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LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

# Quantifying the Agreement between Microstructural Plasticity Simulations and Experiment

Luke N. Brewer, Corbett C. Battaile, Remi Dingreville, and Tim J. Bartel

**Sandia National Laboratories**

Acknowledgements: Thanks for help from Brad Boyce and Tom Buchheit.

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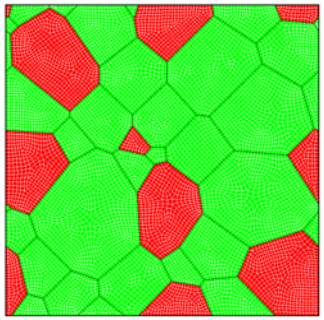
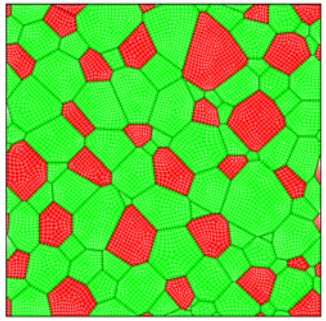
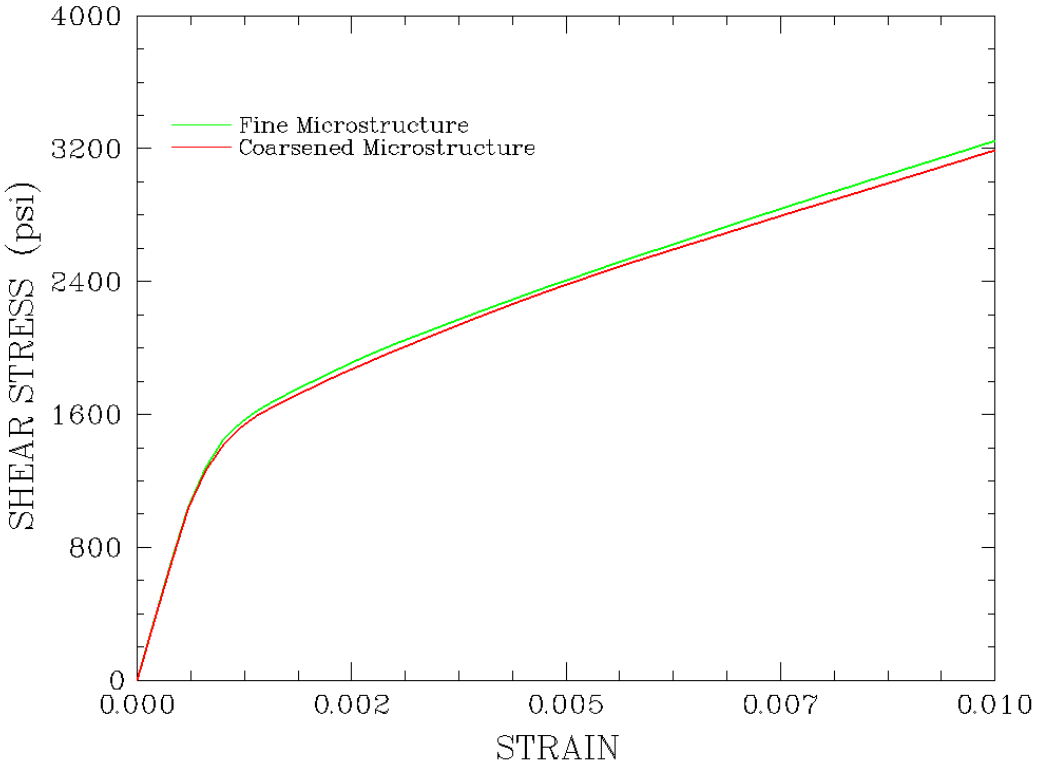
# Modeling Plasticity at the Continuum Scale





150 um 3.4 um

- Structural finite element codes are continuum based—parameterized models
- For local, polycrystalline plasticity (PP) models, predicted σ-ε results from two different grain sizes are similar




We need models and experiments that possess sensitivity to microstructure!

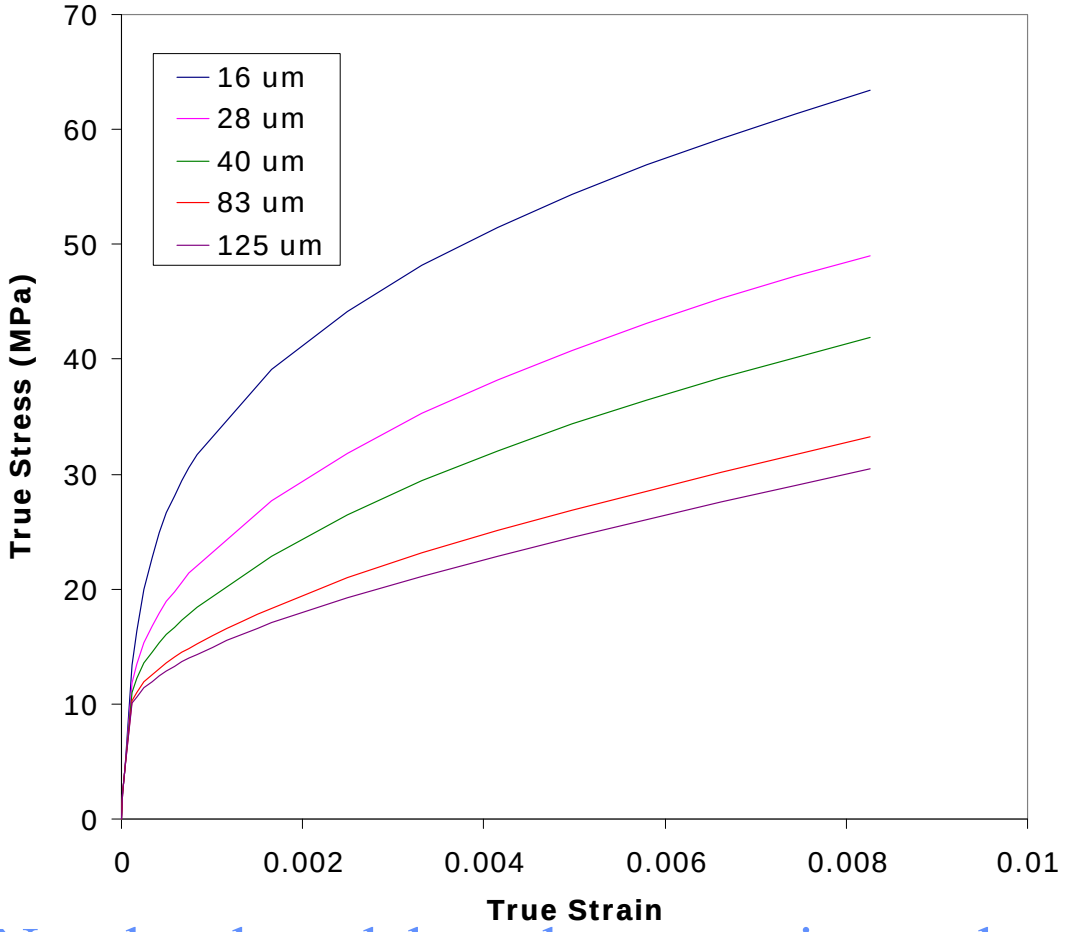
# Non-local Plasticity Model

## Non-Local Model

- Newly implemented with GND* initialization—misorientation at grain boundaries sets GND densities
- Integral of GND densities provides length scale
- Elastic behavior is independent of grain size.
- Yield strength increases as grain size decreases.
- Predicts Hall-Petch behavior with exponent of -1

Counts, WA, et al."Intl. J. Solids and Structures; 2007; vol.44, no.17, p.5742-51

*Geometrically Necessary Dislocations




Non-local model produces continuum level results that resemble experiment, but what about the micro-scale??

# Polycrystal Kinematics

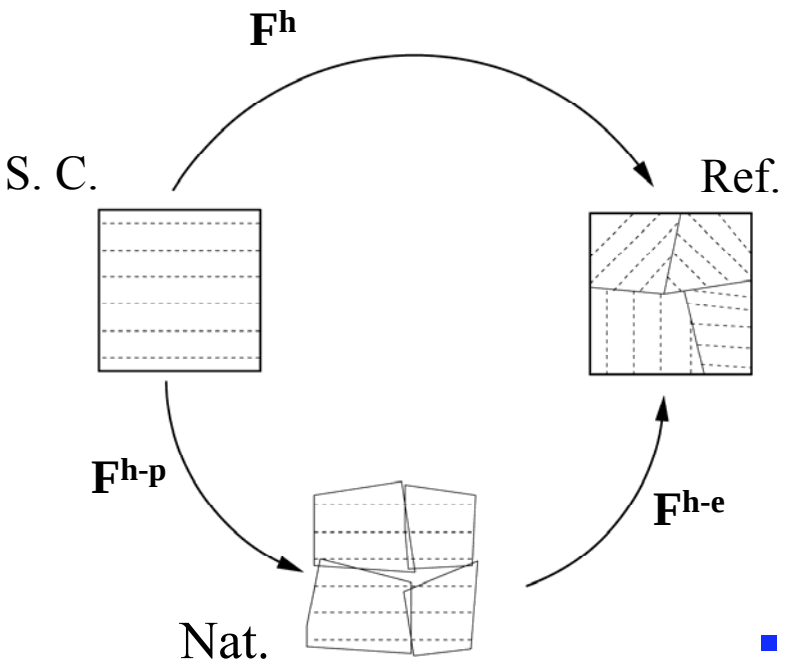
- Define an Initial Dislocation Tensor

$$\tilde{\mathbf{G}}_0 \rightarrow \frac{1}{\mathrm{Det}[\mathbf{F}^{\mathbf{h-e}}]}\,\mathbf{F}^{\mathbf{h-e}^{-1}}\,\mathrm{Curl}\,\mathbf{F}^{\mathbf{h-e}^{-1}}$$

$$\mathrm{Det}[\mathbf{F}^{\mathbf{h-p}}]\,\mathbf{F}^{\mathbf{h-p}}\,\mathrm{Curl}\,\mathbf{F}^{\mathbf{h-p}}$$

$$\tilde{\mathbf{G}}_0 = \frac{1}{\mathrm{Det}[\mathbf{F}^{\mathbf{h-e}}]}\,\mathbf{F}^{\mathbf{h-e}^{-1}}\,\mathrm{Curl}\,\mathbf{F}^{\mathbf{h-e}^{-1}}$$

