SAND2016-5768C

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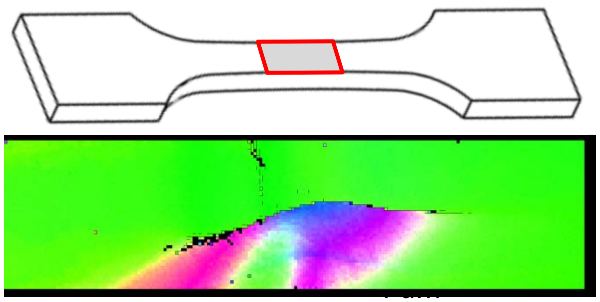

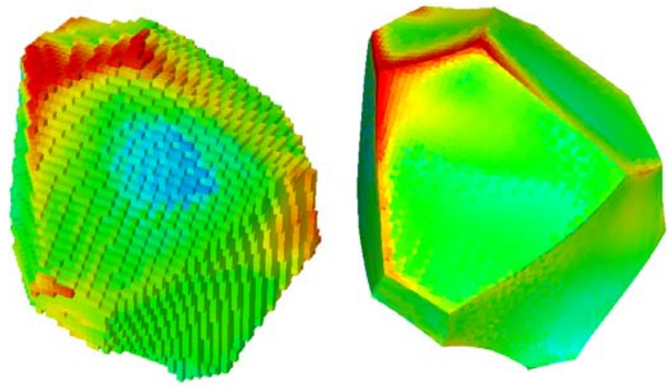

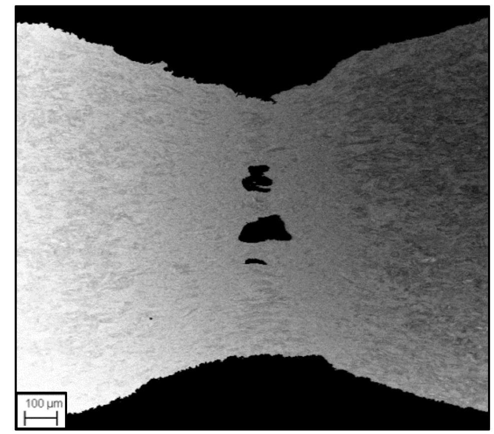

Quantifying Grain-Scale Deformation for Direct Comparison to Crystal Plasticity Predictions

Brad L. Boyce; **Hojun Lim; Jay D. Carroll; Thomas E. Buchheit; Corbett C. Battaile**

Sandia National Laboratories

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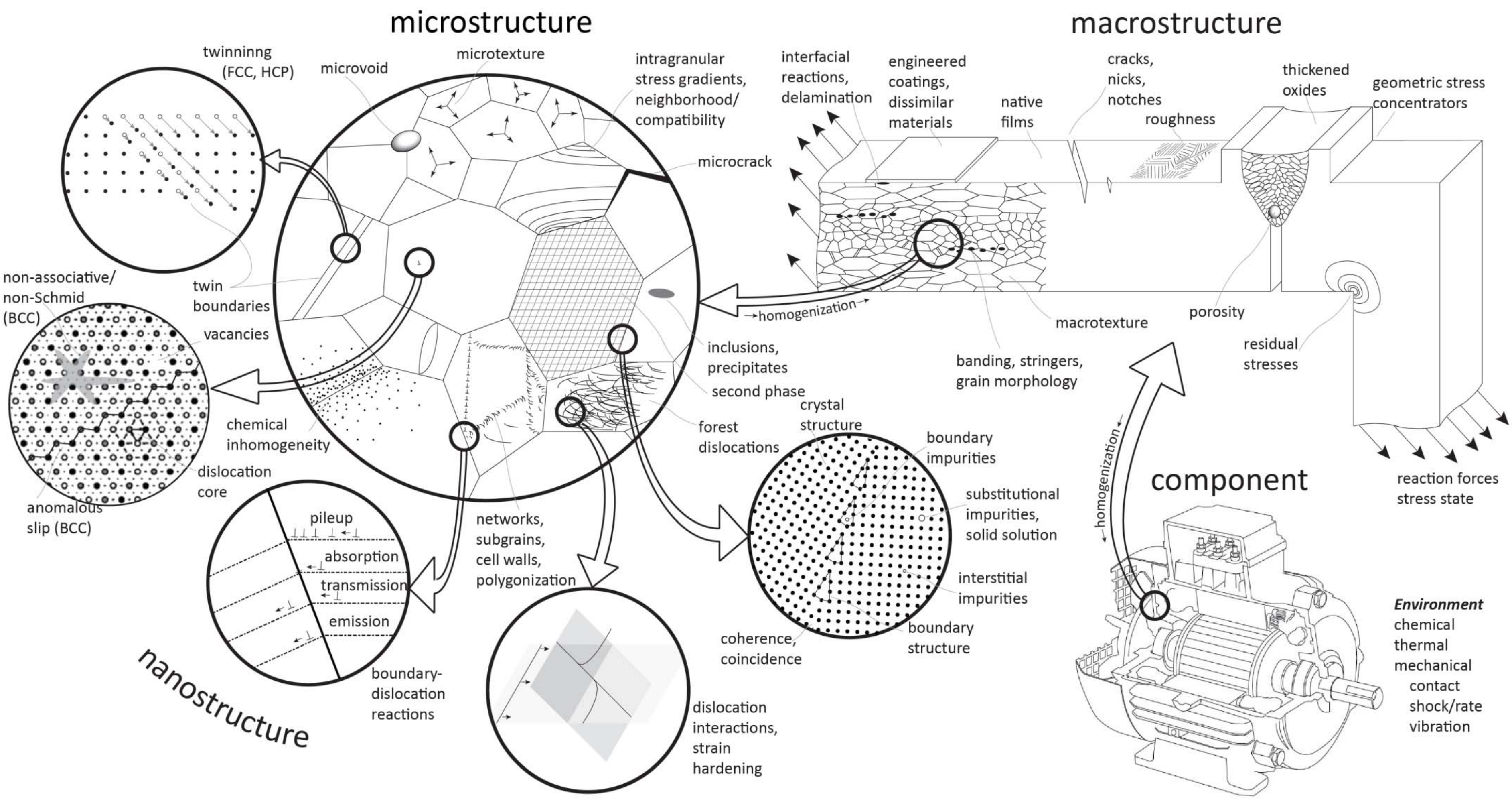
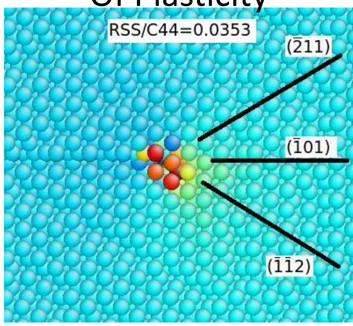
Introduction: Material and length-scale roadmap for deformation and failure of structural metals

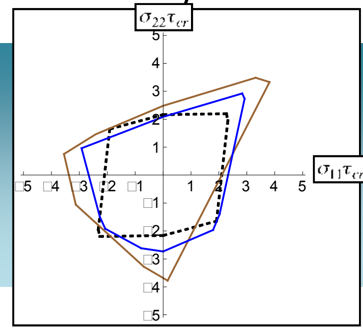


Developing an ***experimentally validated*** model for grain-scale deformation (crystal plasticity)

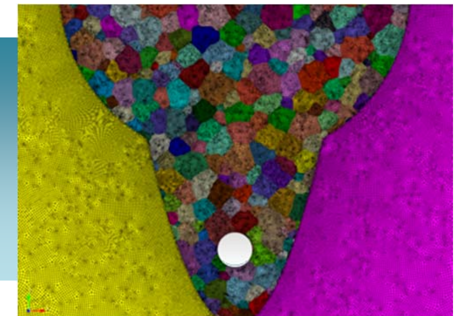
Atomic Mechanisms
Of Plasticity



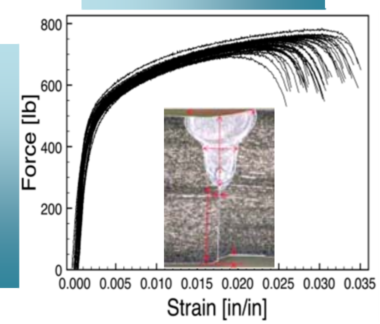
Single-Crystal
Plasticity Models



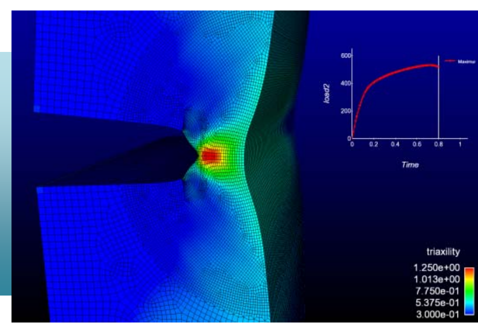
Polycrystalline
Deformation Response



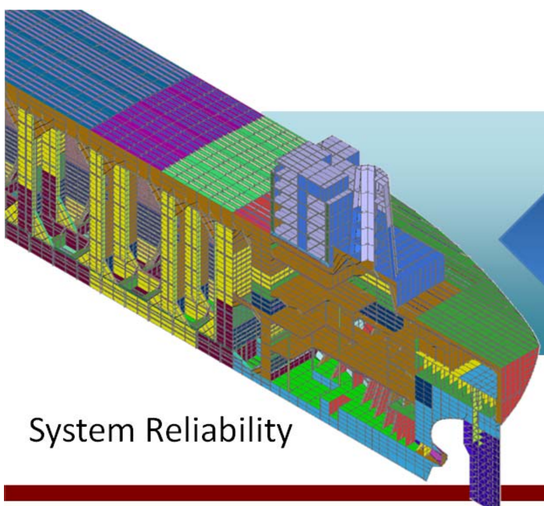
Goal: Provide a science-based foundation for design, analysis, and qualification capabilities that links mesoscopic/microscopic inhomogeneity to property variability.



Stochastic Outcomes
From Different Configurations



Reduced Order Modeling
For Efficient Stochastic Computations



System Reliability

Recent Sandia advances in Polycrystal Plasticity: Phase-Field generated microstructure & smooth meshing

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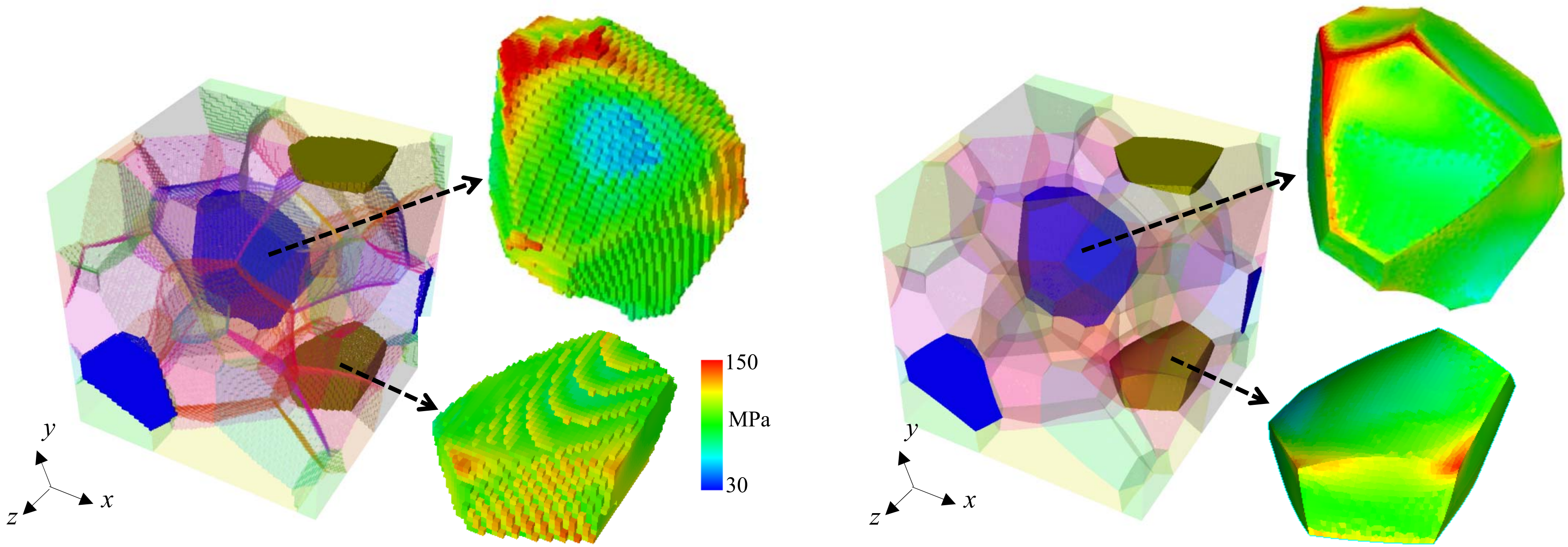
Voxelated FE mesh

