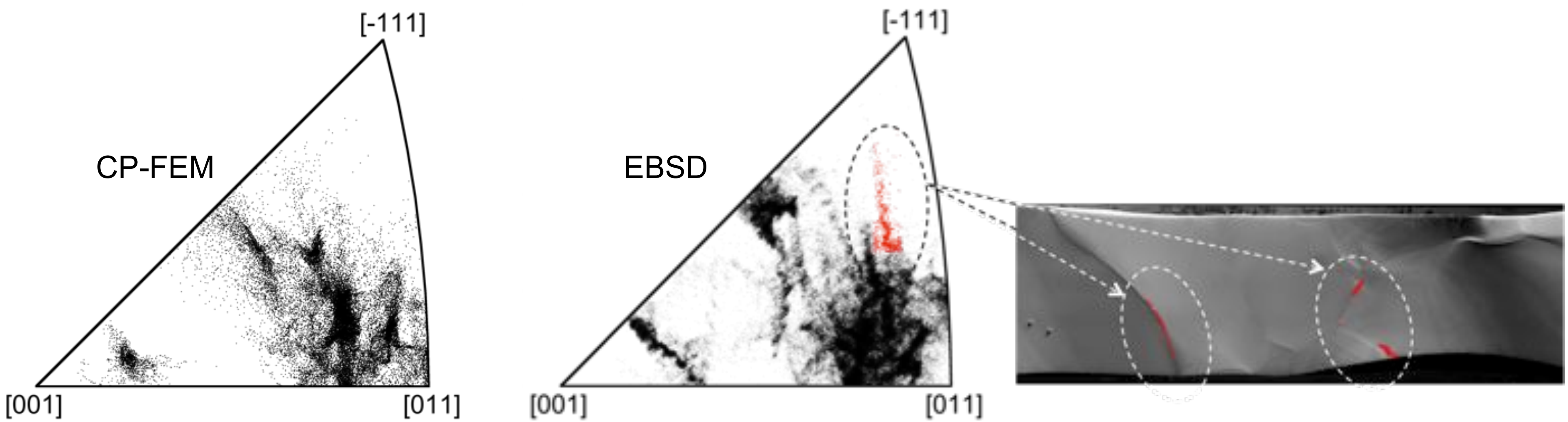
Strain field and texture predictions



Sim. (CP-FEM)



Limitations of the current model



Large deviation observed near grain boundary!

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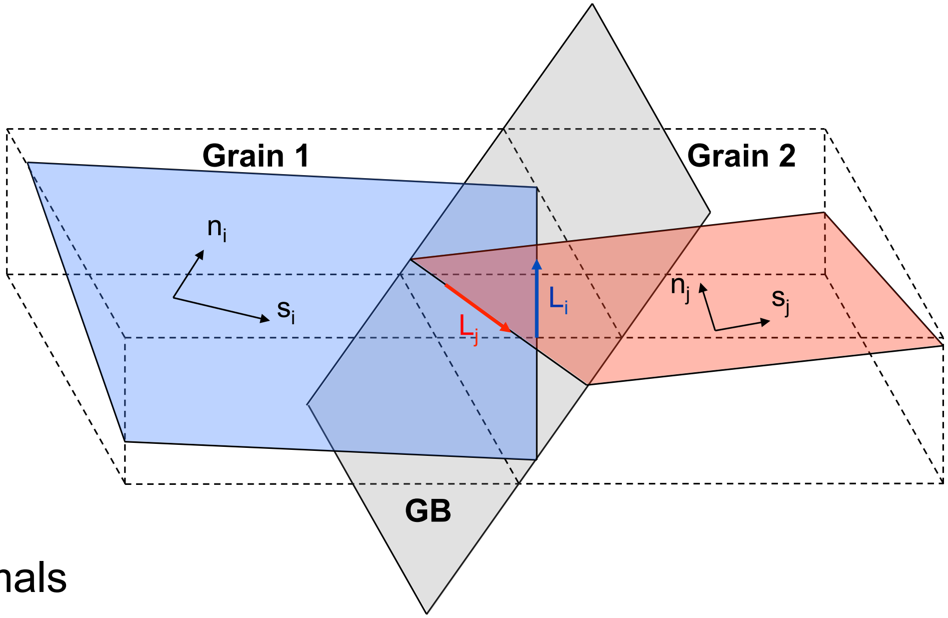
Grain Boundary – Dislocation Interactions

Grain boundary slip transmissivity: *N*

Criteria for predicting the activated slip system across the boundary



Livingstone and Chalmers (1957)

$$N_{ij} = (n_i \cdot n_j)\times(s_i \cdot s_j) + (n_j \cdot s_i)\times(s_i \cdot n_j)$$

Luster and Morris (1995)

$$N_{ij} = (n_i \cdot n_j)\times(s_i \cdot s_j)$$

Shen et al. (1988)

$$N_{ij} = (L_i \cdot L_j)\times(s_i \cdot s_j)$$

n : slip plane normals
s : slip directions
L : intersection line between GB and slip plane normal

$$0 \le N \le 1$$

No transmission — Complete transmission

Grain Boundary Transmissivity

For 24 slip systems, 24 x 24 =576 *N* values!