Preliminary Kinematics




- $\mathbf{F}^{\mathbf{h-e}} = \mathbf{R}^{\mathbf{h-e}}\,\mathbf{U}^{\mathbf{h-e}}$
- Assume Ref. is stress free: $\mathbf{U}^{\mathbf{h-e}} = \mathbf{I}$

$$\tilde{\mathbf{G}}_0 = \mathbf{R}^{\mathbf{h-e}^{-1}}\,\mathrm{Curl}\,\mathbf{R}^{\mathbf{h-e}^{-1}}$$

$\mathbf{R}^{\mathbf{h-e}}$ = orientation of each grain

- Define a Deformation Dislocation Tensor

$$\hat{\mathbf{G}} = \frac{1}{\mathrm{Det}[\mathbf{F}^{\mathbf{P}}]}\,\mathbf{F}^{\mathbf{P}}\,\mathrm{Curl}\,\mathbf{F}^{\mathbf{P}}$$

- Define a Total Dislocation Tensor

$$\hat{\mathbf{G}}^{\mathbf{Tot}} = \mathbf{F}^{\mathbf{P}}\,\mathbf{R}^{\mathbf{h-e}}\,\tilde{\mathbf{G}}_0\,\mathbf{R}^{\mathbf{h-e}^{\mathrm{T}}}\,\mathbf{F}^{\mathbf{P}^{-1}} + \hat{\mathbf{G}}$$

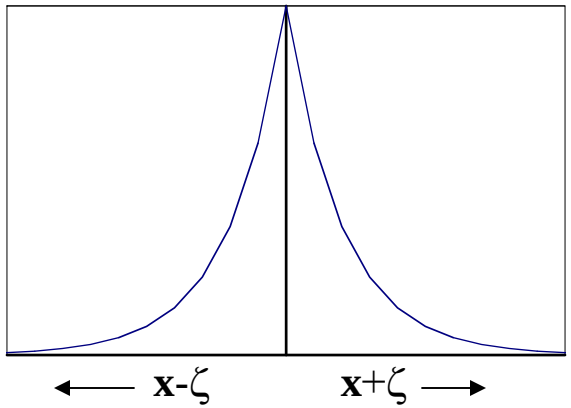
# Non-Local Integral Method

**Define a non-local curl**

$$\{\text{Curl } \mathbf{H}\}_{jk} \equiv \varepsilon_{irs} \frac{\int_V \left(H_{js}(\mathbf{x}+\zeta) - H_{js}(\mathbf{x})\right)\zeta_k \ \text{Exp}\left[-\frac{1}{\omega}\sqrt{\zeta_1^{\,2}+\zeta_2^{\,2}+\zeta_3^{\,2}}\right] dV}{\int_V \zeta_r \zeta_K \ \text{Exp}\left[-\frac{1}{\omega}\sqrt{\zeta_1^{\,2}+\zeta_2^{\,2}+\zeta_3^{\,2}}\right] dV}$$

$\zeta$ = local coordinates centered at $\mathbf{x}$

- Exponentials ensure $\{\text{Curl } \mathbf{H}\}$ is convergent
- $\omega$ represents the distance over which interactions are felt ➡ LENGTH SCALE



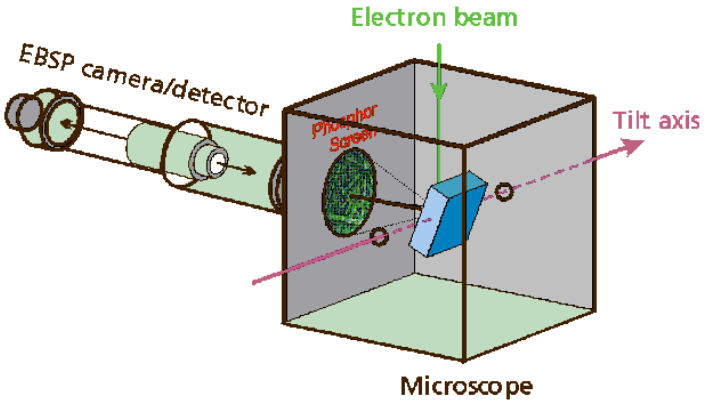

The Non-Local Integral Based Dislocation Tensors

$$\{\hat{\mathbf{G}}\} = \frac{1}{\text{Det}[\mathbf{F^P}]}\ \mathbf{F^P}\ \{\text{Curl } \mathbf{F^P}\} \qquad \{\tilde{\mathbf{G}}\} = \mathbf{R}^{\mathbf{h-e}^{-1}}\ \{\text{Curl } \mathbf{R}^{\mathbf{h-e}^{-1}}\}$$

# Combined Study of Microstructural Plasticity Evolution

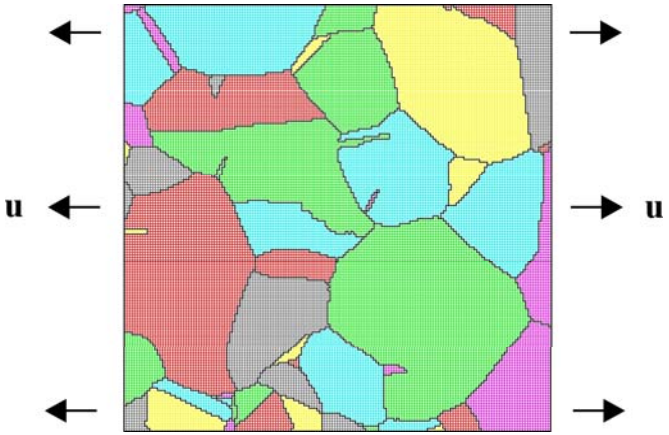
## Experimental

- Annealed Ni (99.9%) polycrystal
- Interrupted Tensile Test
  - 0%, 1%, 5%, 10% Strain
- EBSD data @ same location
  - Zeiss Supra 55 VP-FEG SEM
  - 20keV, 0.5μm steps, 500x500
  - 3 areas on three tensile samples

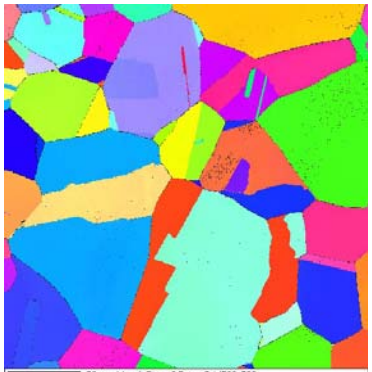



## Simulation

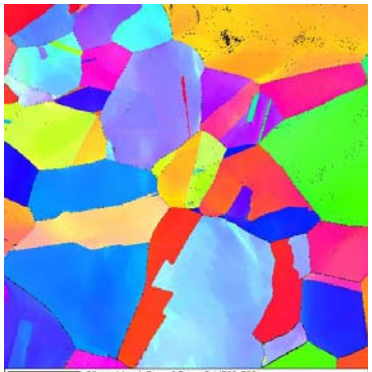
- Meshed the initial microstructure from EBSD*
- Ran both the local and non-local models to 10% strain
- Sandia JAS3D FEM platform, periodic boundary conditions in z.



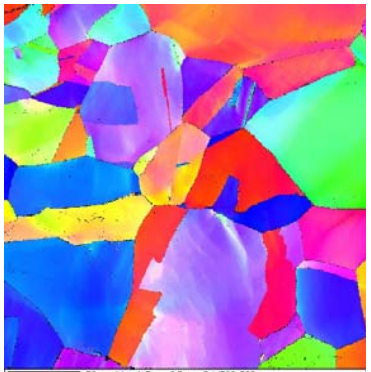

1% strain



5% strain



10% strain



*Electron backscattered diffraction

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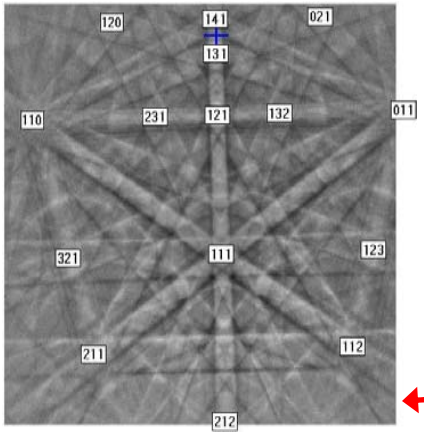
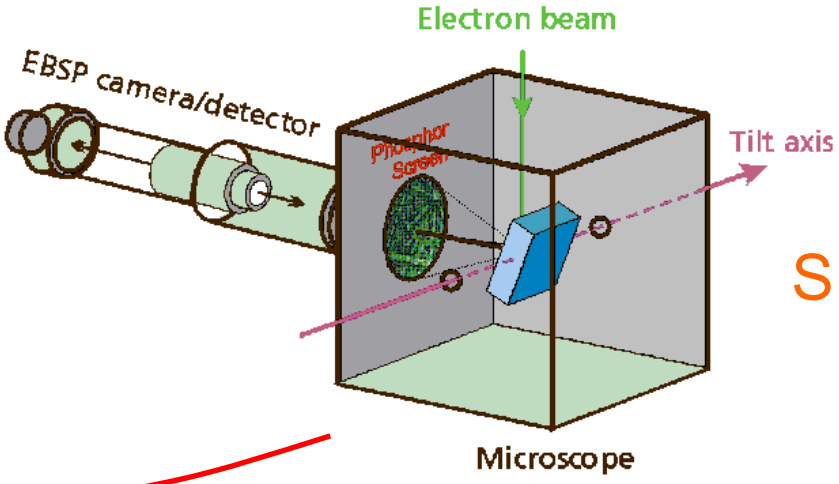
# EBSD: A technique for crystallography in **SEM**