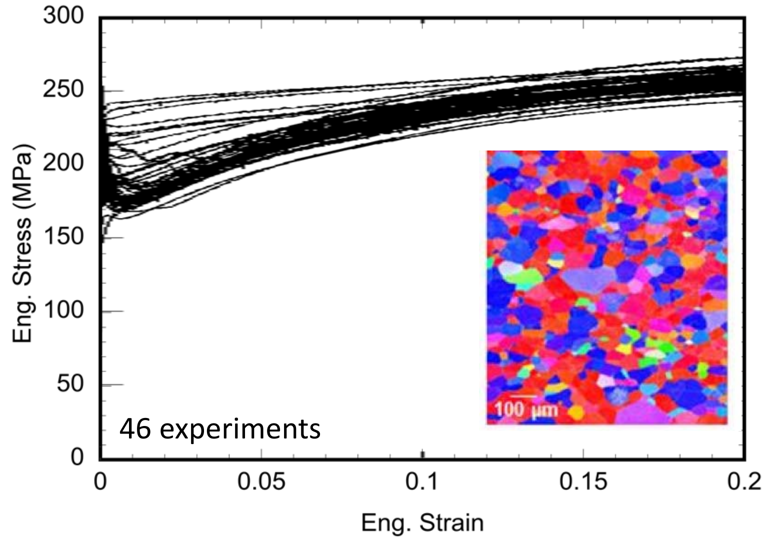
Conformal FE mesh

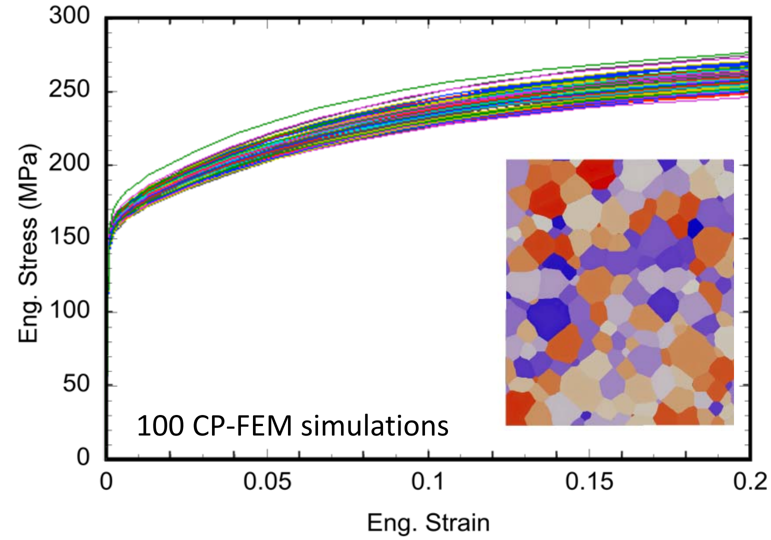


Von Mises stress contours at 10% deformation

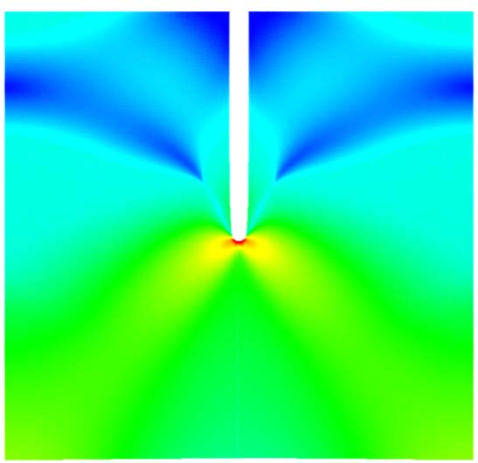
ABSTRACT	SYMPOSIUM	SESSION	WHEN	WHERE
Developing Physically-based Three Dimensional Microstructures: Bridging Phase Field and Crystal Plasticity Models *Hojun Lim*[1]; Fadi Abdeljawad[1]; Steven J. Owen[1]; Byron W. Hanks[1]; Corbett C. Battaile[1]; [1]Sandia National Laboratories	Computational Materials Discovery and Optimization: From 2D to Bulk Materials	Microstructure and Mechanical Properties	**Thursday 11:10 AM - 11:30 AM**	Music City Center 207D

Predicting Stochastic Behavior of Polycrystals

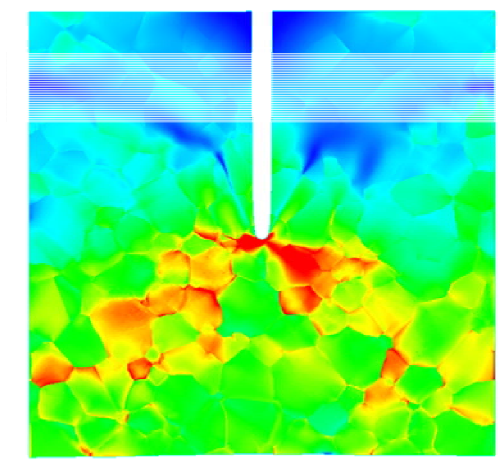




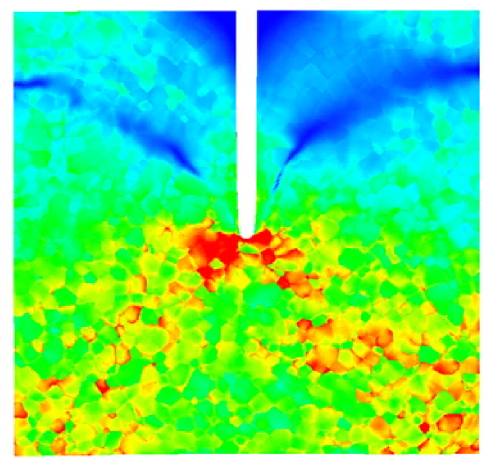
Grain-scale variability in macroscale response



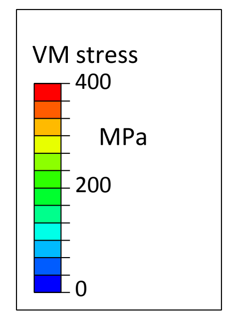
Continuum simulation (J2)



CP-FEM simulation (~200 grains)



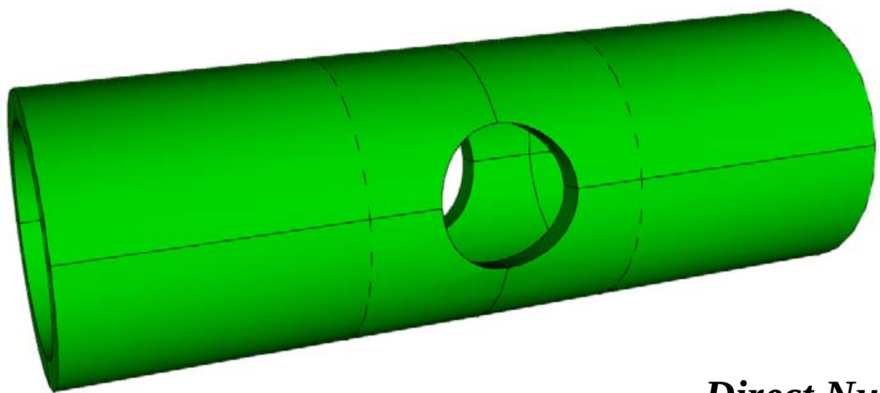
CP-FEM simulation (~1000 grains)

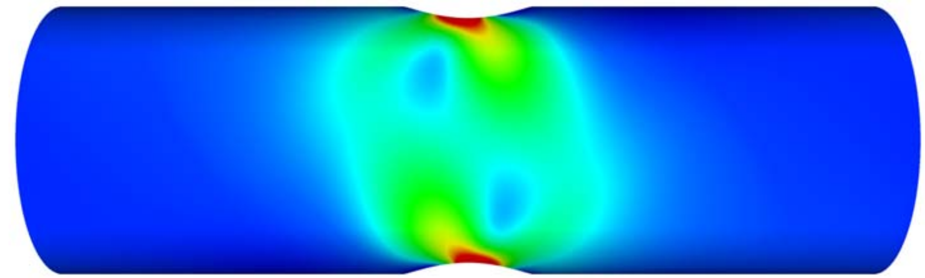


VM stress fields after 3% deformation

On the horizon: System-scale simulations with explicit microstructural representations.