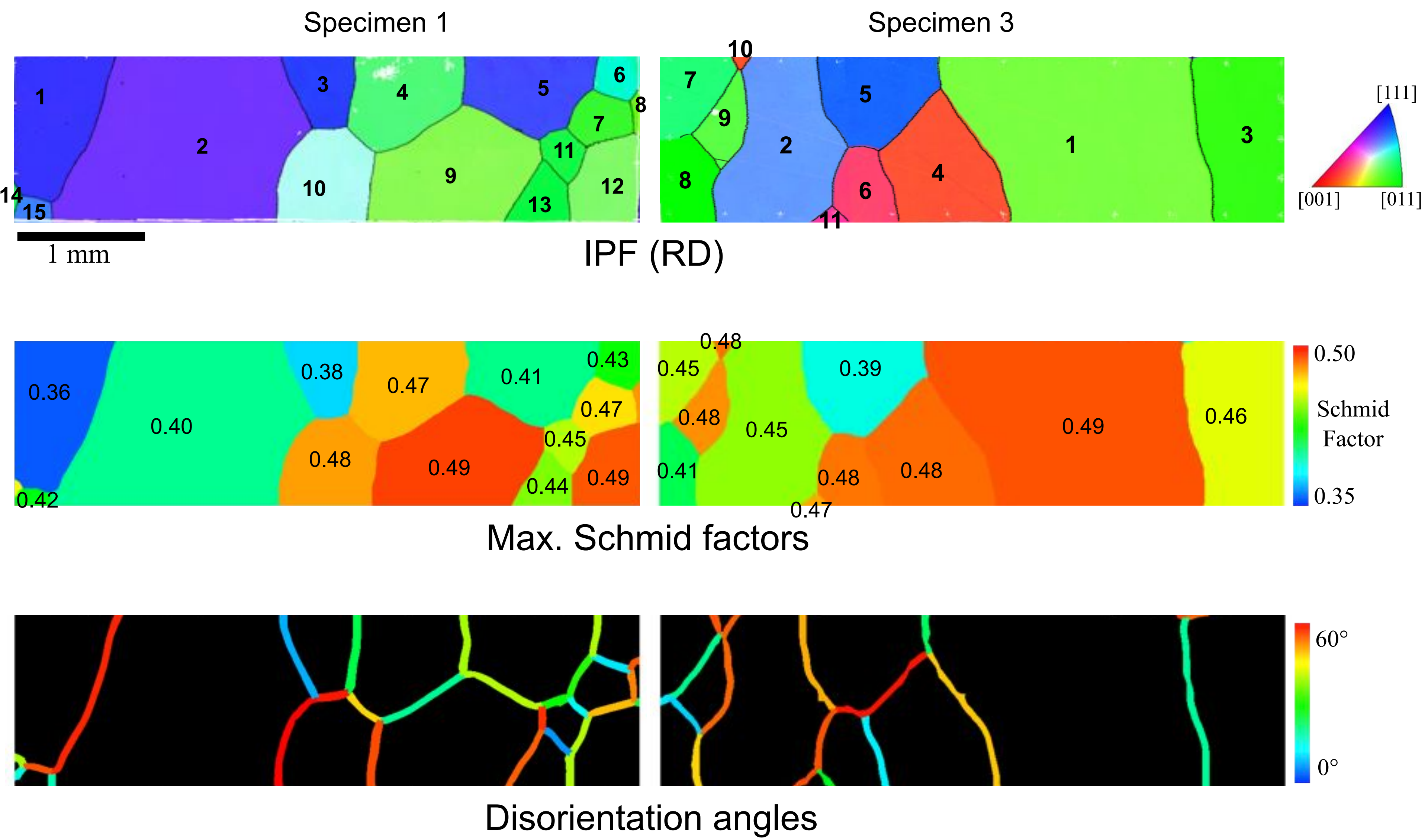
- ❖ Maximum *N* (Shen et al., 1988)
- ❖ Schmid factor (Bieler et al., 2014)
- ❖ Slip activity (Current work)

$$m = \sum_{i=1}^{24} \left(\sum_{j=1}^{24} \left(N_{ij} \frac{\gamma_j}{\sum \gamma_j} \right) \frac{\gamma_i}{\sum \gamma_i} \right)$$