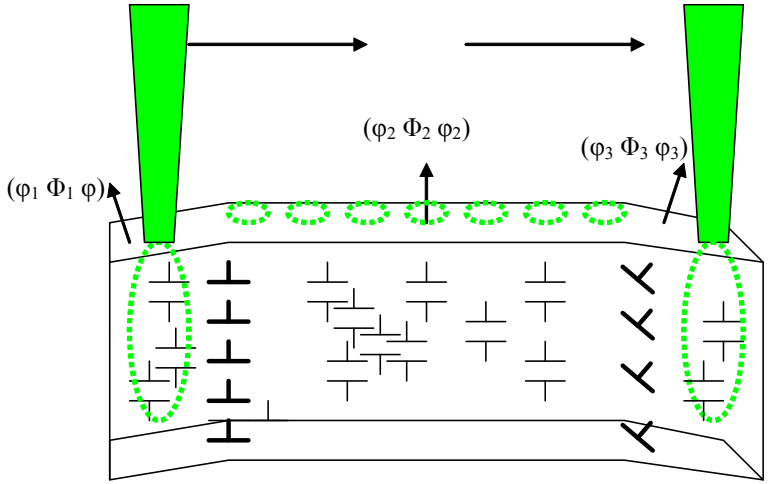



SEM

Figure courtesy of J. Sutliff

$$G_i = \begin{pmatrix} \cos(\phi_1)\cdot\cos(\phi_2) - \sin(\phi_1)\cdot\sin(\phi_2)\cdot\cos(\Phi) & \sin(\phi_1)\cdot\cos(\phi_2) + \cos(\phi_1)\cdot\sin(\phi_2)\cdot\cos(\Phi) & \sin(\phi_2)\cdot\sin(\Phi) \\ -\cos(\phi_1)\cdot\sin(\phi_2) - \sin(\phi_1)\cdot\cos(\phi_2)\cdot\cos(\Phi) & -\sin(\phi_1)\cdot\sin(\phi_2) + \cos(\phi_1)\cdot\cos(\phi_2)\cdot\cos(\Phi) & \cos(\phi_2)\cdot\sin(\Phi) \\ \sin(\phi_1)\cdot\sin(\Phi) & -\cos(\phi_1)\cdot\sin(\Phi) & \cos(\Phi) \end{pmatrix}$$




$$M = G_1^{-1} \cdot G_2$$

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

# Some Major Concerns (among many) when comparing experimental and computational microstructural plasticity….

- **Fidelity of physical model (usually where all of the effort goes)**
- **Dimensions of volumes to be compared (experiments usually plane stress, simulations usually plane strain)**
- **Boundary Conditions (are the tractions on the edges of the grain the same as the macro tractions applied on the edges of the bar???)**
- **Coordinate Systems (Eulerian vs Lagrangian)**
- **What do I compare and how do I compute it???**
  - **Average microstructural metrics**
  - **Microscale comparisons**

Quantitative comparison at microstructural level

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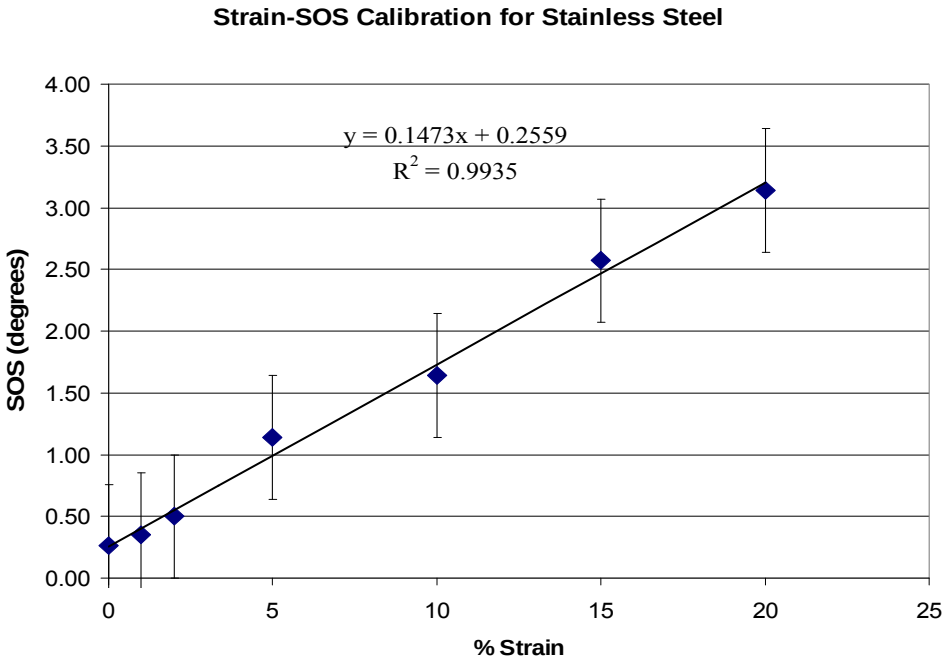
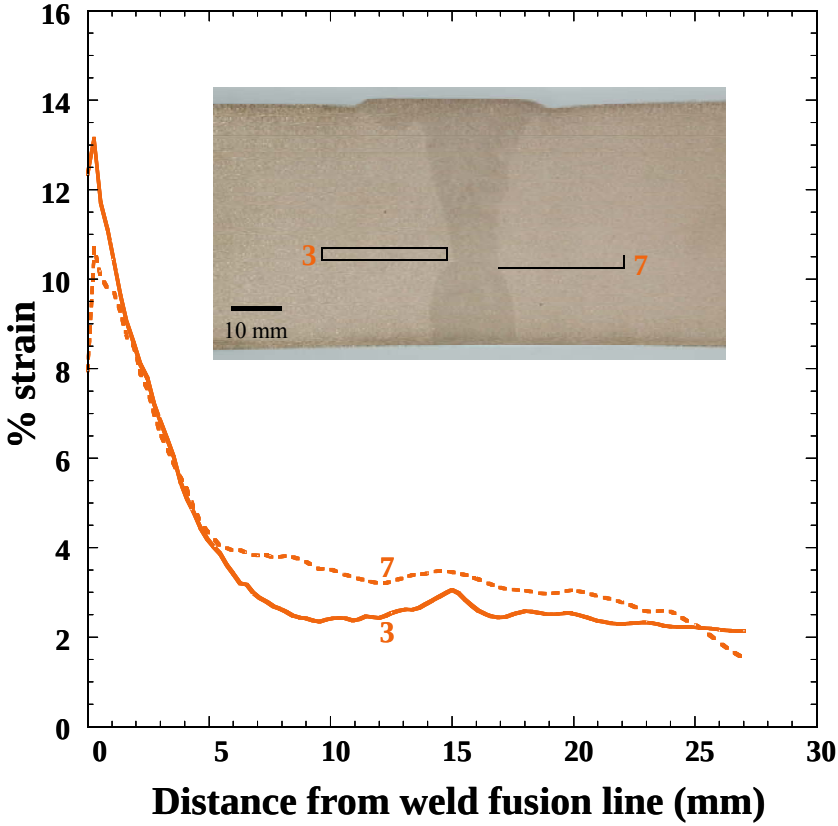
# Average Microstructural Metric for plastic deformation

Scalar orientation spread (SOS)--or--

Average (Intragrain) Misorientation—AMIS




$$SOS^{\text{grain segment}} = \frac{\Sigma(pixel - pixel\ misorientations)}{N^{pixel\ pairs}}$$