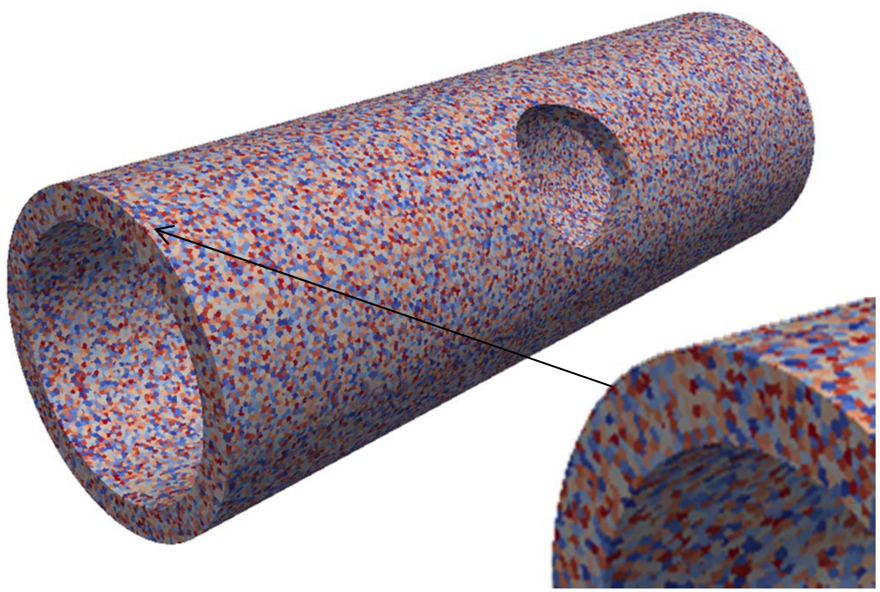
Homogenization

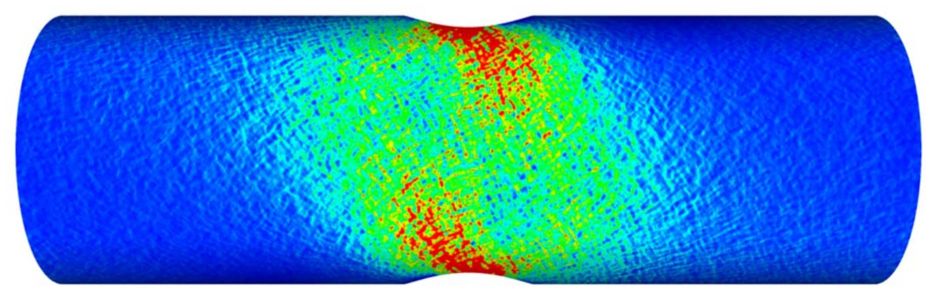




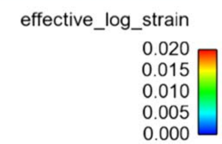
8K elements

Direct Numerical Simulation

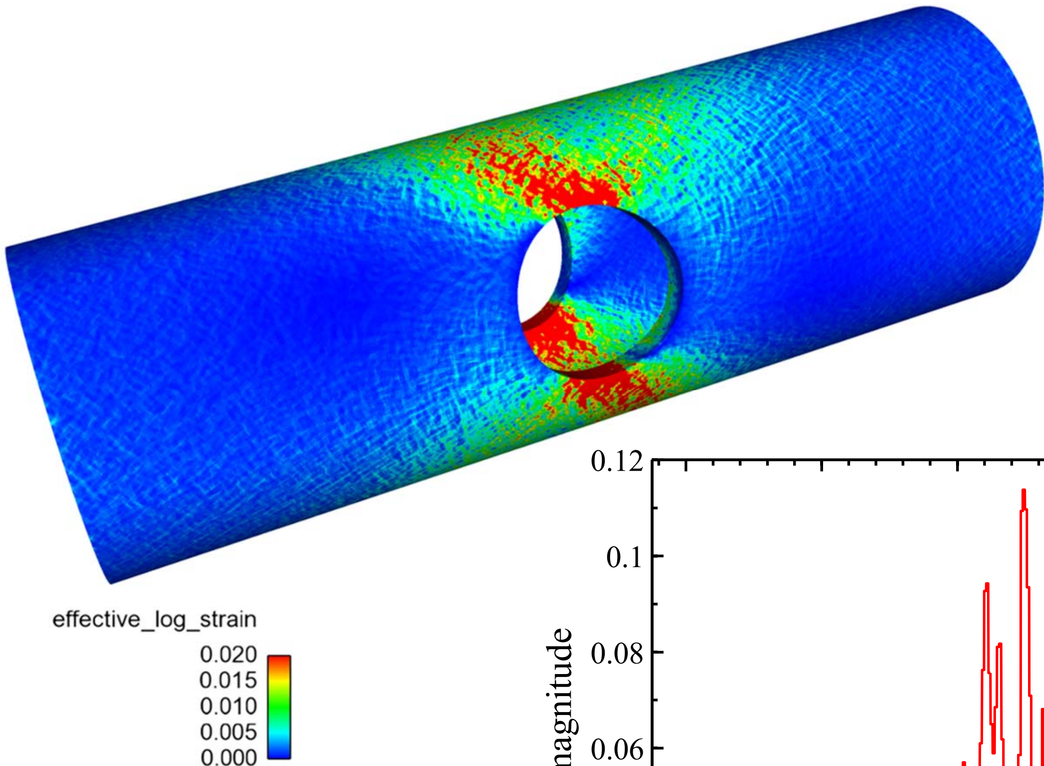


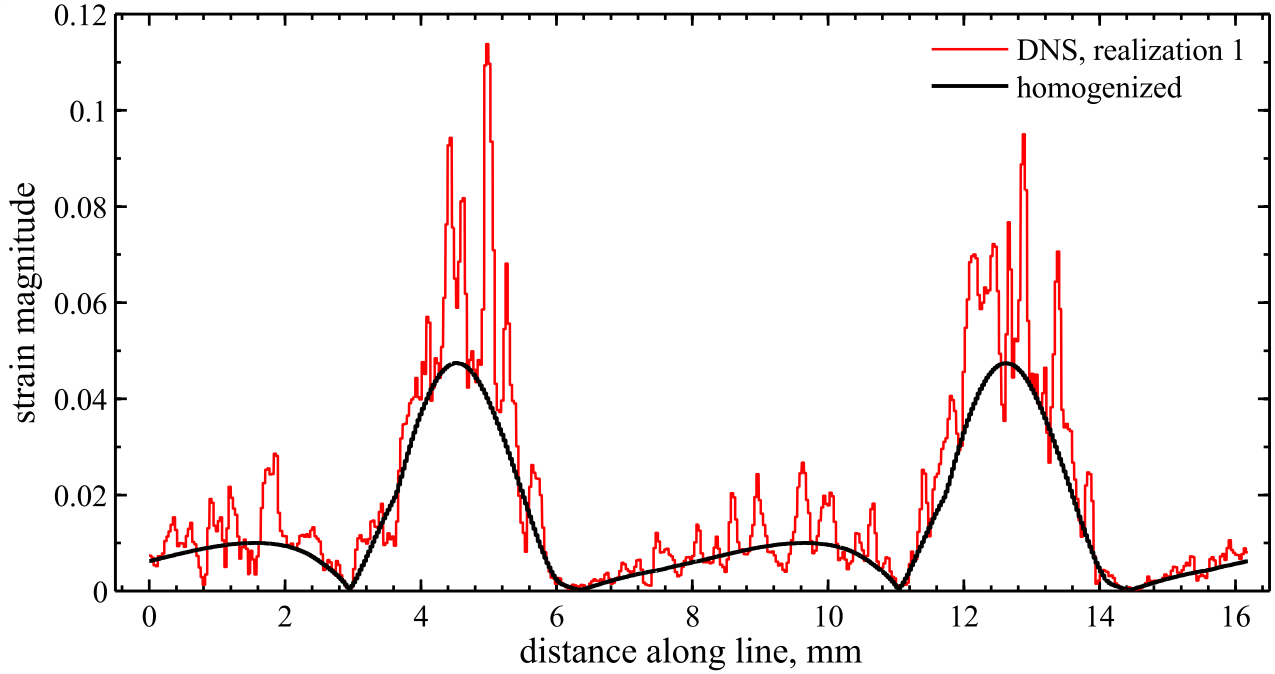


35M elements, 350K grains
2400 processors (Chama)



On the horizon: System-scale simulations with explicit microstructural representations.





Polycrystal plasticity employs finite element method to discretize crystallographic slip at the crystallographic-level.

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

- $\tau_{\mathrm{obs}}^{\alpha}$ → Obstacle stress
- $\tau_{\mathrm{ns}}^{\alpha}$ → Lattice friction

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

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

Options for Experimental Validation at Grain-Scale

Deformation gradient can be decomposed into a product of stretch and rotation

$$\boldsymbol{F} = \boldsymbol{UR}$$

stretch

rotation

Analagously, experimentally we measure shape change and rotation

Digital Image Correlation Surface Profilometry Synchrotron X-ray microdiffraction	Electron Backscatter Diffraction Precession Electron Diffraction Synchrotron X-ray microdiffraction

Quantifying Shape Change

Previous Work on Sim.- Exp. Comparison

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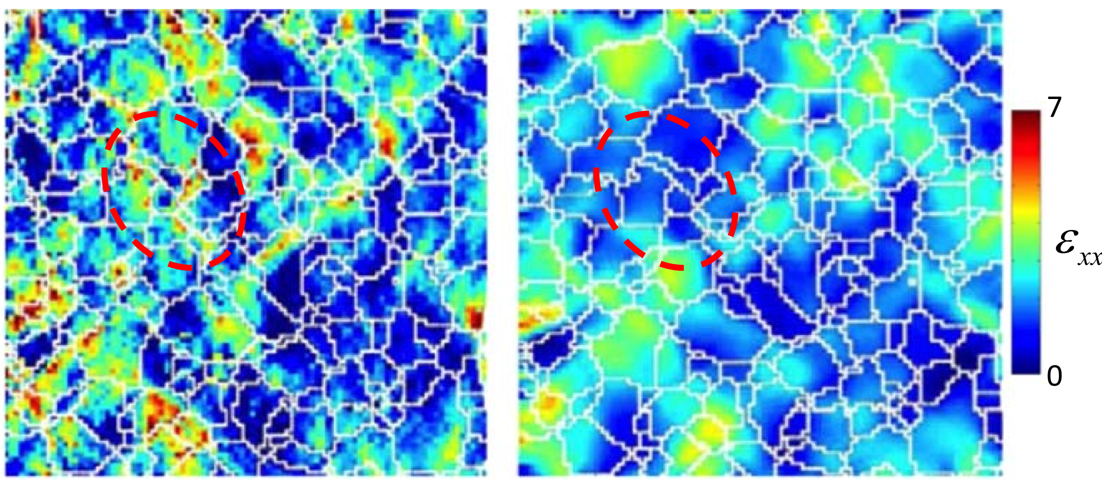
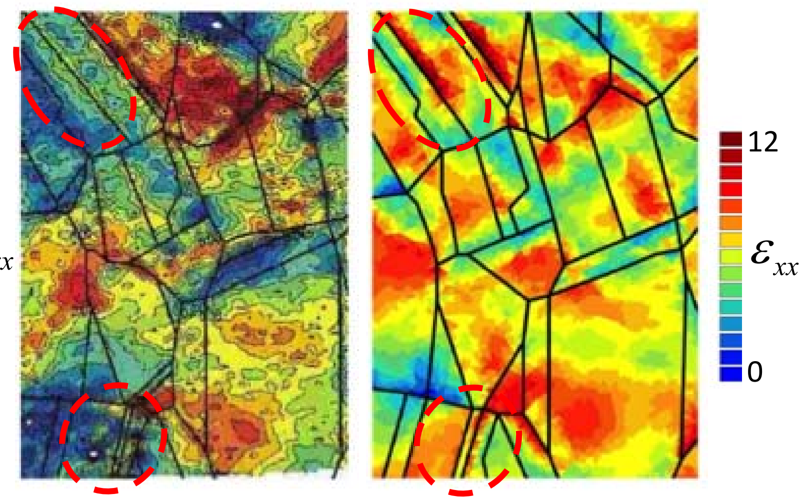
"Quantitative comparisons between the model and experiments"

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



Experiment Simulation

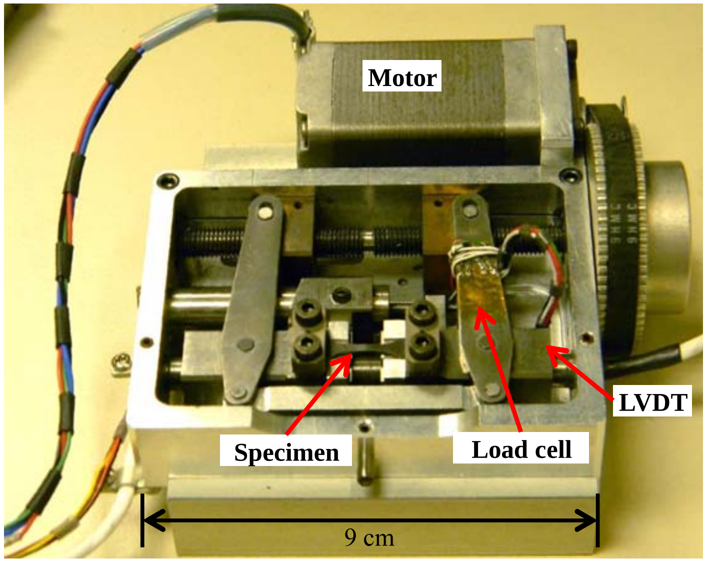
OFHC Cu polycrystal (Musienko et al, 2007)
(5 % strain)



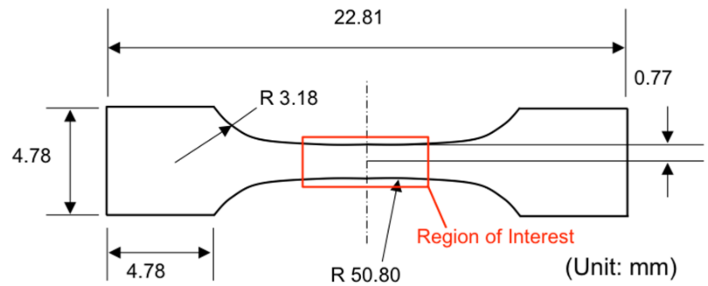
Experiment Simulation

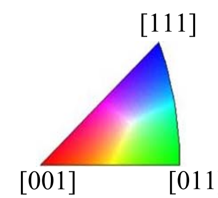
Limited success has been achieved in modeling polycrystal deformation behavior due to unknown subsurface grains