γ_i : slip activity obtained from CP-FEM

Advantages
- Considers effects of local strain field (no assumptions for uniaxial loading)
- Considers effects of crystal rotation (not using initial crystal orientations)

Tantalum oligocrystals



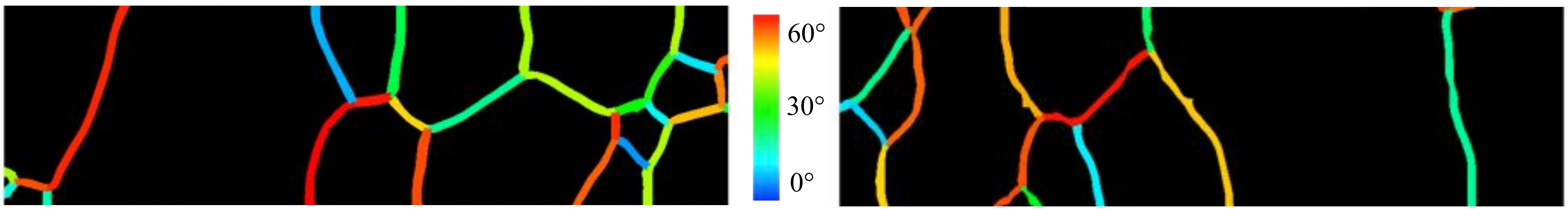
Disorientation analysis

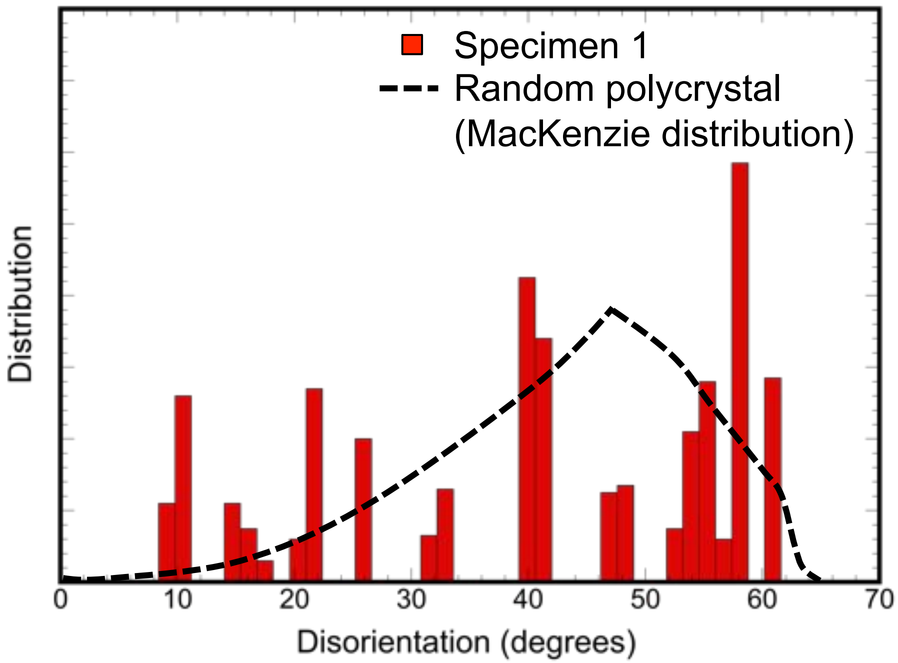
$$\Delta g_{AB} = g_B g_A^{-1}$$

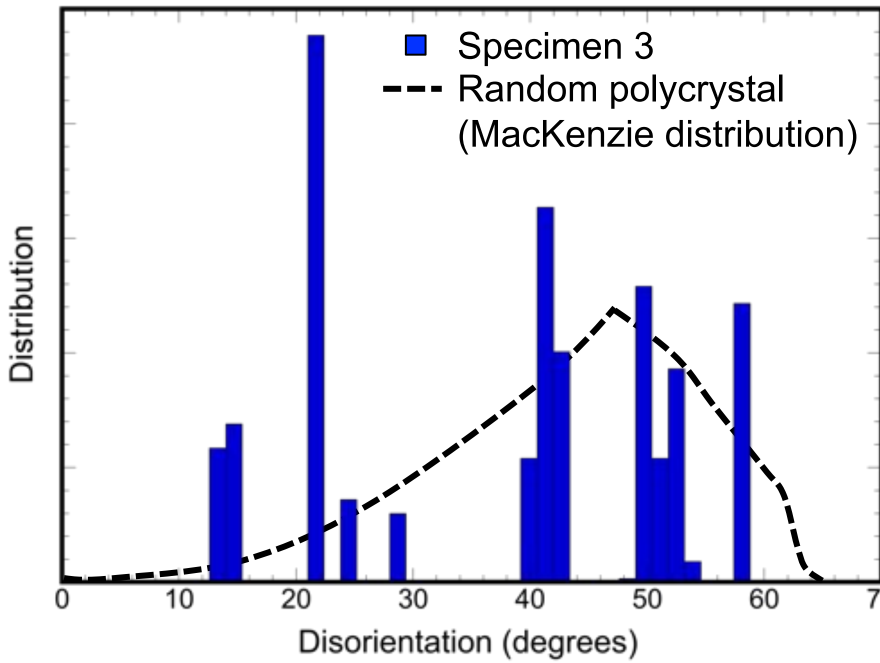
$$\cos\theta = \frac{1}{2}\left(\Delta g_{11} + \Delta g_{22} + \Delta g_{33} - 1\right)$$