$$SOS^{\text{Test Line}} = \frac{\Sigma(SOS^{Segment_i})}{N^{Segments}}$$


**J.A. Sutliff, Microscopy &Microanalysis Proceedings 1999, pp. 236.**
**S.I. Wright ICOTOM 12, NRC Research Press 1999**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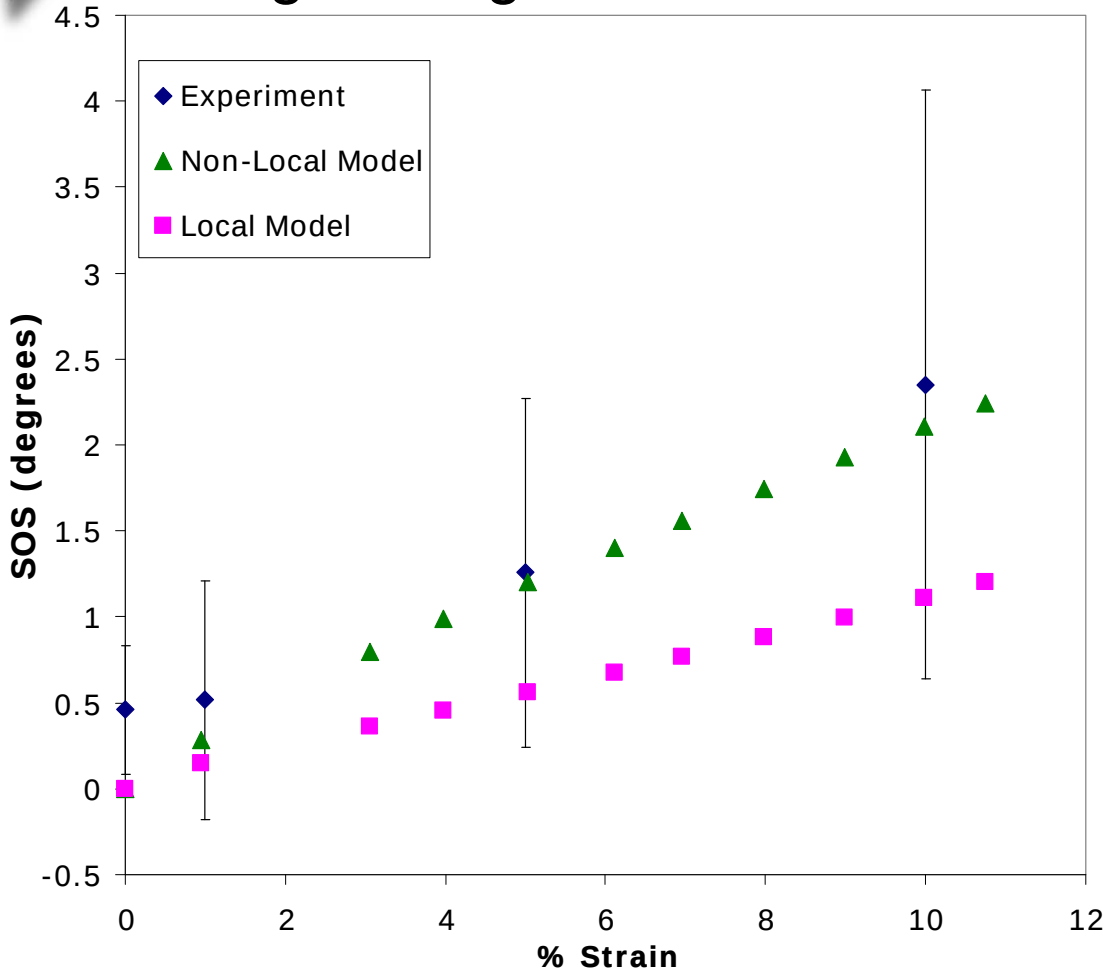
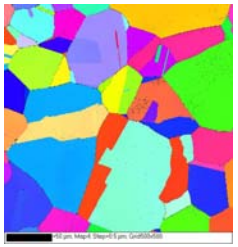
# Scalar Orientation Spread
# (aka Average Intragrain Misorientation: AMIS)





1% strain

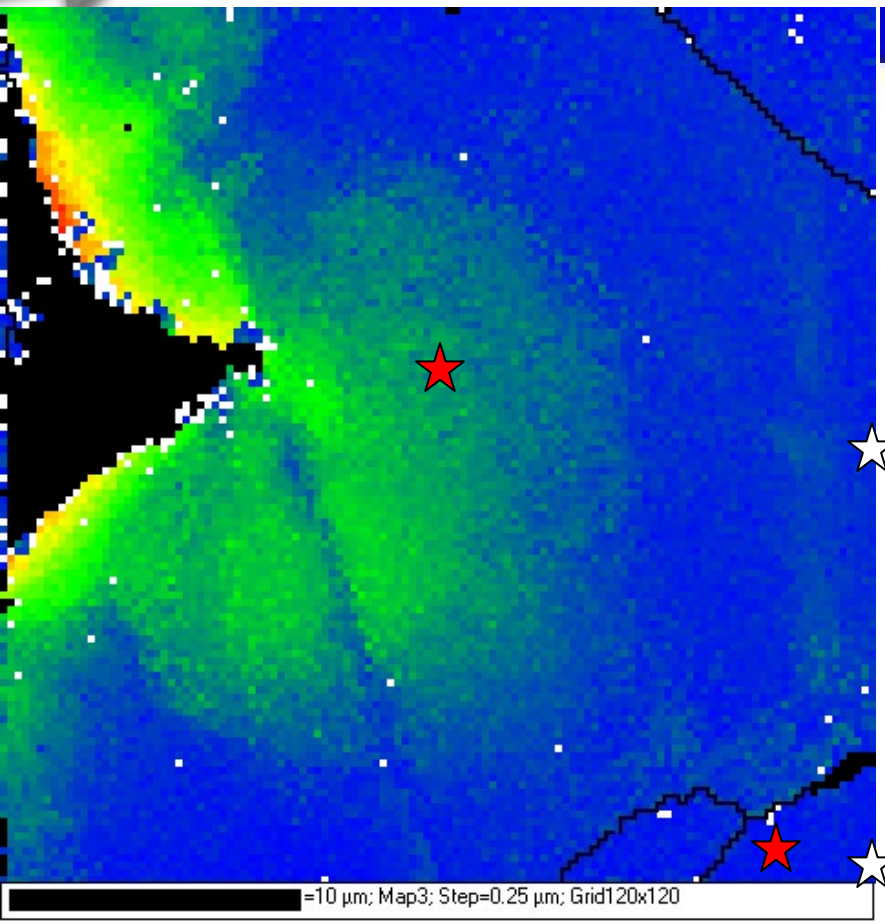

5% strain


10% strain

- Experimental error bars because of small number (<100) of grains sampled
- Linear trend consistently observed for FCC metals deformed in tension
- SOS values for local model lower than experimental value.

# Local Misorientation Mapping

L.N. Brewer et al., Microscopy and Microanalysis, 2006




0° 10°

- Locate grain boundaries using standard misorientation calculations
- Assign each pixel in map to a grain
- Locate reference pixel in each grain (minimum distortion)
  - Calculate misorientation for an 8-pixel cluster
  - Choose cluster with least misorientation as reference
- For a given grain, calculate the misorientation between each pixel and the reference pixel.
- Map this misorientation for each pixel using a color table.

Blue represents small internal misorientation "relaxed"

Red represents large internal misorientation "strained"

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# Local Misorientation Spread from Simulations

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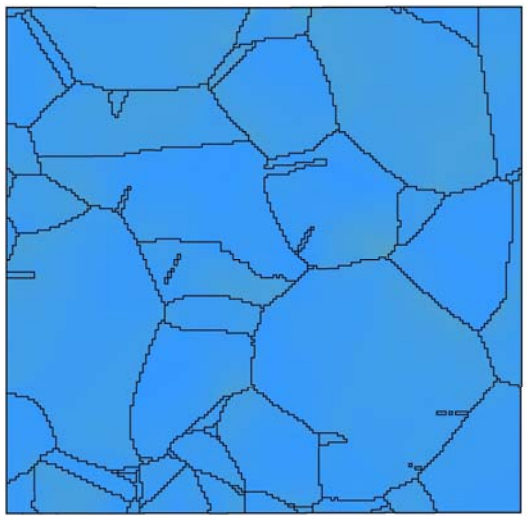
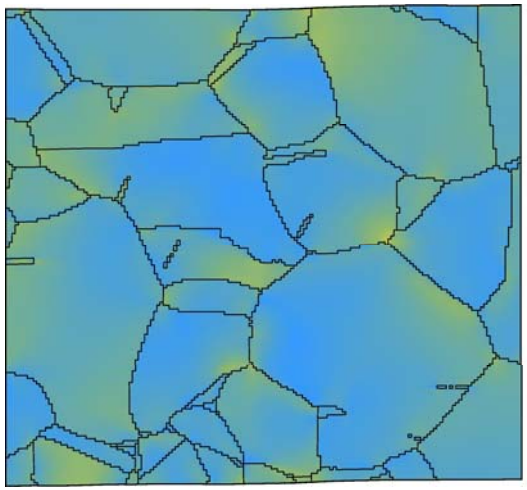
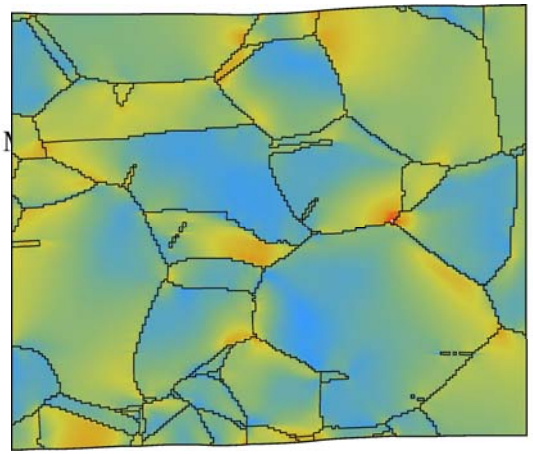
Local Model