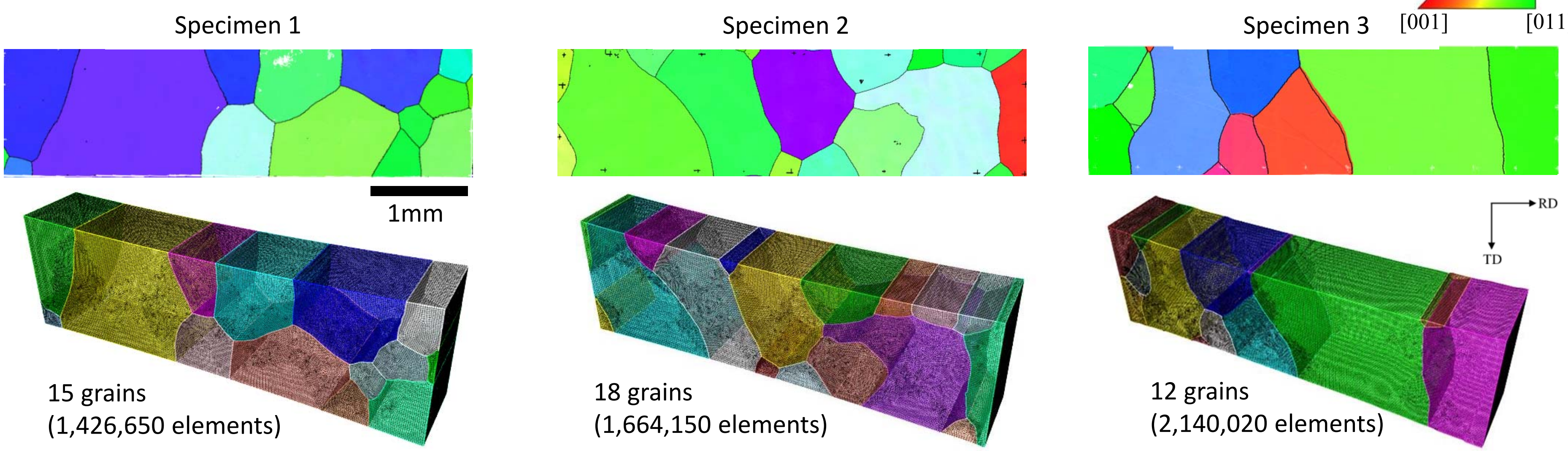
Experimental Setup



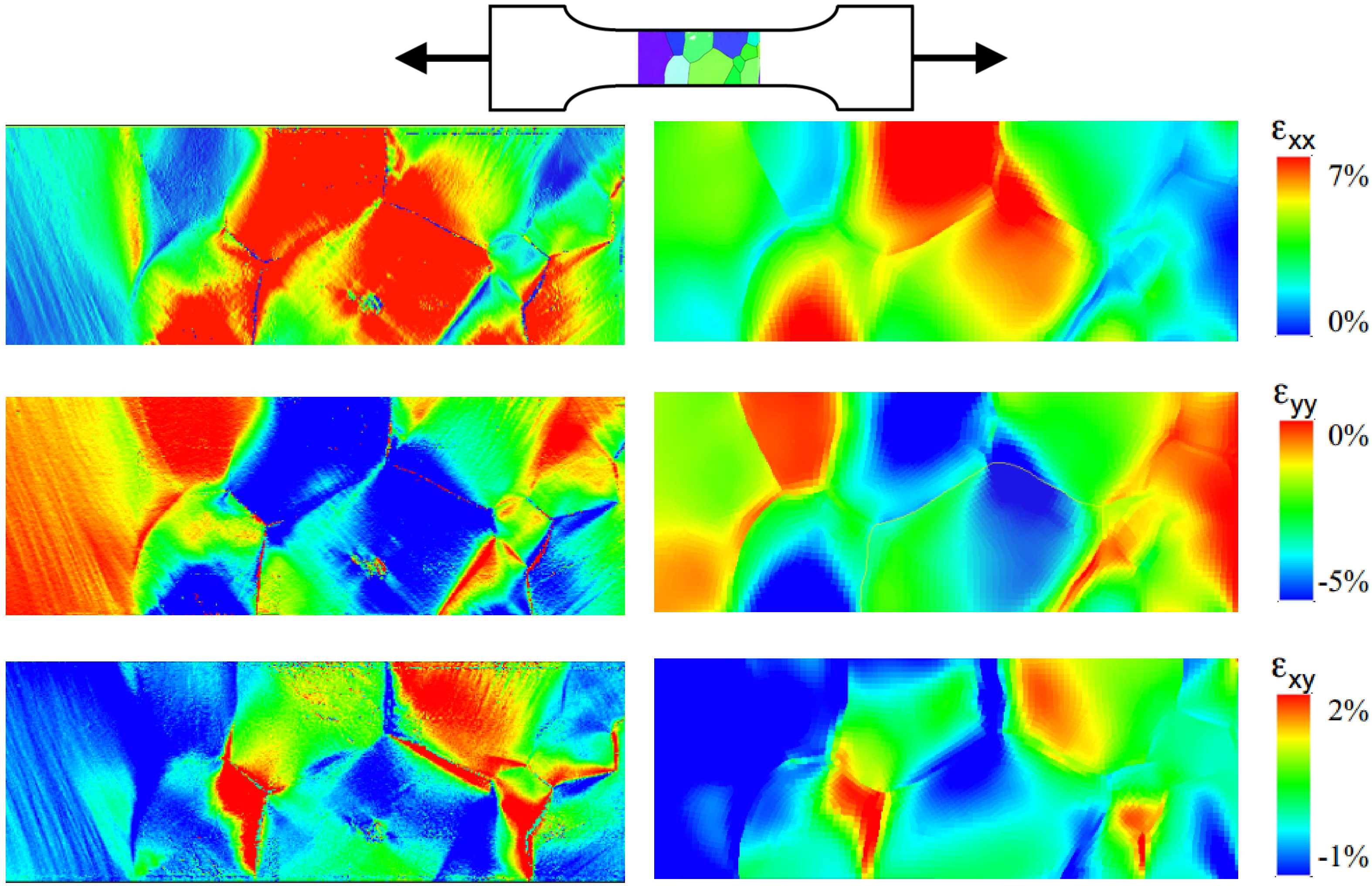
- Tantalum oligocrystals with mostly columnar 2D grain structure eliminate unknown subsurface grain morphology.
- *In-situ* load frame developed at Sandia
- HR-DIC (surface strain fields) and EBSD (crystal orientations) measurements at load inside SEM







Side-by-side qualitative comparison

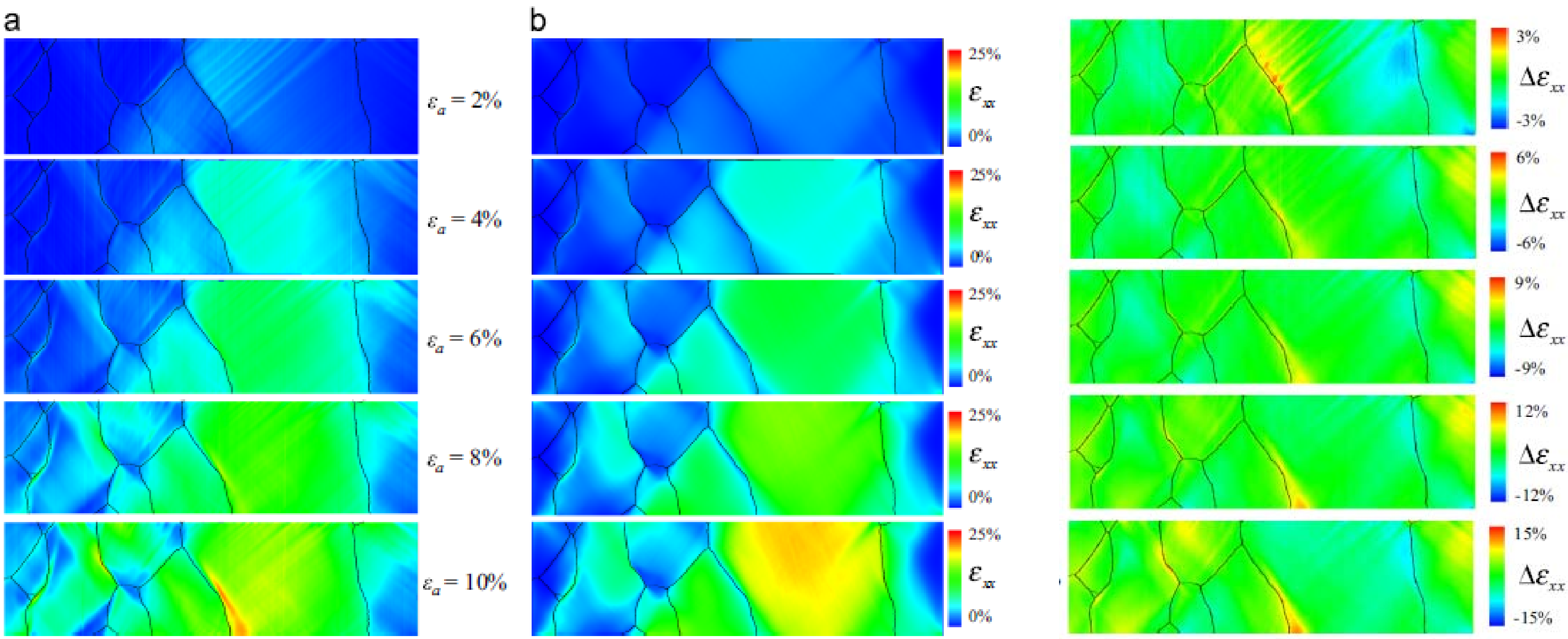


Experimental measurement of strains within individual grains using SEM Digital Image Correlation

2D slice of a 3D simulation of strain inhomogeneity based on crystal plasticity finite element modeling.

A Quantitative Model-Experiment Difference Map

$$\varepsilon_{xx}{}^{DIC} \quad - \quad \varepsilon_{xx}{}^{CPFEM} \quad = \quad \Delta\varepsilon_{xx}$$



Lim *et al.*, *Int. J. Mechanical Sciences*, 2015

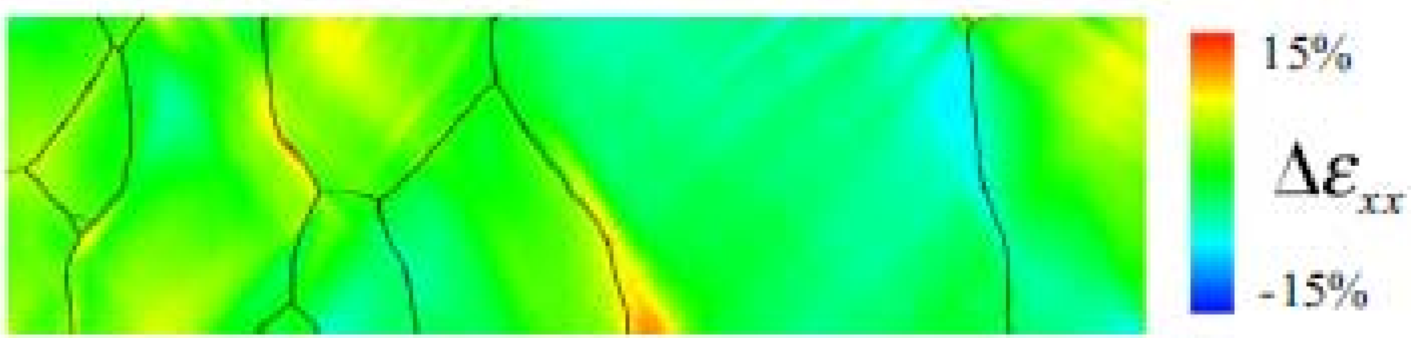
The advantage of quantitative difference mapping:

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

- **A rational RMS goodness-of-fit metric to compare and discriminate effectiveness and locate deficiencies.**

Deviation	Applied strain (ε_a)				
	2%	4%	6%	8%	10%
$\Delta\varepsilon_{xx}^{avg}$	0.0073	0.0102	0.0143	0.0215	0.0344
$\Delta\varepsilon_{yy}^{avg}$	0.0059	0.0097	0.0116	0.0142	0.0180
$\Delta\varepsilon_{xy}^{avg}$	0.0031	0.0071	0.0104	0.0136	0.0159

$\varepsilon_a = 10\%$

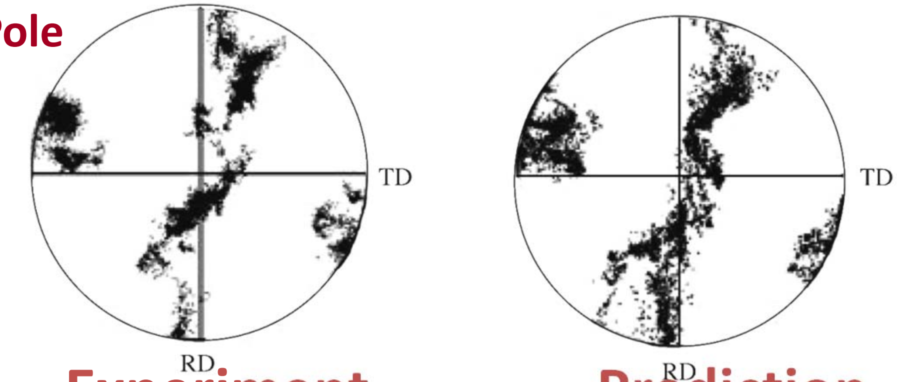


Quantifying Rotation Change

Global vs Local Rotation Measurements

Global Texture Evolution

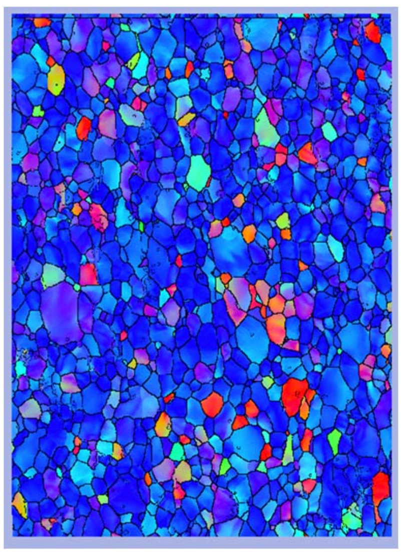
(100) X-ray Pole Figures



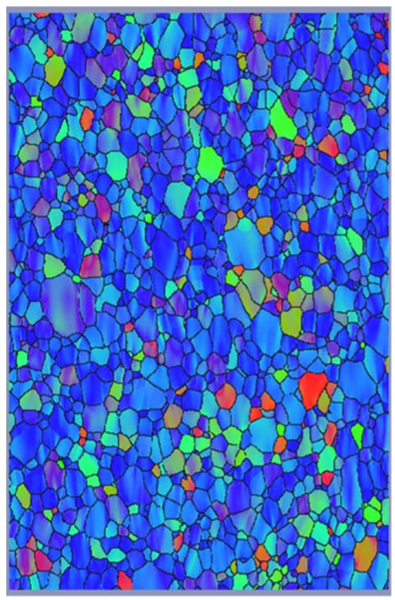
Experiment   Prediction

S.R. Kalidindi, A. Bhattacharyya, and R.D. Doherty, *Proc. Roy. Soc. Lond. A* **460** (2004) 1-22.