Specimen 1

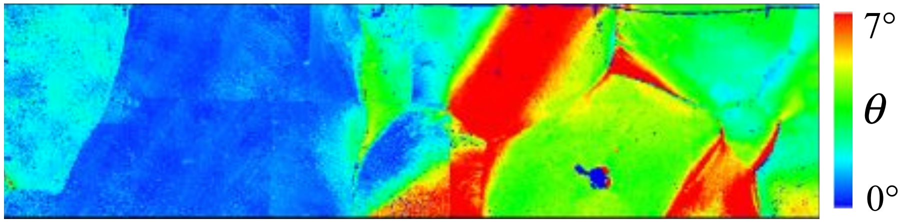
Specimen 3



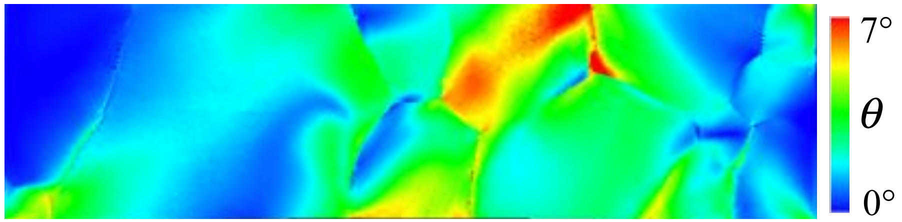




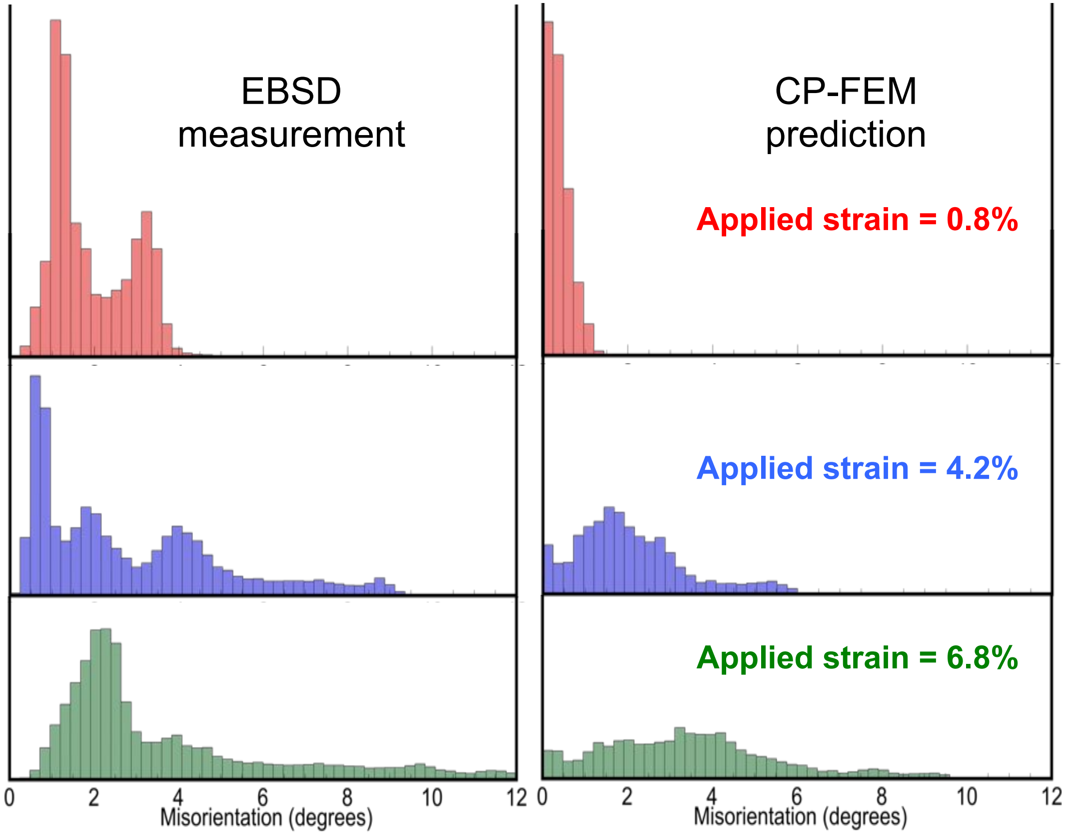
Misorientation analysis

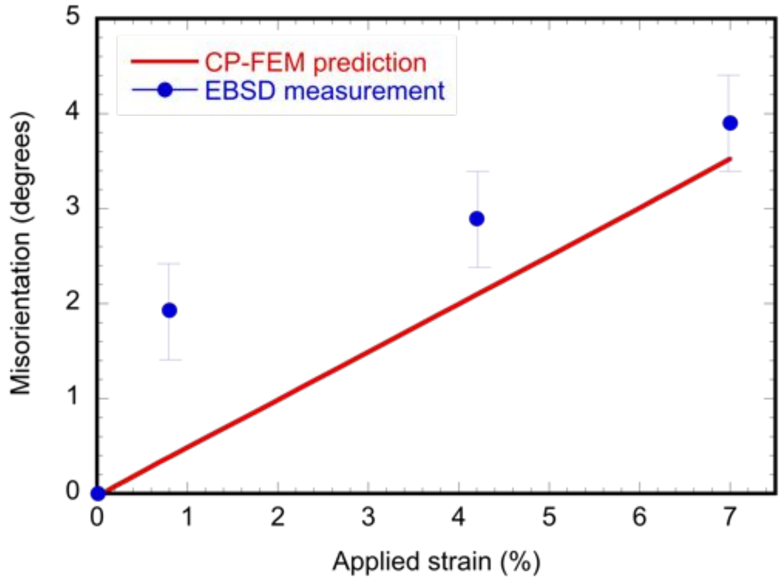


EBSD measurement



CP-FEM prediction



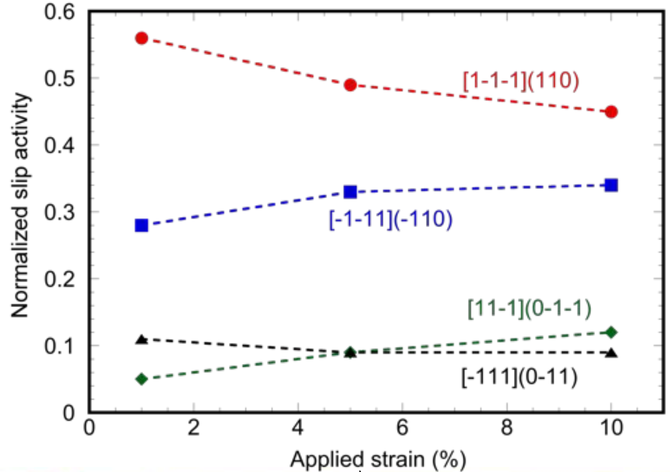