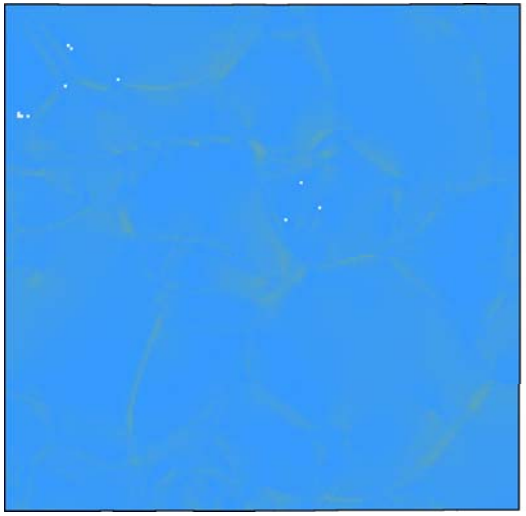


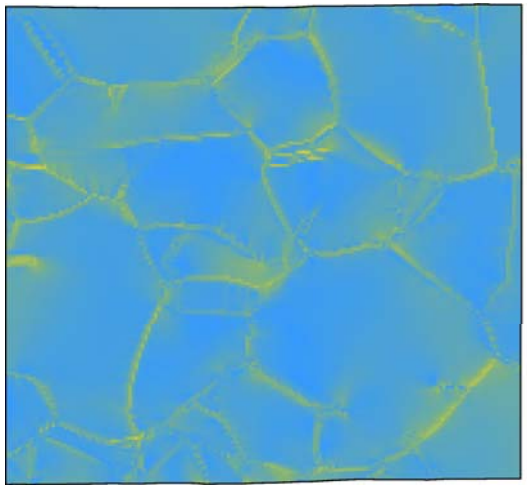


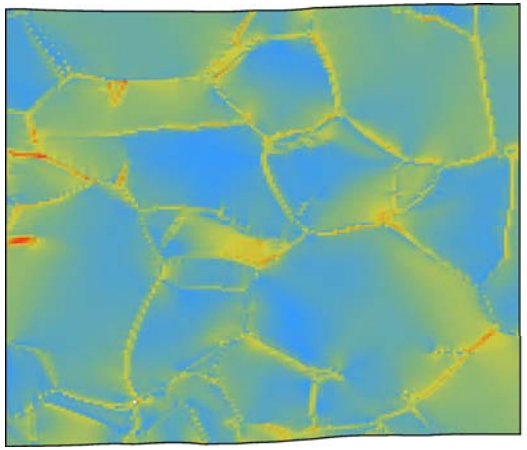

1% strain

5% strain

10% strain








Non-Local Model

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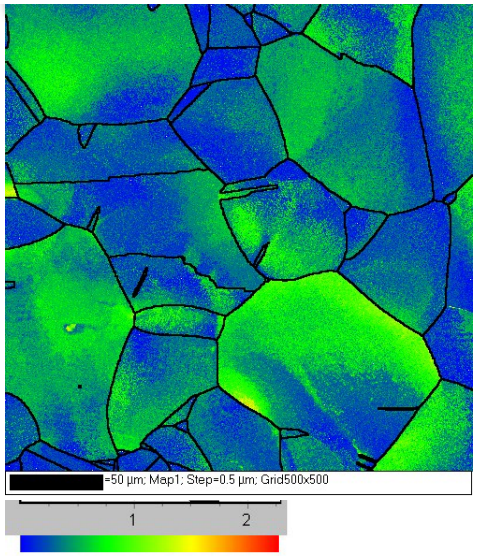
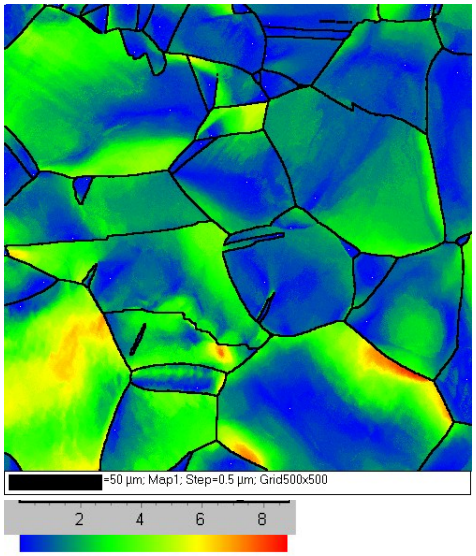
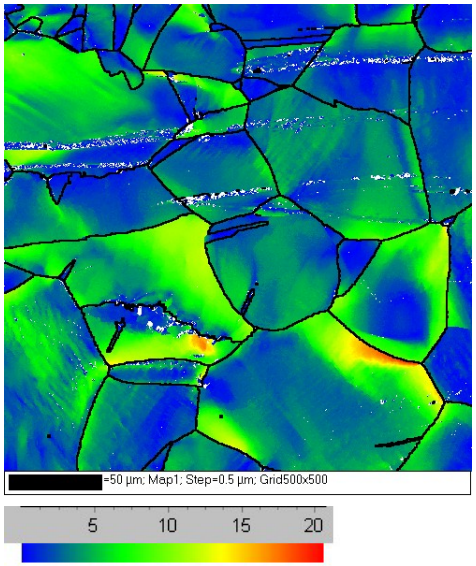
# Comparison of Local Model and EBSD: Local Misorientation Distributions



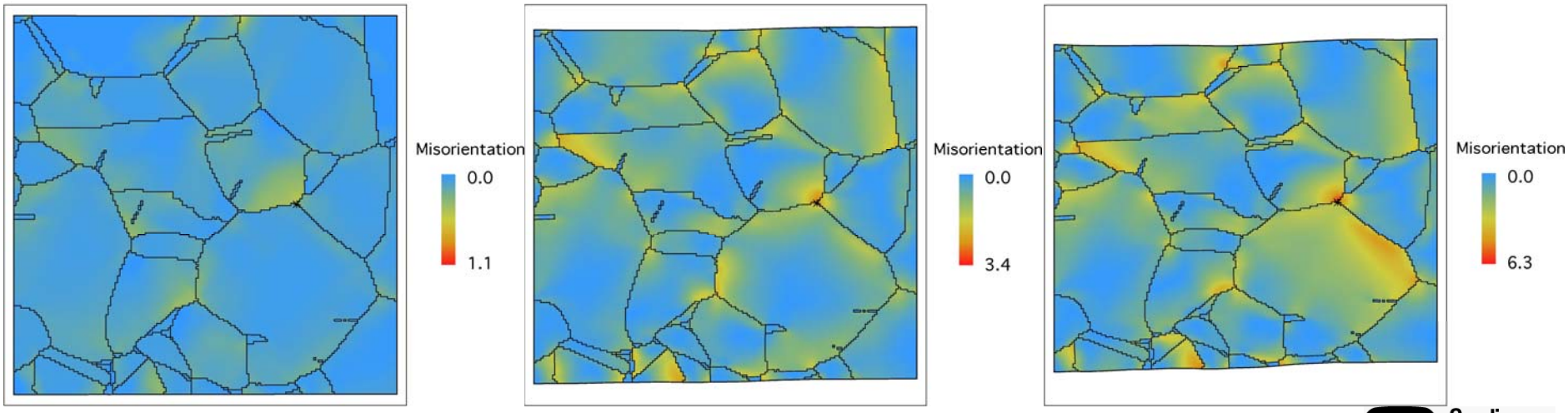




1% Strain

5% Strain

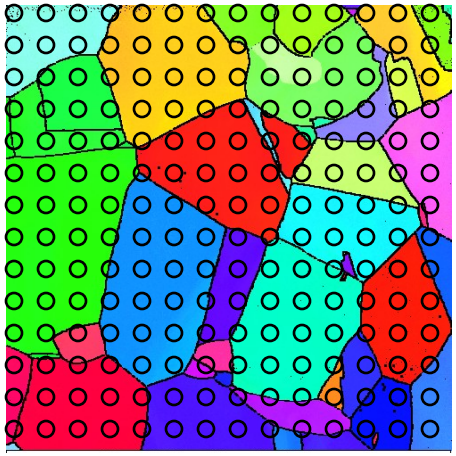
10% Strain



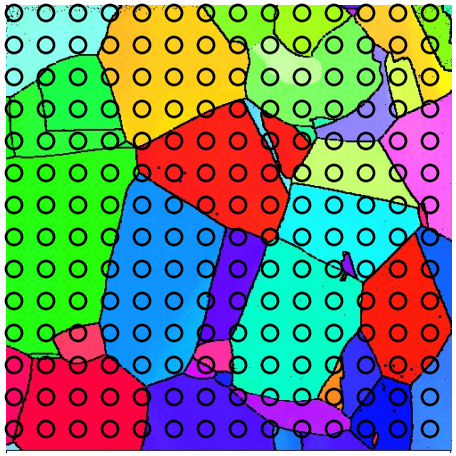

How do we go about comparing these microstructures quantitatively?

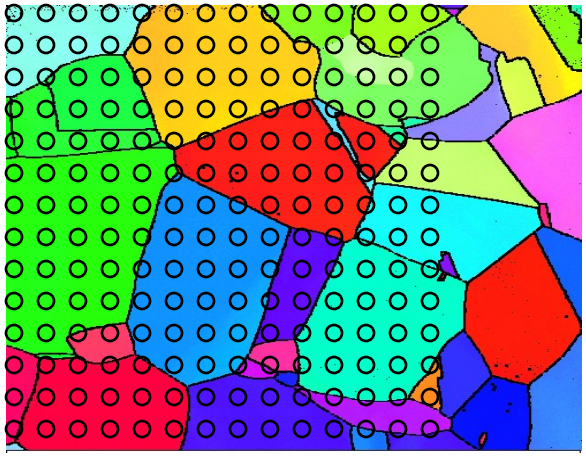
# Coordinate Systems for Comparing Experiment and Simulation

Experiment Initial

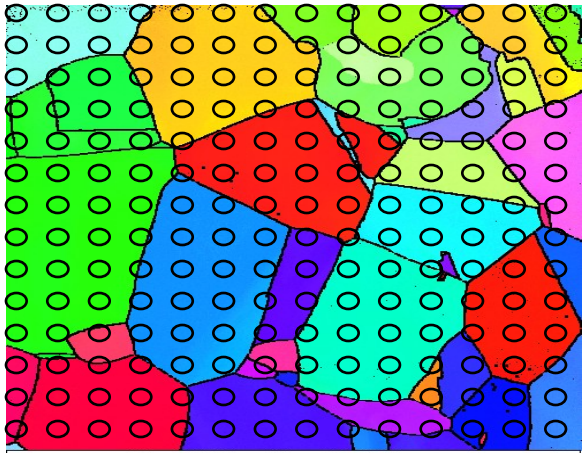


Simulation Initial





Eulerian---points move outside of analysis area



Lagrangian---points analysis area stays with points

Need to match these coordinate systems in order to quantitatively compare the results, point by point…