Local Crystal Orientation

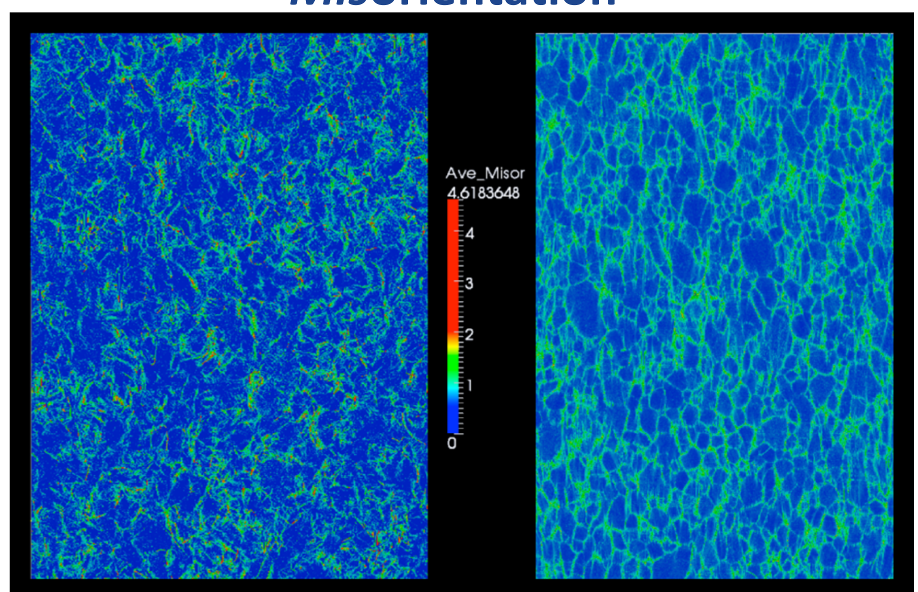


Experiment



Simulation

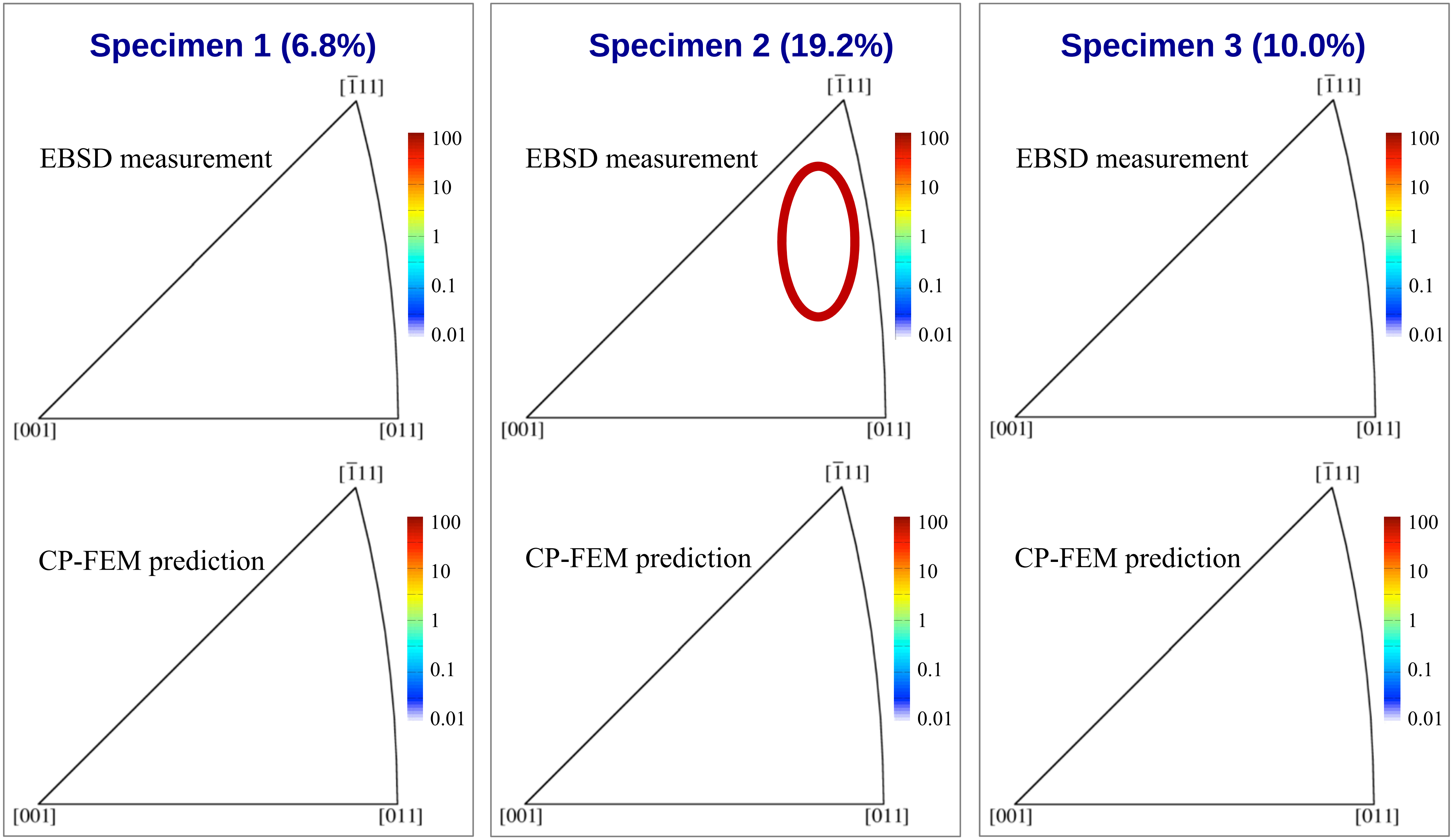
***Mis*orientation**



Experiment   Simulation

Courtesy of A.D. Rollett

Texture Predictions

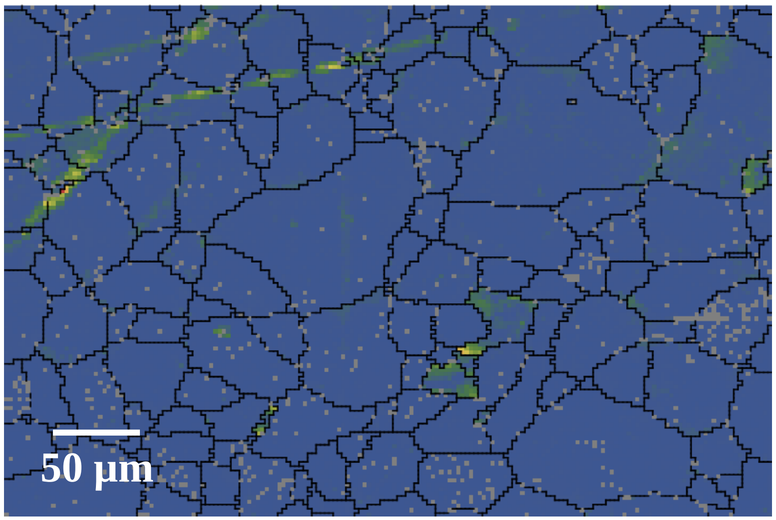


IPF contour plots indicate very good agreement between model and experiment.

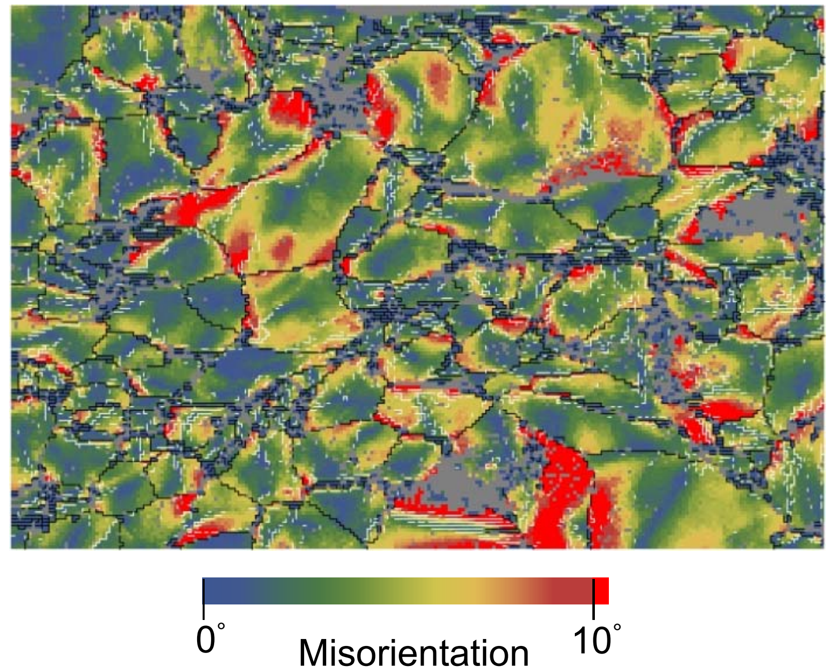
Reference Orientation Deviation Map (ROD) – reference pixels to a specific orientation in a grain

<u>Misorientation between all pixels in a grain and the grain's **current average orientation**</u>

Original Configuration



Deformed Configuration
~22% Strain (4th strain step)



- Conventional approach –does not require a correlation between maps
- deformation history not captured

Legend:
- Grain boundaries
- 2.5º threshold exceeded between adjacent pixels
- Pixels not indexed

Buchheit *et al.*, *Microscopy and Microanalysis*, 2015

A new type of ROD map, **referencing to the average orientation of *originally defined grains***

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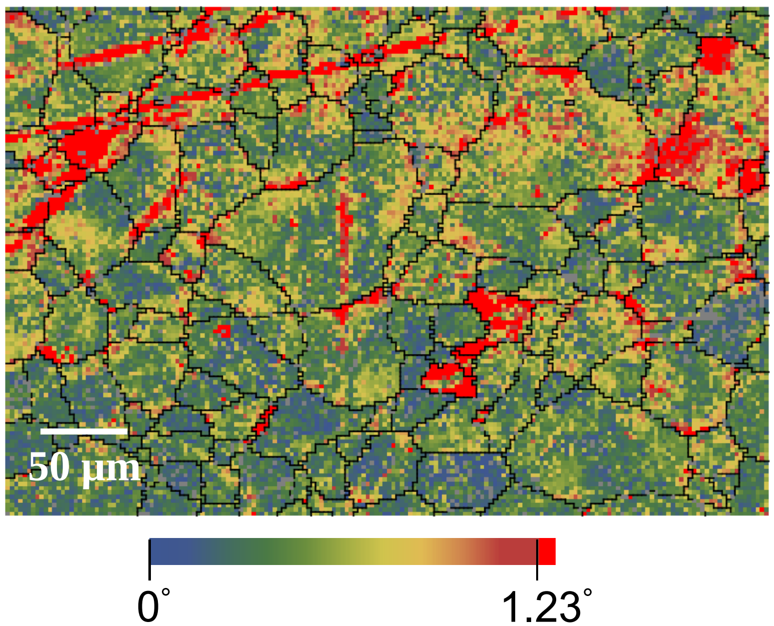
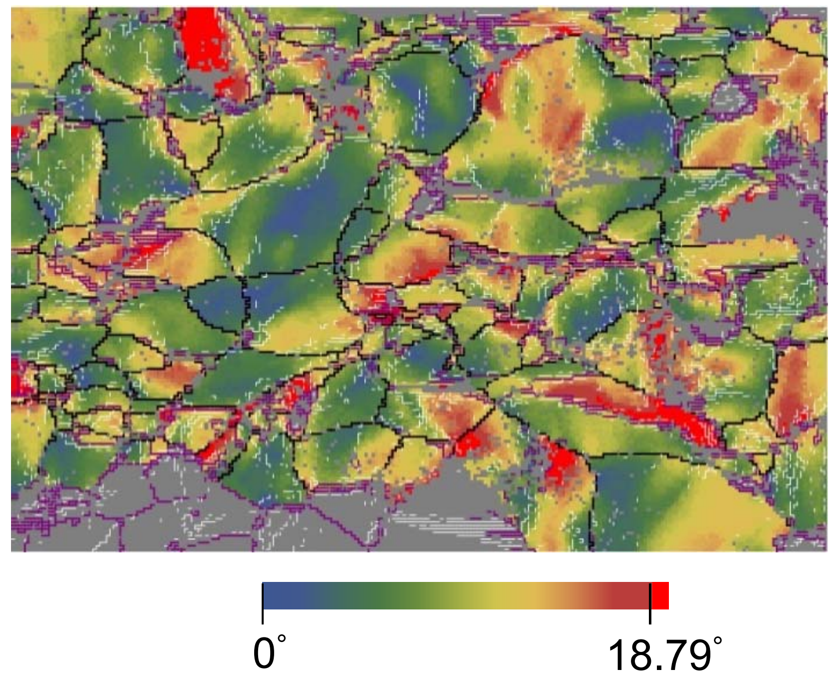
Original Configuration



Deformed Configuration
~22% Strain (4th strain step)



- Must track grain ID during deformation to allow orientation relative to original
- Requires ability to perform in-situ EBSD measurements during deformation
- Easily compared to a CPFEM model