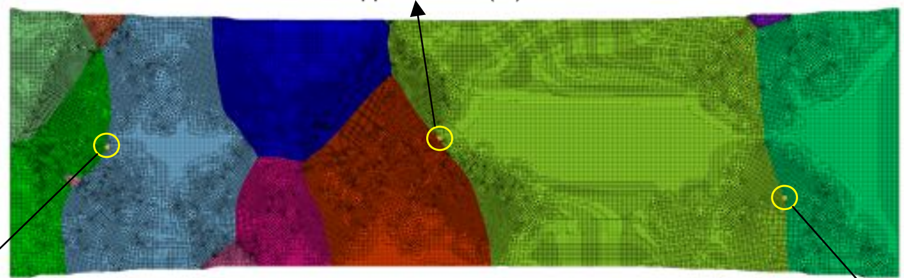
Average misorientations

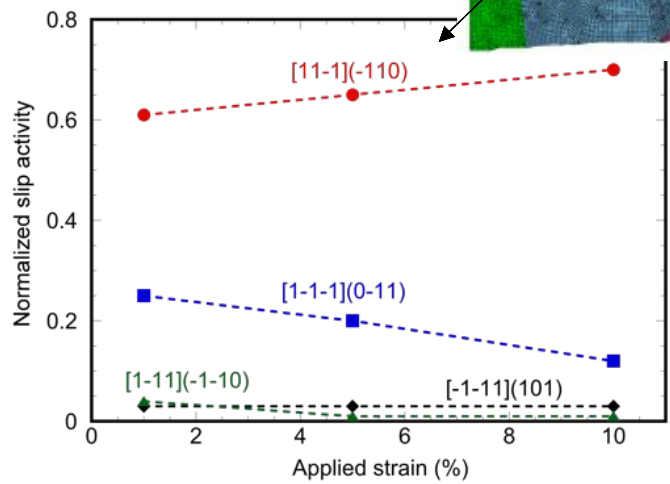
Slip activities

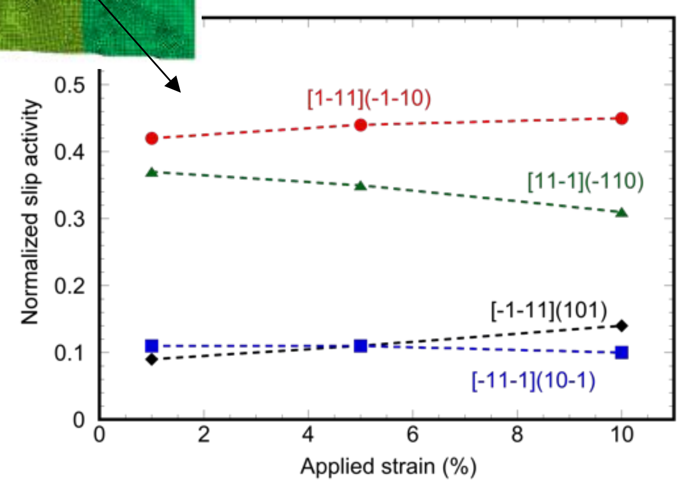
Normalized slip activity

$$\bar{\gamma}_i = \frac{\gamma_i}{\sum \gamma_j}$$

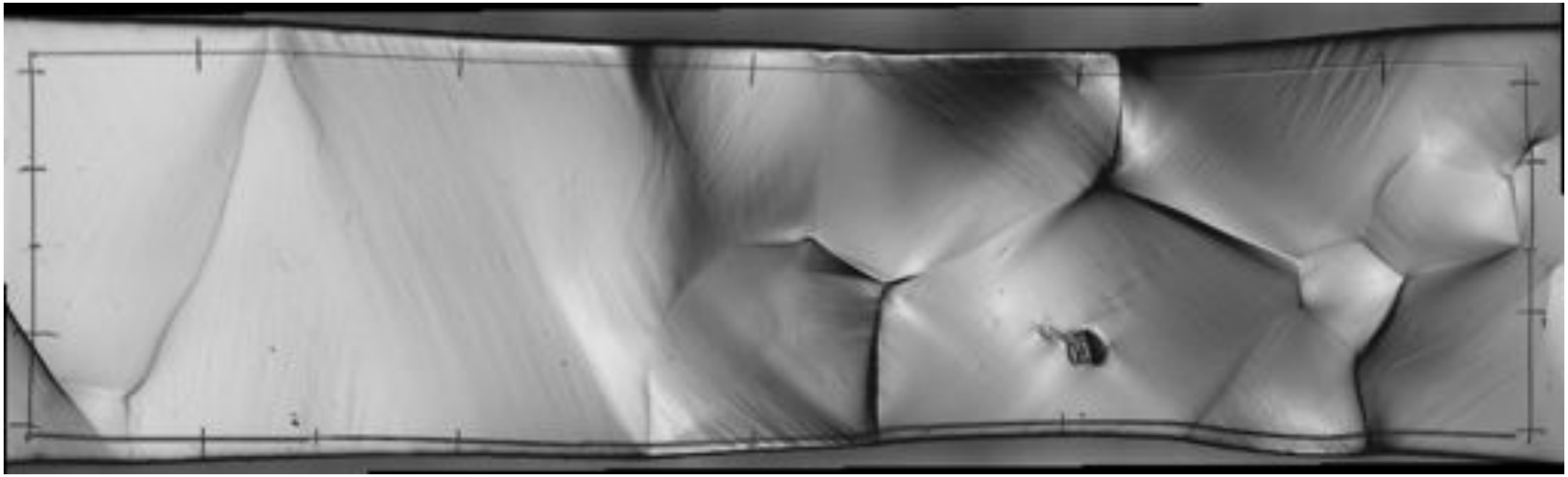


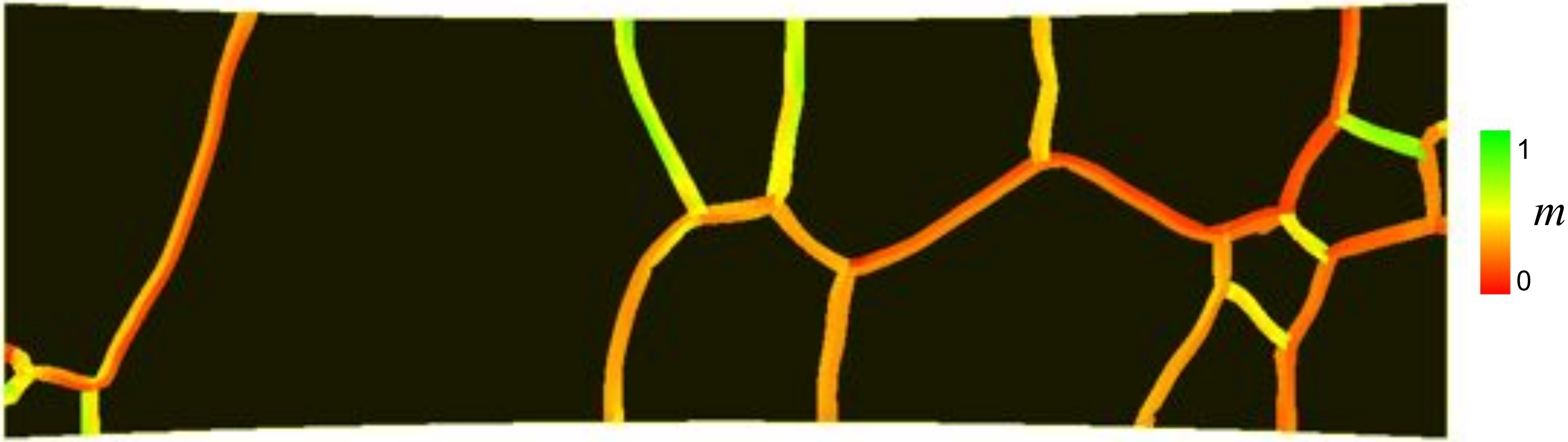