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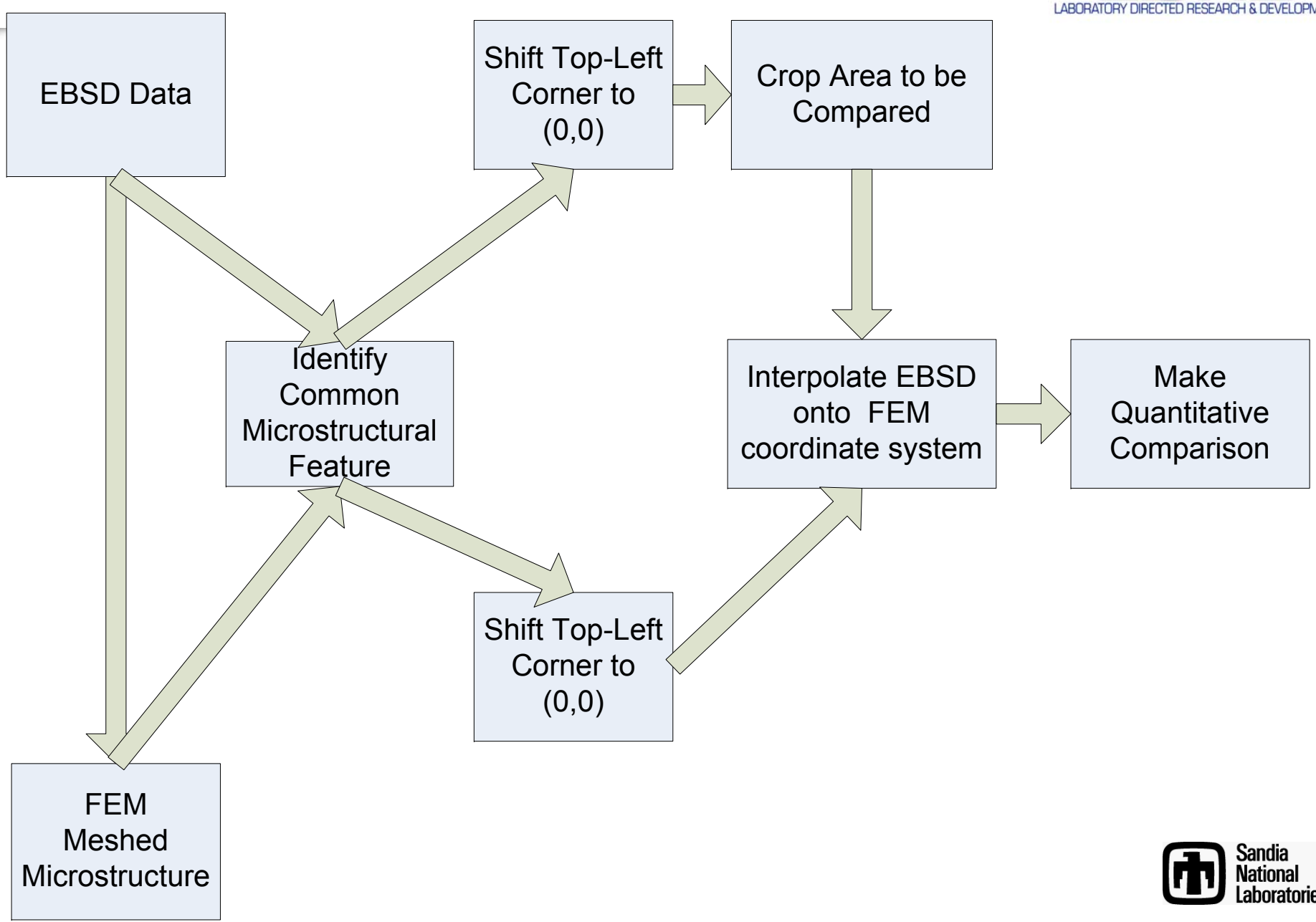
# Remapping the Coordinate Systems

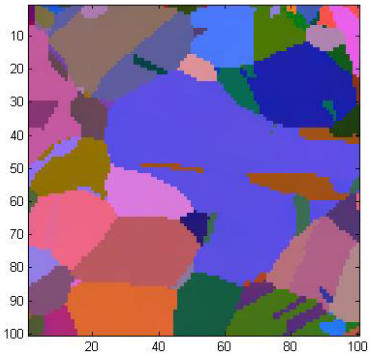


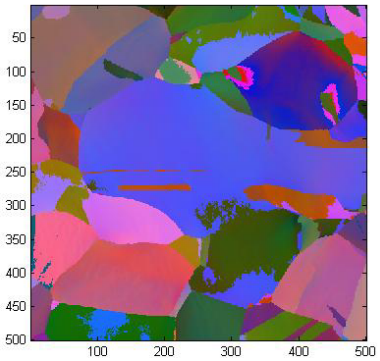
# Example: 10 percent strain (Non-local model vs EBSD)

FEM

EBSD

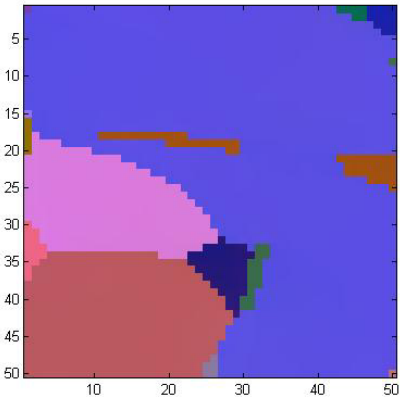
FEM Mesh from Experimental data

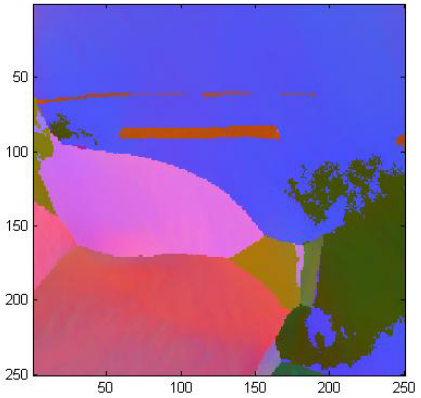



Experimental data

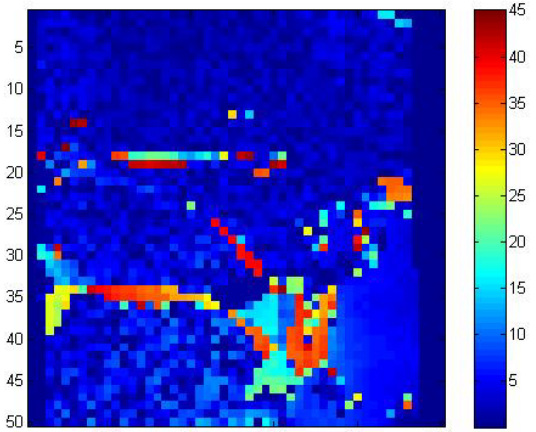
Cropped and shifted areas



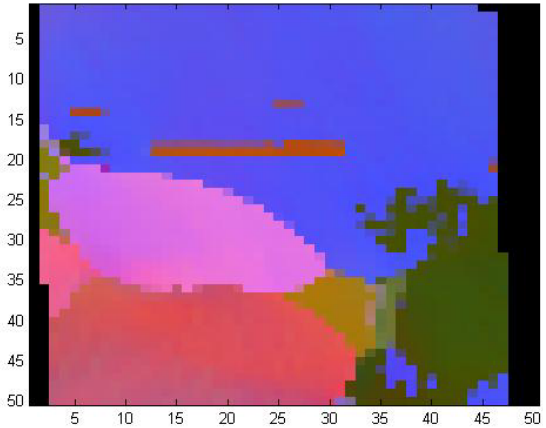

Comparison

(misorientation angle)

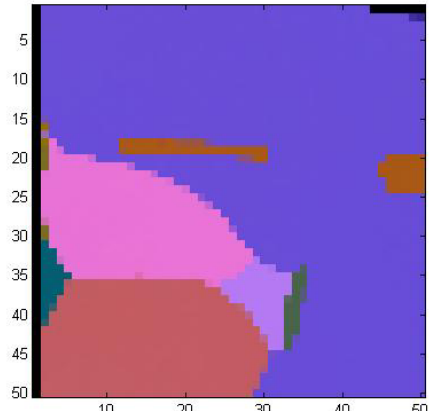



Interpolated

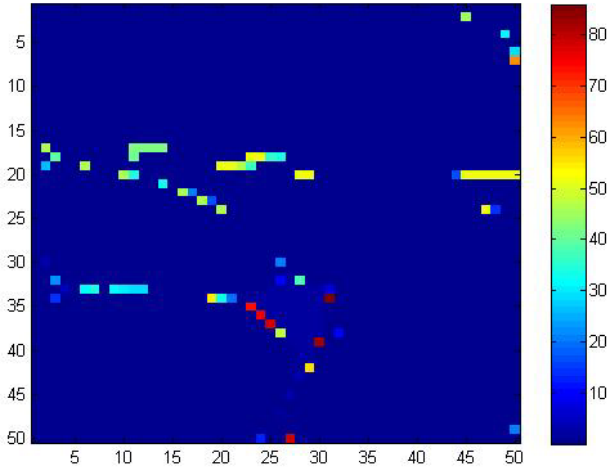
EBSD data



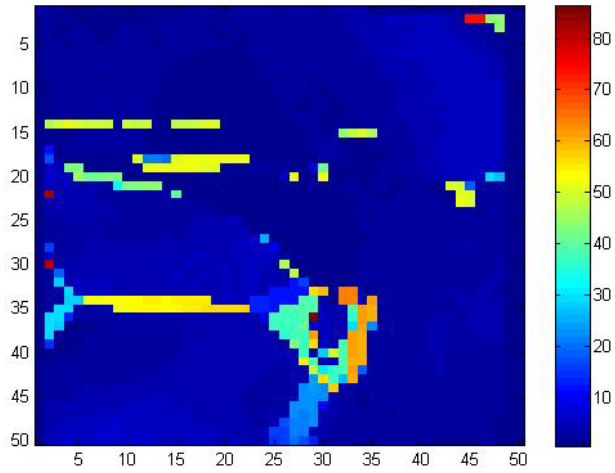
# Misorientation maps show local deviation between experiment and model.