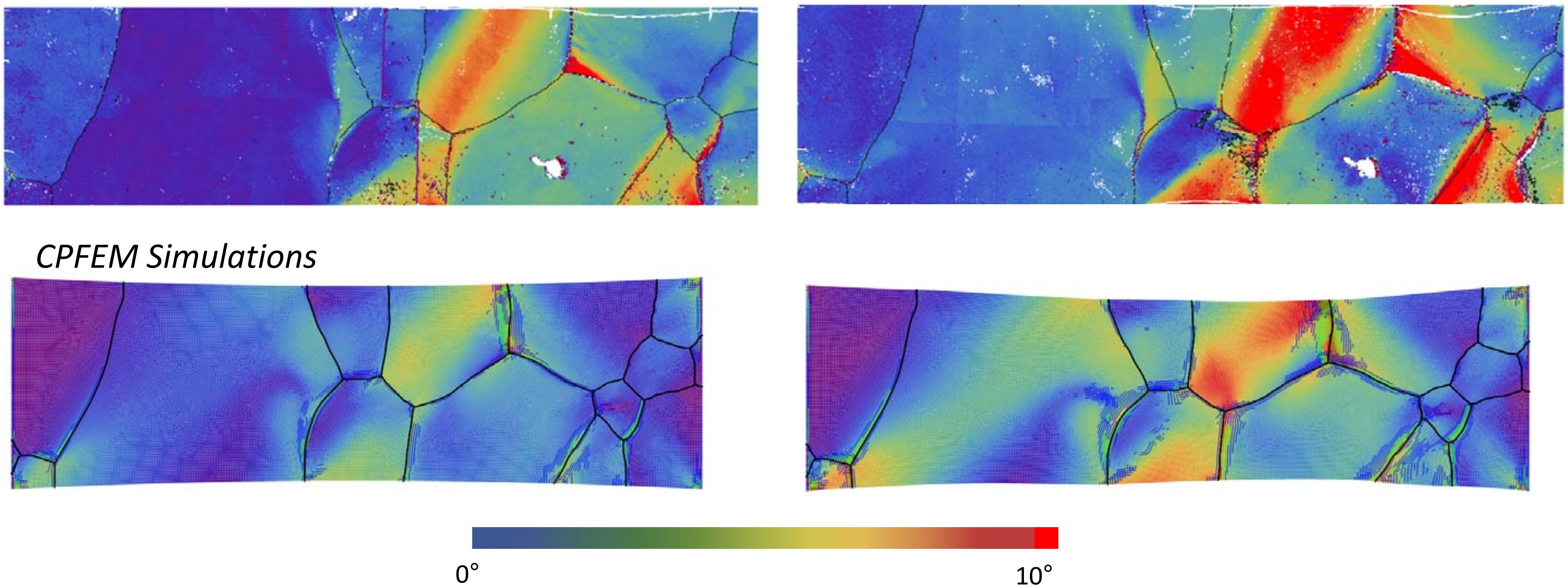
Boundaries of originally defined grains
Boundaries of new grains
2.5º threshold exceeded between adjacent pixels
Pixels not correlated or indexed

Comparison of pixel misorientation ***relative to original average grain orientation***

4.2% Strain **6.8% Strain**

Experiments (EBSD Maps)

CPFEM Simulations



2.5°
1.0°
0.5°

Minimum misorientation angle
relative to the undeformed grain orientation

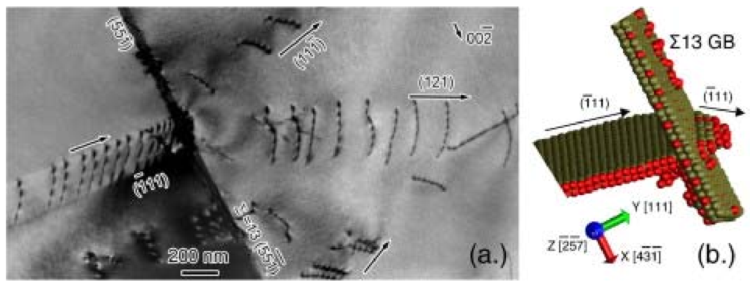
Grain boundary transmissivity

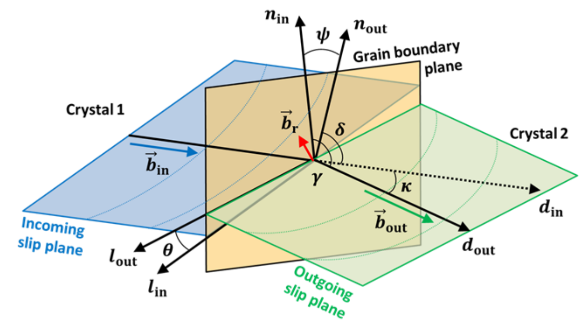
There are many models for grain boundary slip transmissibility

How does slip transfer across GBs? Dependence on GB type?

- Explicit MD examination
  - Sangid-Ezaz-Sehitoglu-Robertson, Acta Mater. 2011

    (3 boundaries)

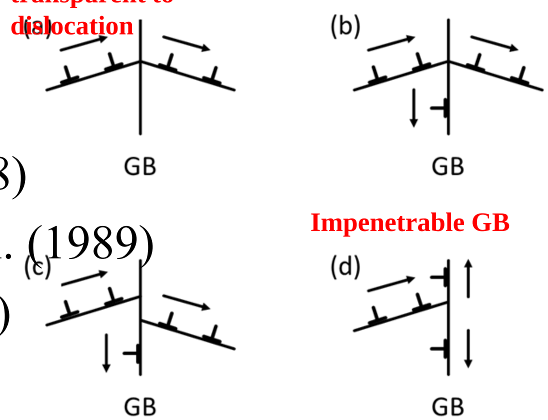




- Geometrical criteria:
  - *N factor* from Livingston-Chalmers, Acta Metall. (1957)
  - *SWC factor* from Shen-Wagoner-Clark, Acta Metall. (1988)
  - *LRB factor* from Lee-Robertson-Birnbaum, Scripta Metall. (1989)
  - *m' factor* from Luster -Morris, Metal. Mat. Trans. A (1995)
  - *The residual Burgers vector*, Metal. Trans. (1970)
  - *The λ function* from Werner and Prantl, Acta Metall. (1990)

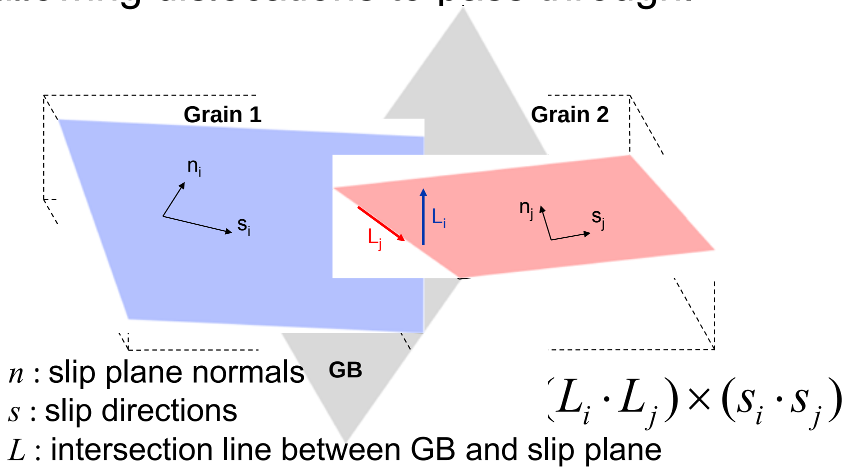
GB transparent to dislocation

Impenetrable GB

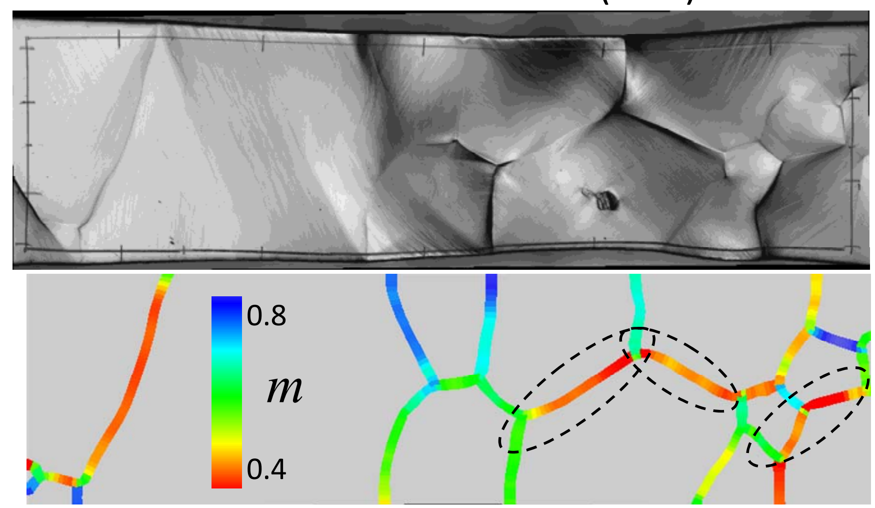


Surface profile for interpreting grain boundary transmissivity

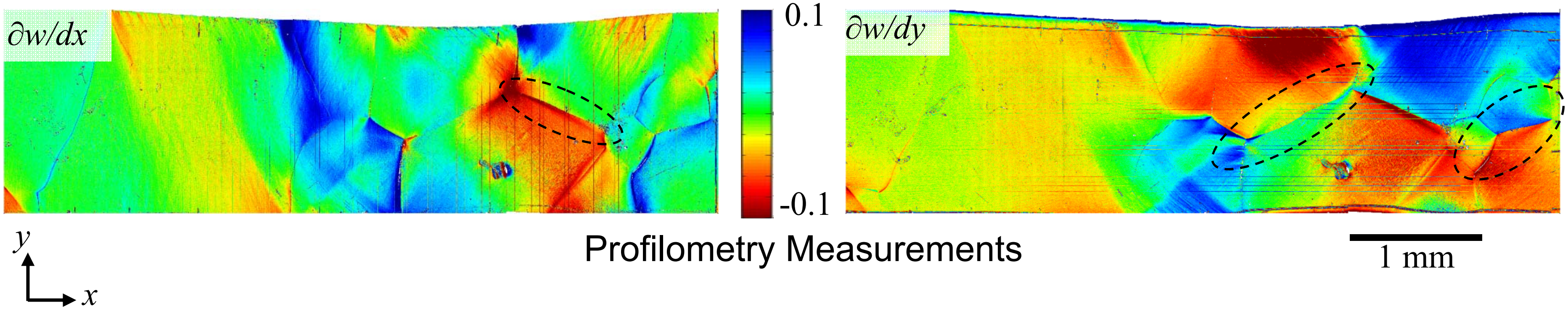
Grain boundary slip transmissivity provides an estimate for how resistant a grain boundary is to allowing dislocations to pass through.



Deformed surface (10%)



Transmissivity (SWC)

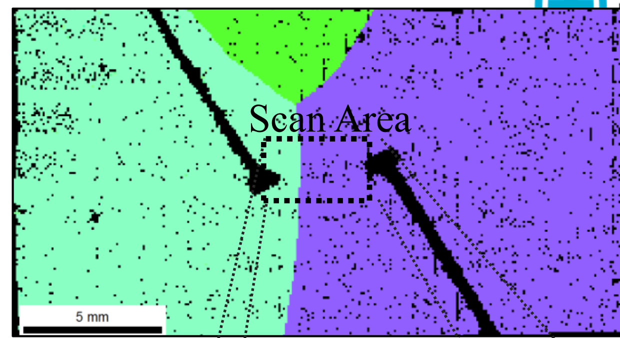


Profilometry Measurements

Our transmissivity-based model for boundary – dislocation interactions provides qualitative agreement with measurements of slip band formation and surface profilometry.