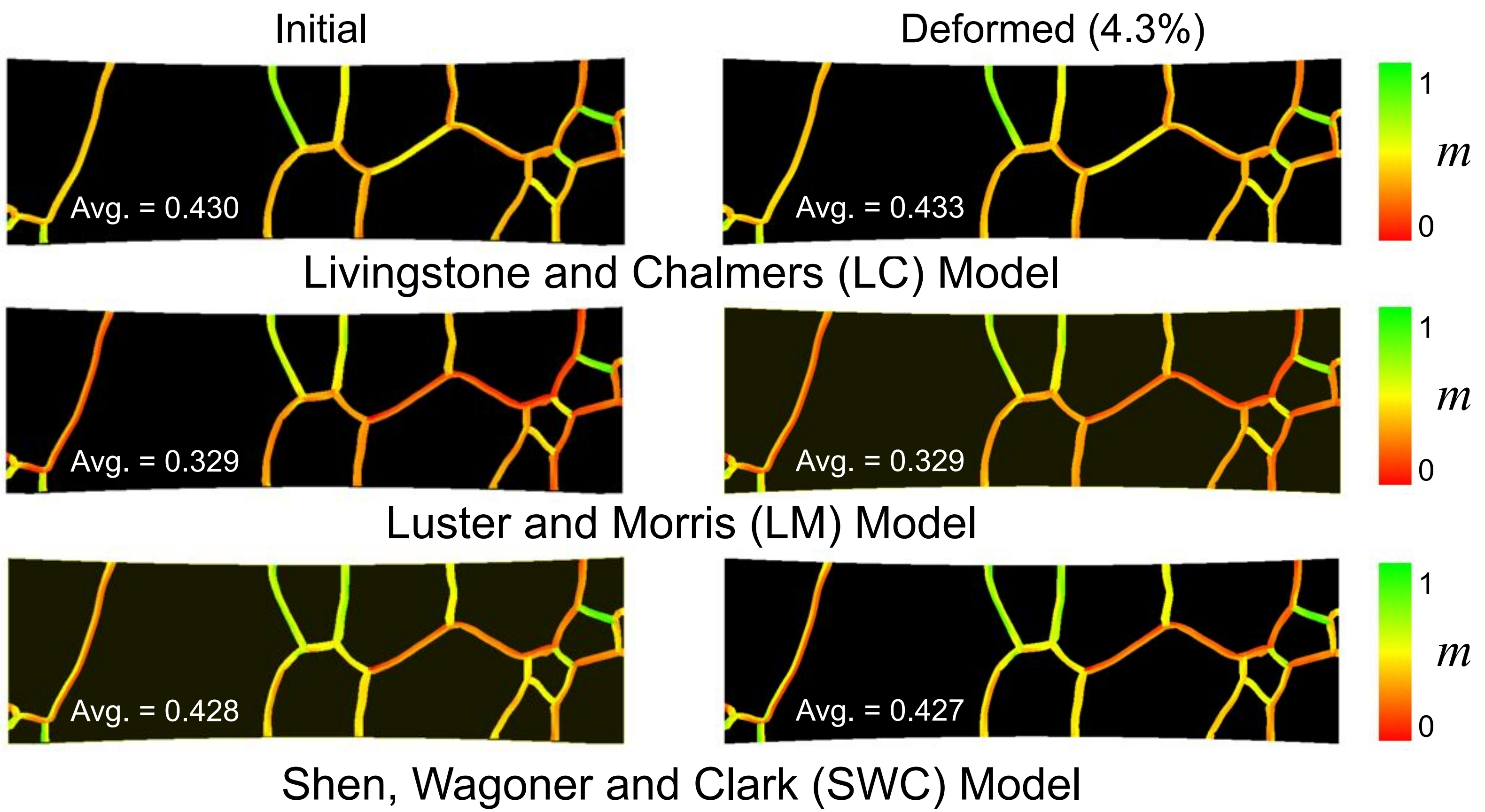


Transmissivity vs. exp. measurements





Transmissivity Calculations



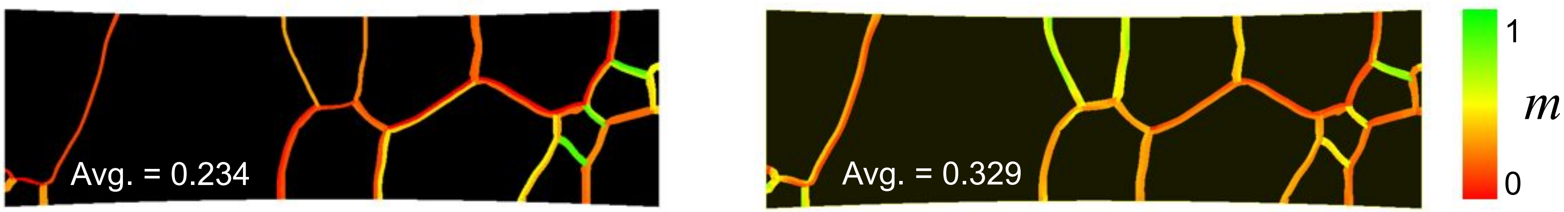
Tantalum oligocrystal specimen 1

Transmissivity Calculations

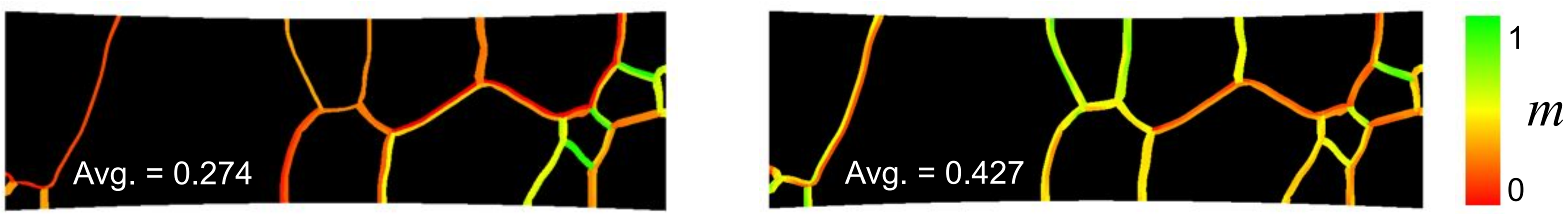
Schmid factor based calculations

Slip activity based calculations

Livingstone and Chalmers (LC) Model



Luster and Morris (LM) Model



Shen, Wagoner and Clark (SWC) Model

Summary

- CP-FEM predictions of Ta oligocrystals showed good agreement with measured surface strain fields (HR-DIC) and deformed textures (EBSD).
- GB transmissivity, *m*, characterizes geometries for the slip transfer.
- No clear correlation between GB disorienation and transmissivity is observed.
- Contributions from crystal rotations and slip activities does not change *m* significantly with applied strain.

THANK YOU !

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