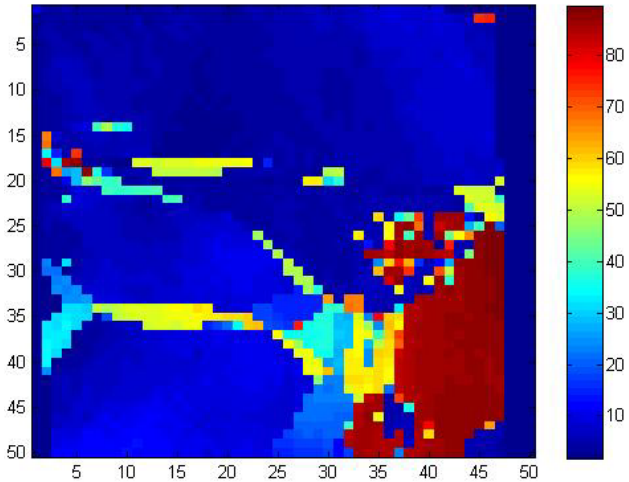
Local model



1%



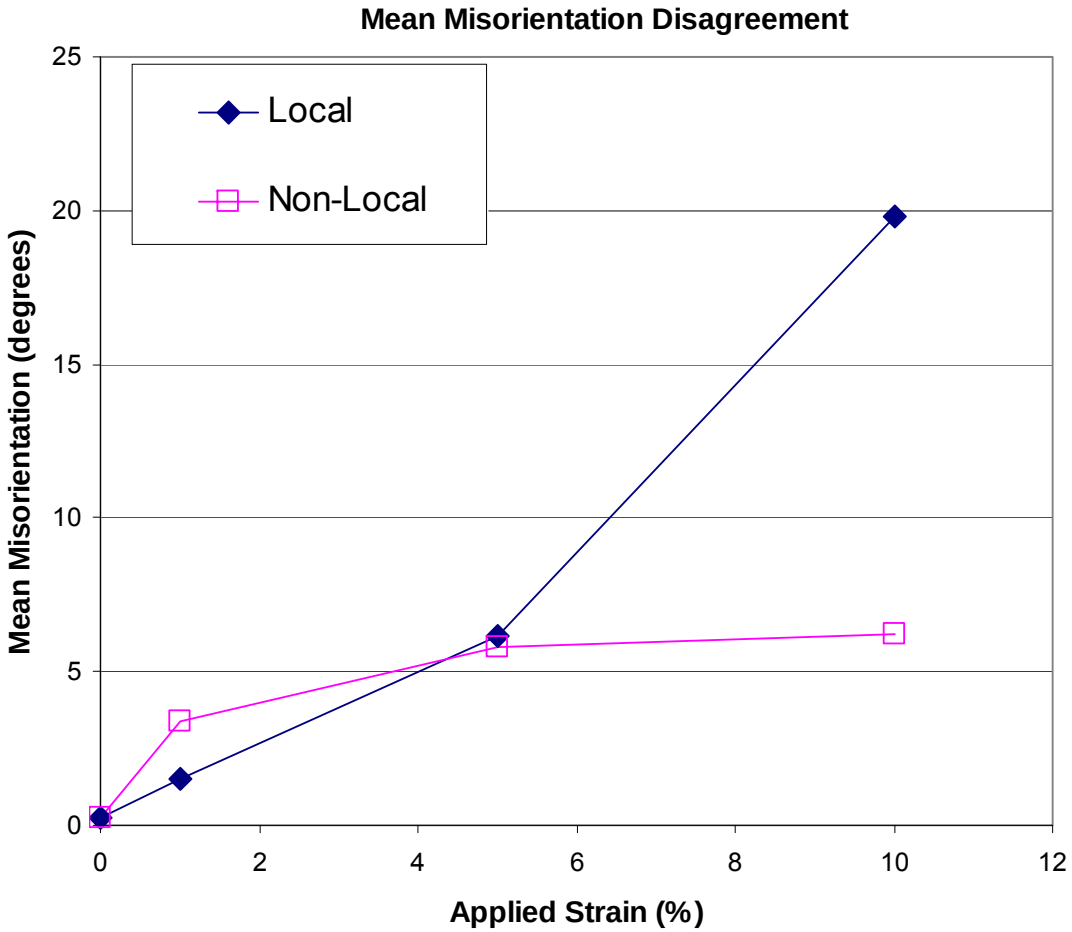
5%



10%

Misorientation (scalar, in degrees)

# Mean misorientation comparison of Local and Non-Local Models with Experiment

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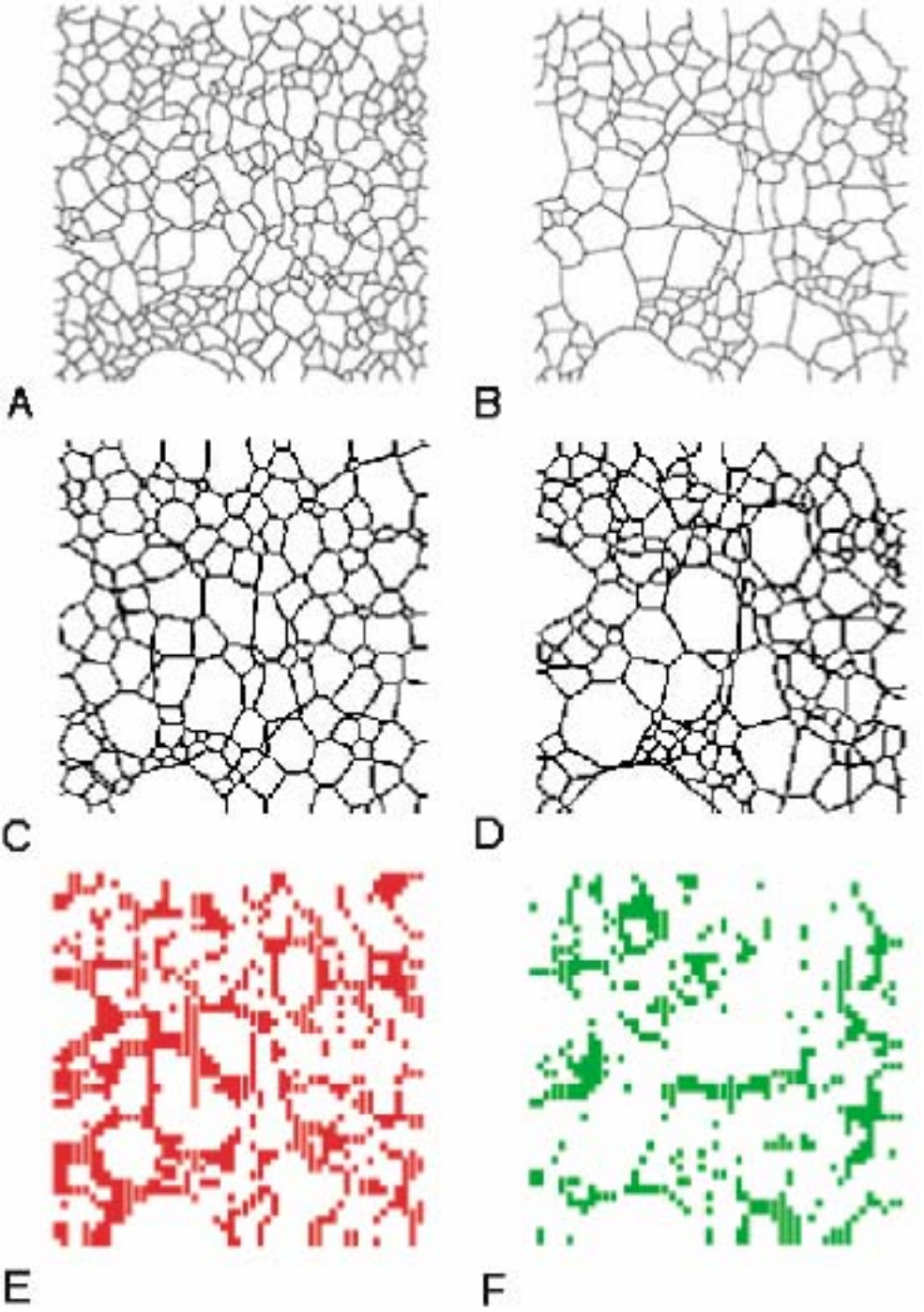


# Normalized Area Match Fraction

$$\mathrm{NAMF}_i = \frac{1}{Z}\sum_{x,y} \delta[s_i(x, y) - s_{\exp}(x, y)],$$

- What percentage of pixels agree?
  - Agreement is binary [0,1]
  - Simple “spin” comparison for grain growth

M.C. Demirel et al., P.R.L., Vol. 90 No. 1, 2003.