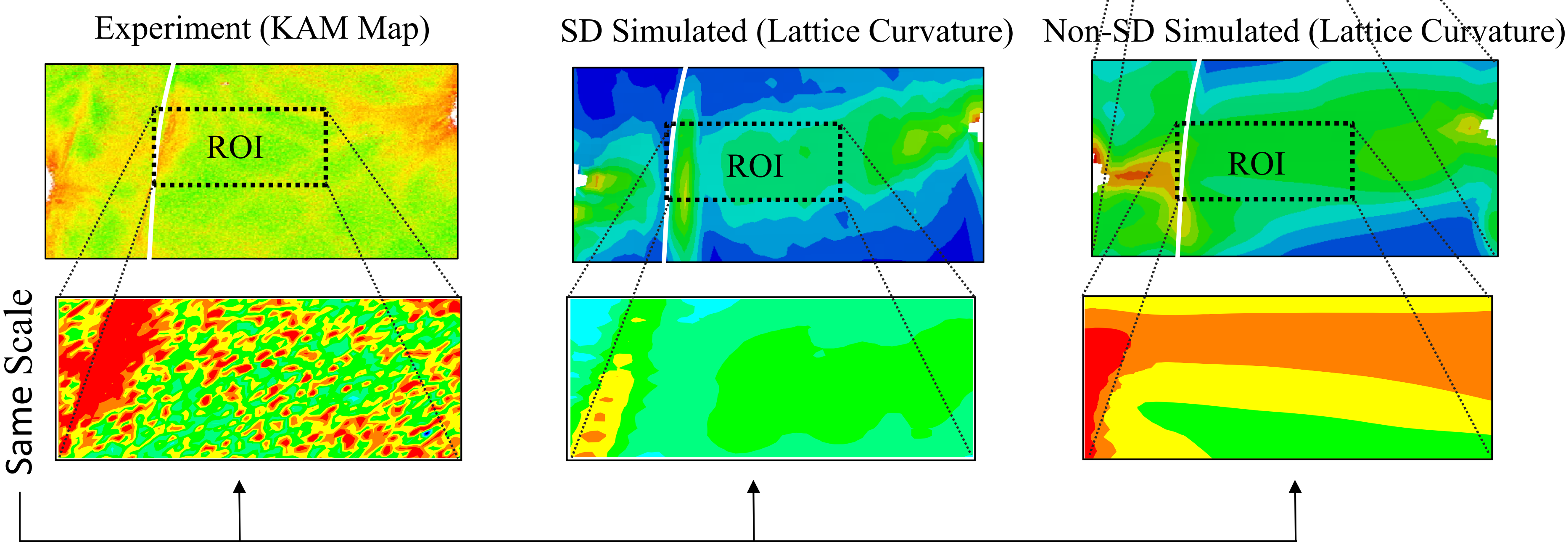
See also, Bieler, *et al.*, JOM, 2014

Fullwood/Wagoner/Homer Collaboration: Quantitatively validate transmissability laws at individual boundaries



Ta Bicrystal – Lattice Curvature

*** 0.1 mm Plastic Extension in Mini Instron**



ROI Lattice Curvature (rad/mm)	Experiment	SD Model	Non-SD
Average	1.20	0.91	1.98
Maximum	2.15	1.33	2.56

Grain boundaries are not always as simple as 'just' 5 degrees of freedom!!!

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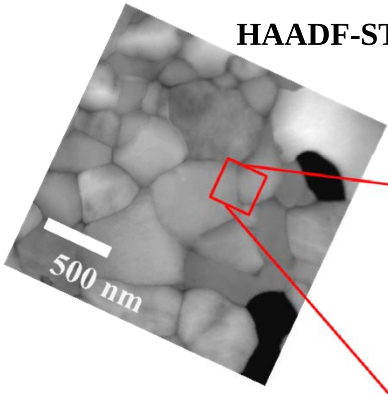
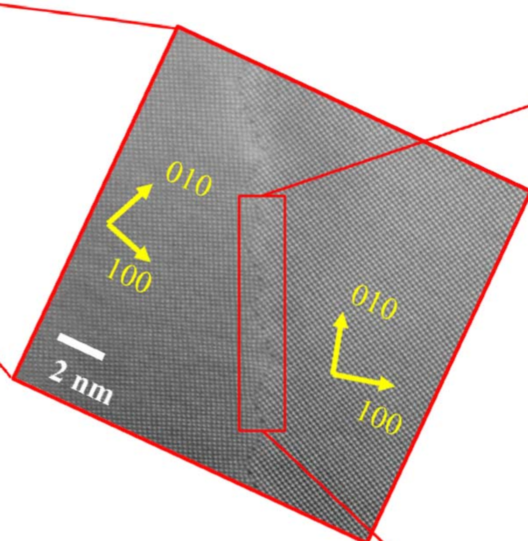
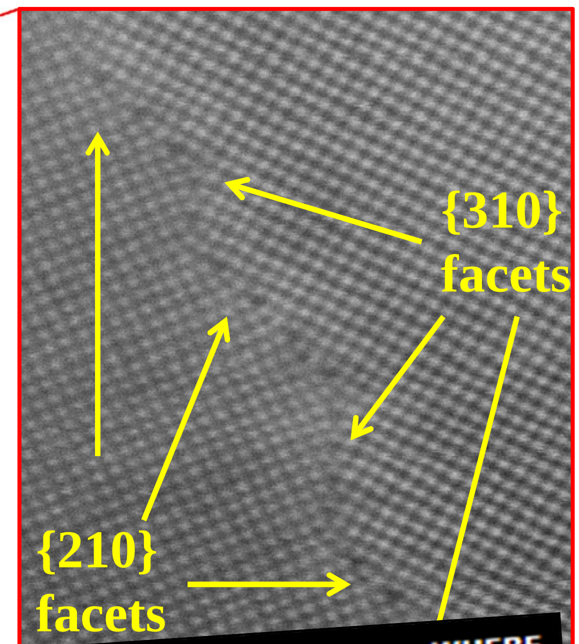
HAADF-STEM





HAADF-STEM Σ 5
<001> GB in Fe

Inclination from {310}: 26.3°



Observations

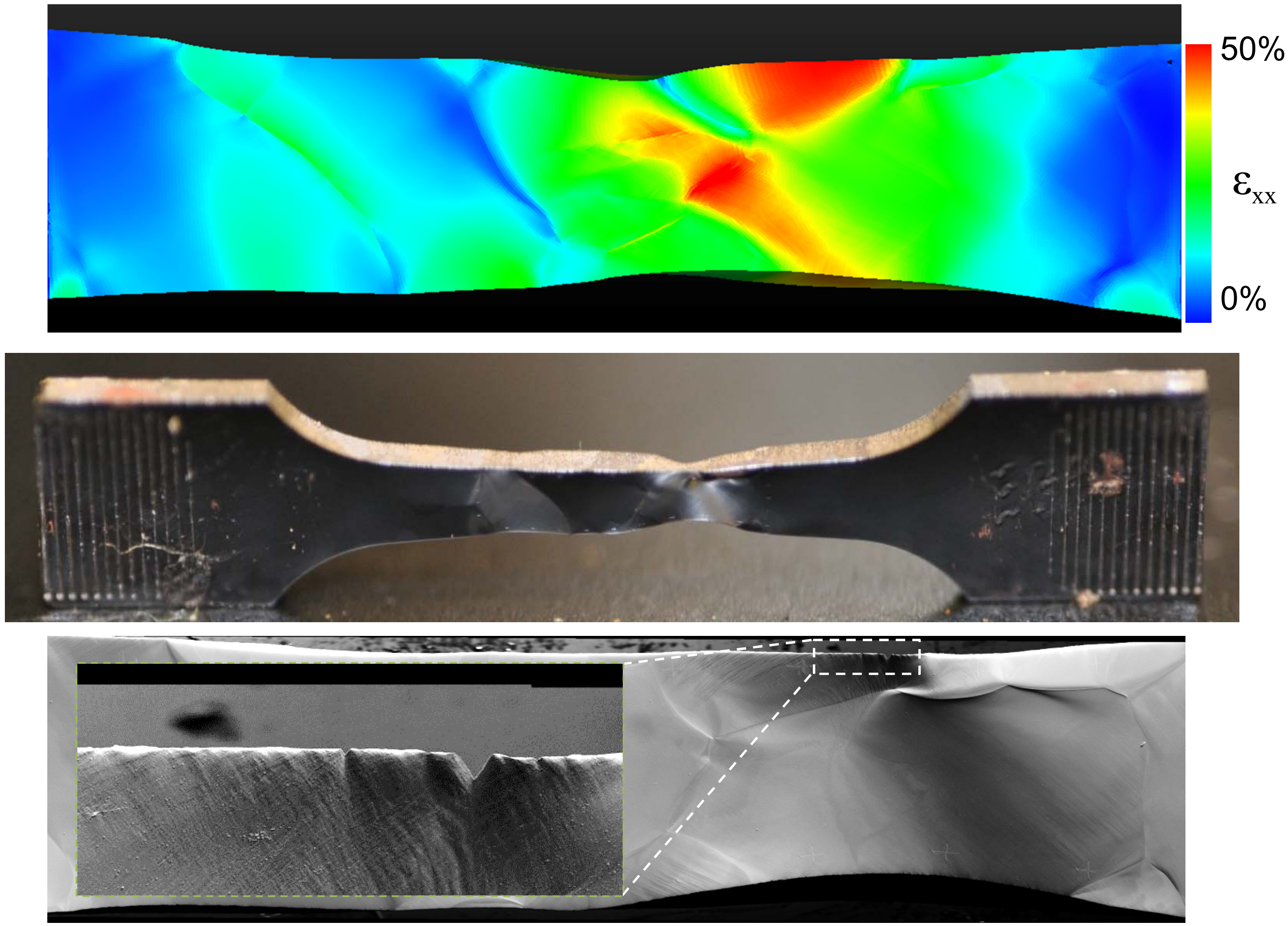
- Thermal faceting into "hill-and-valley" morphology
- Boundary is faceted on {210} and {310} inclinations

ABSTRACT	SYMPOSIUM	SESSION	WHEN	WHERE
Experimental Observations and Modeling of Interfacial Defects at an Asymmetric Σ=5 Grain Boundary in Fe *Douglas L. Medlin*[1]; K. Hattar[1]; J. A. Zimmerman[1]; F. Abdeljawad[1]; S. M. Foiles[1]; [1]Sandia National Labs	Interface-driven Phenomena in Solids: Thermodynamics, Kinetics and Chemistry	Structure-Property Relations	Tuesday 9:30 AM - 9:50 AM	Music City Center 108

Void Behavior and Damage

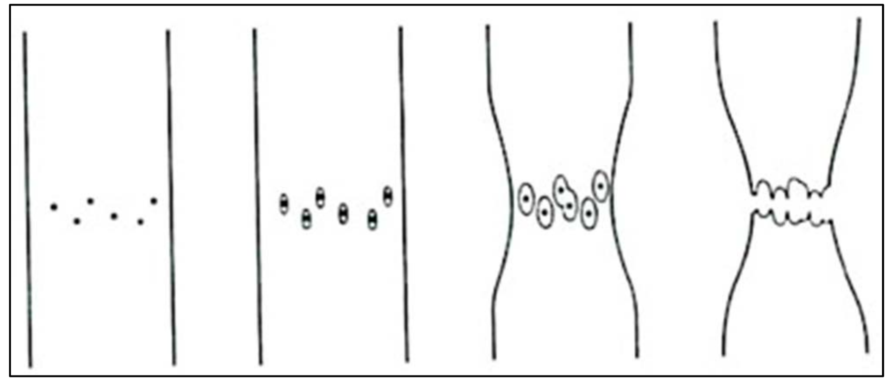
The crystal plasticity model predicts localized hot spots in strain at the same location where cracking is observed…

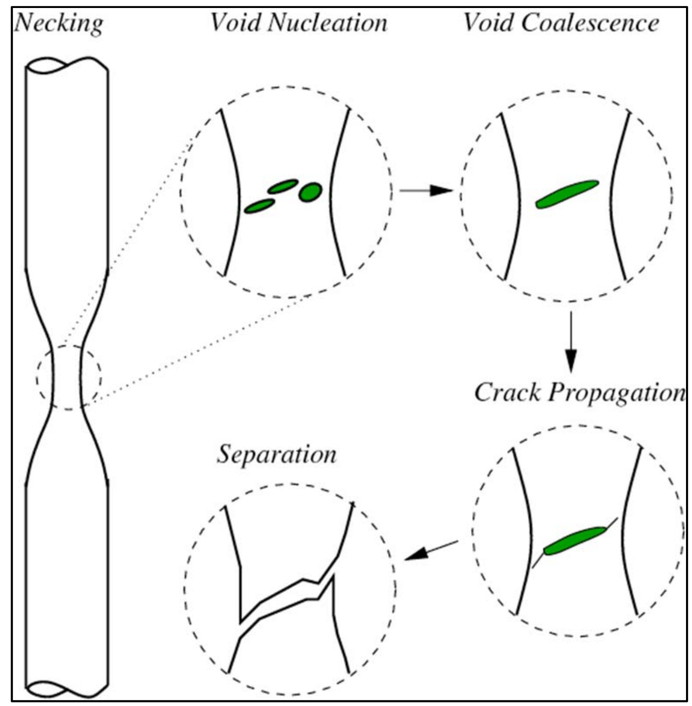
Sandia National Laboratories



Background: Ductile Fracture

- Initiation of voids through decohesion at second-phase particles or inclusions
- Voids continue to grow in response to high stresses
- Eventual coalescence of voids, leading to failure

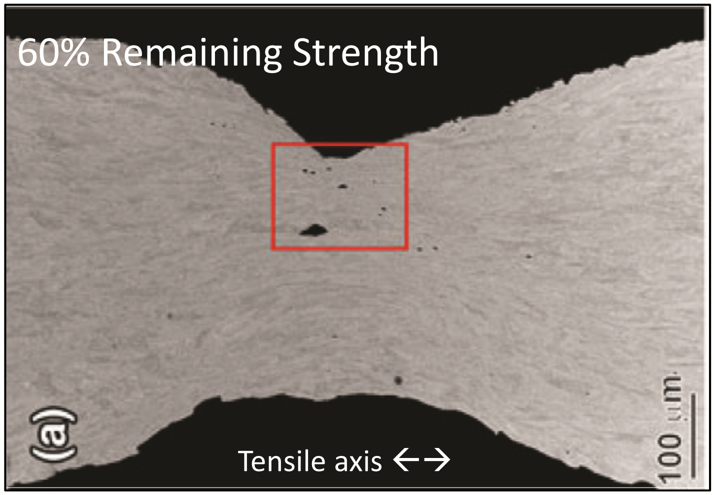




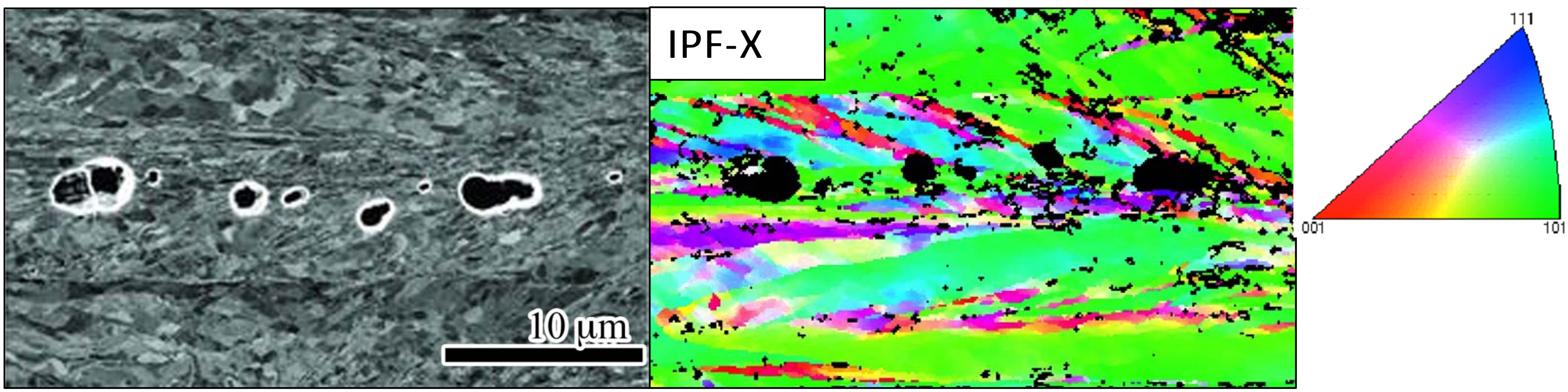
How do voids initiate in pure metals?

 http://en.wikipedia.org/wiki/Fracture; http://www.weck.ca

Void Formation in 99.9%Ta

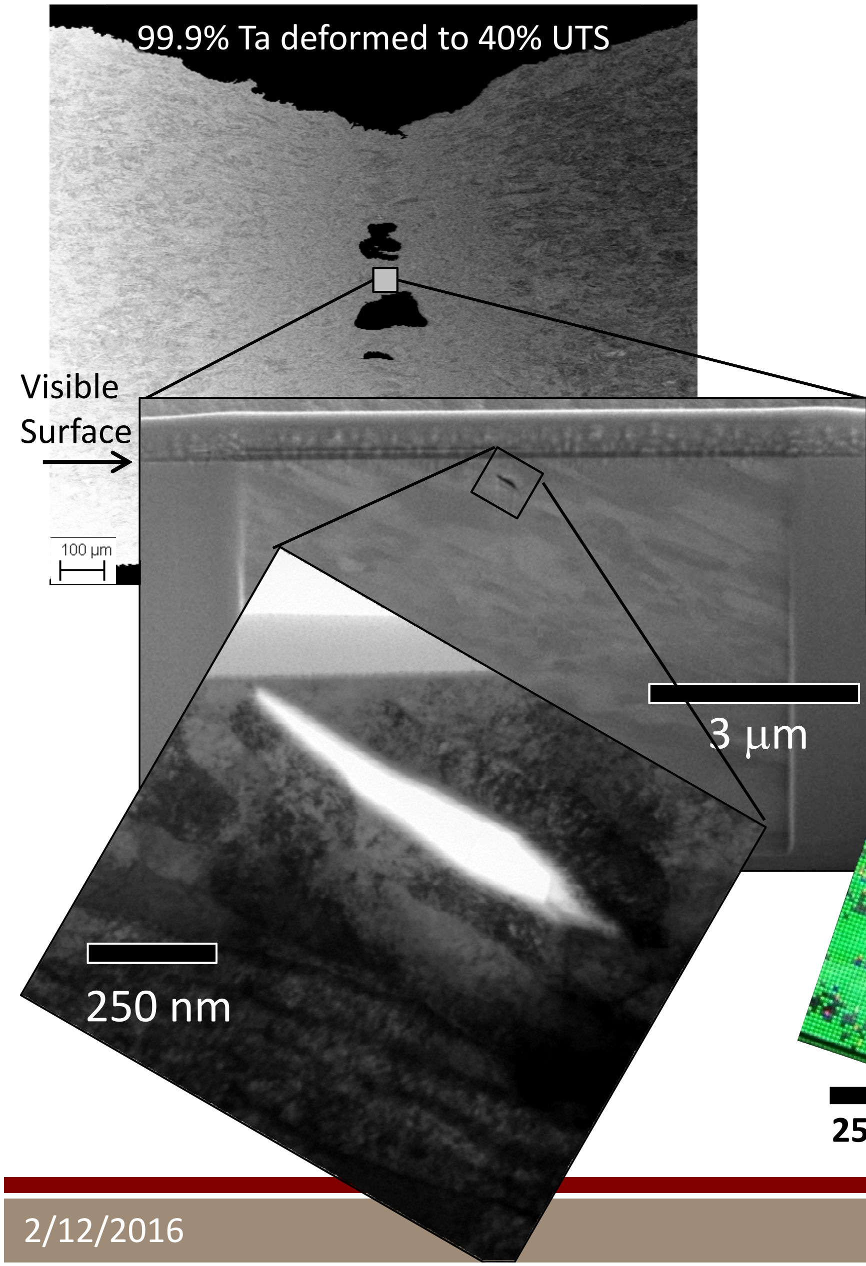


- Arrays of voids aligned along tensile axis
- EBSD shows elongated, inclined [001] subgrains associated with each void
- Alternating regions of [122] indicates high angle GBs

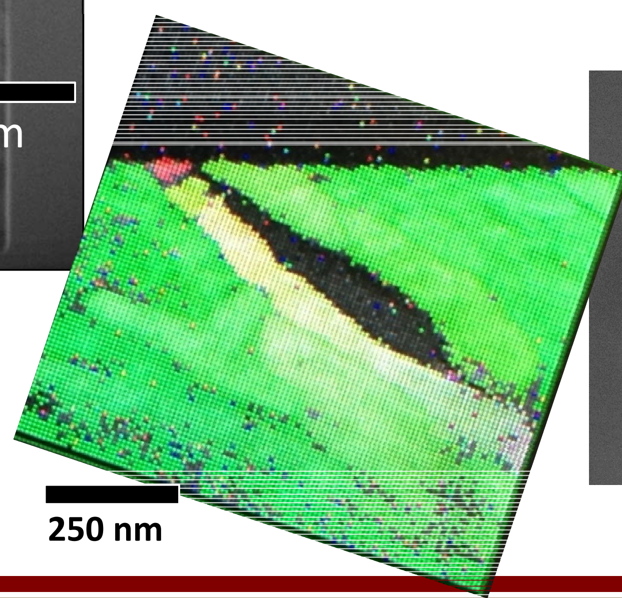


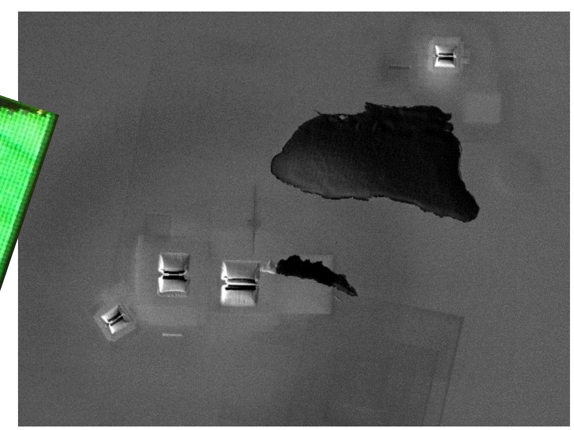
Ta failure is void-driven, with deformation-induced microstructural changes and stress state controlling the initiation/growth of voids

Nanoscale Analysis of Void Initiation

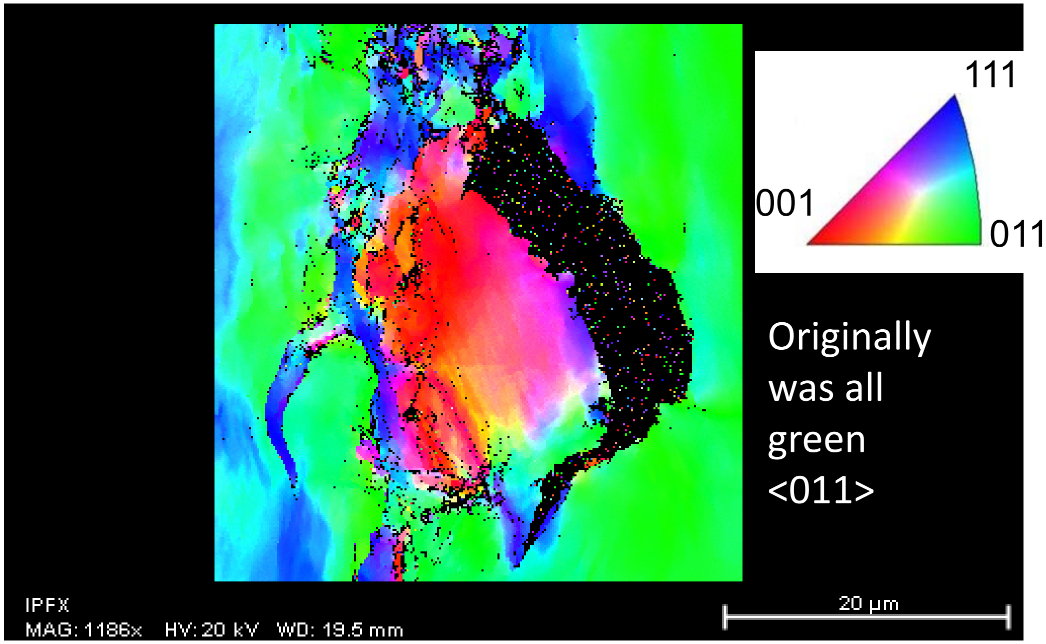


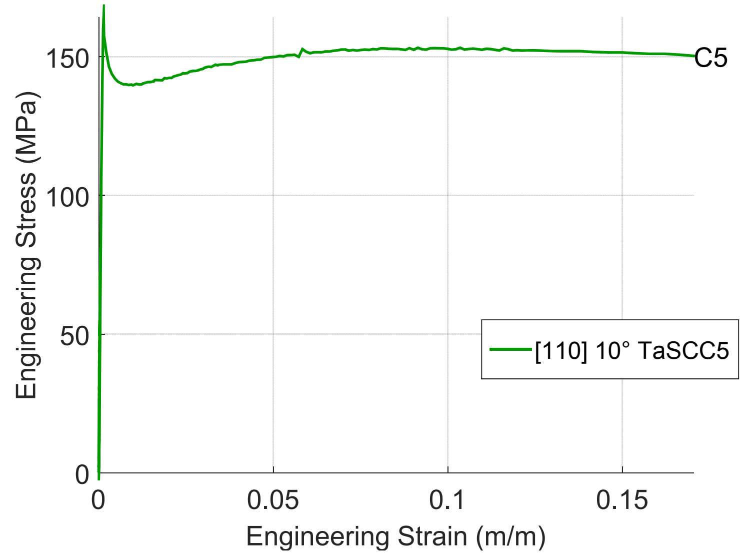
- Focused Ion Beam (FIB) used to locate subsurface, deformation-induced voids in interrupted tensile bar.
- Preliminary TEM shows void shape aligned with angle of sub-boundaries
- Transmission Kikuchi Diffraction (TKD) to determine crystallographic orientation near void.
- Orientations are consistent with EBSD analysis showing void nucleation along high angle misorientation boundaries





Probing relationships between void formation and crystallographic orientation





- **Investigated a void formed during tensile testing of a Ta single crystal <011>. Imaging at the specimen midplane.**
- **Crystallographic rotations near a void in single crystal specimens improve our understanding of void formation in polycrystals.**
- **Void formation is associated with developing <001> and <111> crystallographic orientations.**
- **We are investigating whether substructure leads to these crystallographic rotations which leads to voids or whether the formation of voids causes the crystallographic rotations.**

Summary

- **Grain-scale validation of crystal-plasticity models is still largely qualitative**

- **Both distortion and rotation can be mapped relative to the original undeformed configuration**

- **With an ability to map back to the original undeformed configuration, it is possible to begin to assess quantitative difference metrics.**

- **These new statistical metrics may help identify and address gaps in CP-FEM theory:**
  - **Grain boundary slip transmissibility**
  - **Void nucleation and growth**