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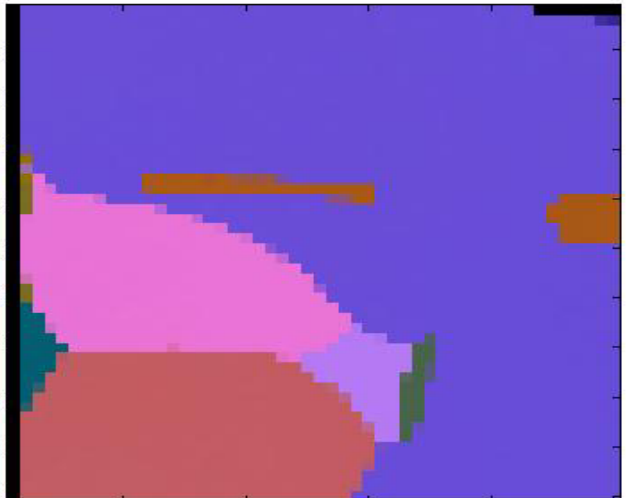
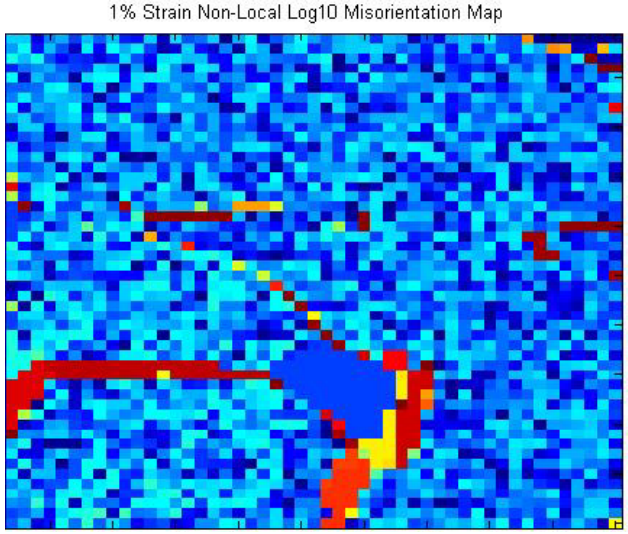
# NAMF for Plasticity

$$NAMF = \frac{1}{Z}\sum_{x,y}\begin{cases}1 \text{ if } \theta < threshold\\ 0 \text{ if } \theta \geq threshold\end{cases}$$

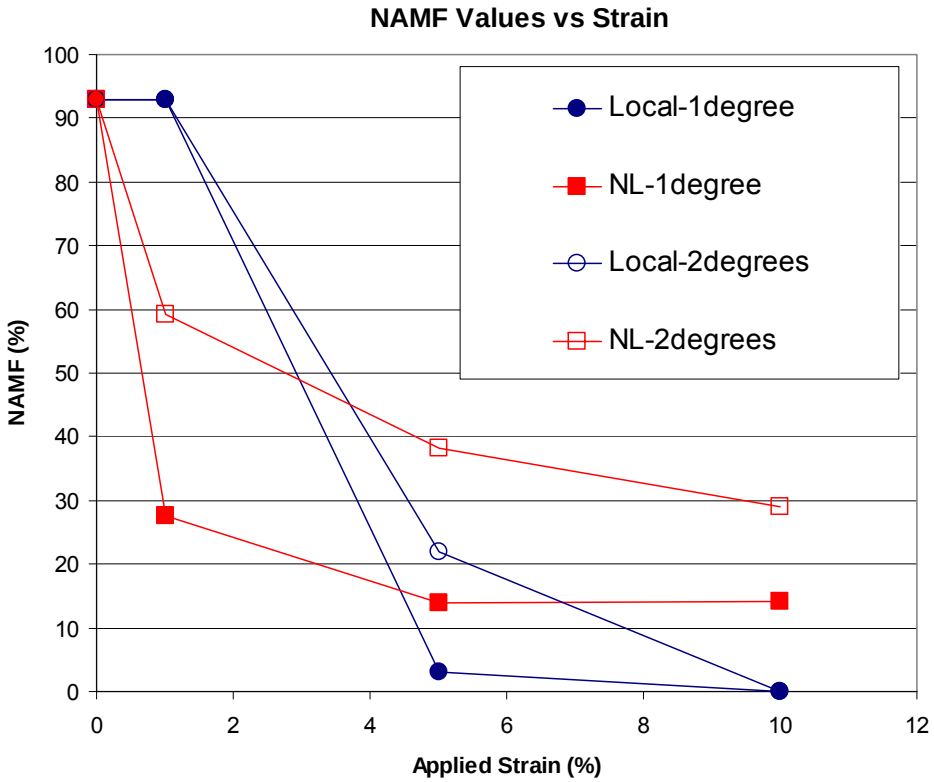
θ is the scalar misorientation between the orientations at a given pixel for the FEM and EBSD data.

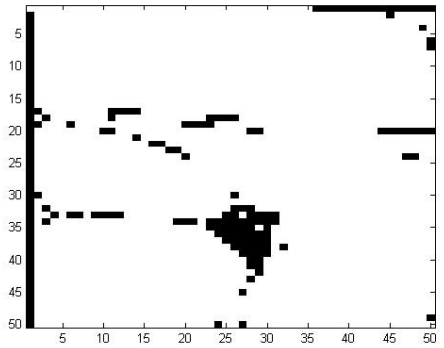
Note that the noise floor for θ measured with standard EBSD is 0.3-0.5˚. 1-2˚ may be a better choice



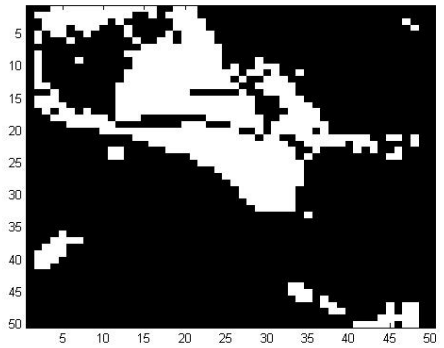



# NAMF for Plasticity Comparison



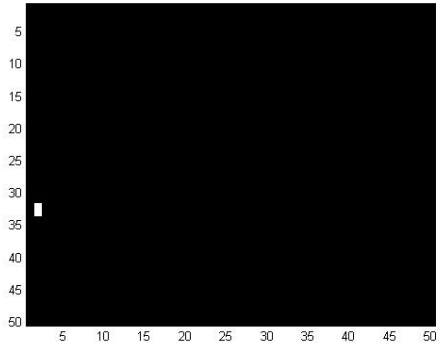



1% strain



5% strain

Local model, 2˚ threshold



10% strain

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# Conclusions

- **Meaningful development of microstructural-level models requires careful comparison with experiment at the microstructural length scale.**

- **Often, the models may give collective stress-strain responses that look acceptably good, but the details microscale of the plasticity are not as stable or as accurate**

- **We are developing methods for quantitatively comparing microstructural simulations and experiment on the same microstructures.**

- **Both average metrics and local plots of simulation-experiment difference are important**

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# Crystal Plasticity: Theoretical framework

**Kinematics of slip systems** $\mathbf{L}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p-1} = \sum_{\alpha=1}^{Nslip} \dot{\gamma}^a \left( \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha \right)$

Crystallographic slip

=

Dominant plastic deformation mechanism

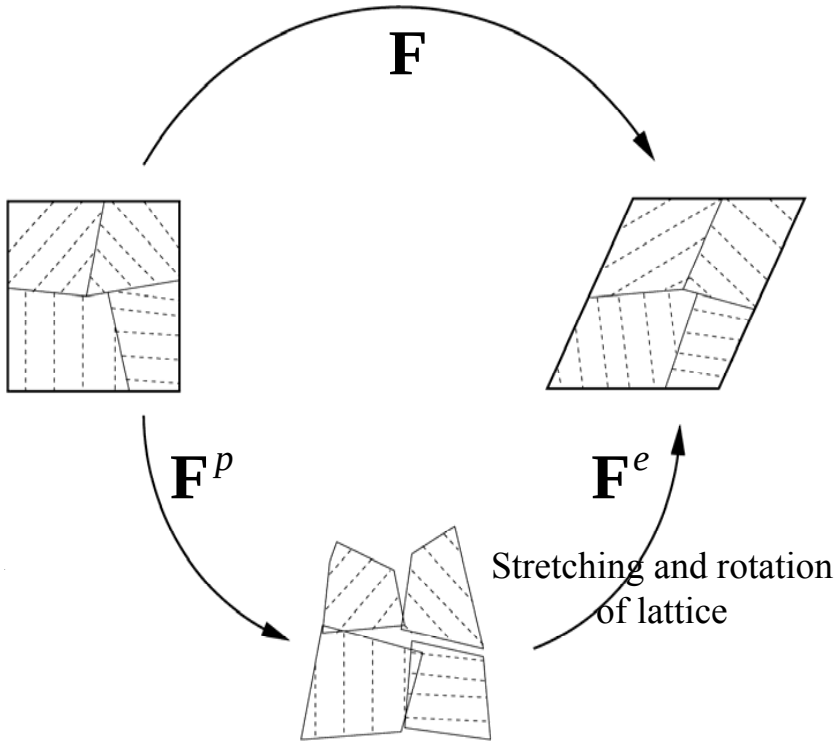
**Elasticity** $\sigma^{PK2} = \mathbf{C}^e : \tilde{\mathbf{E}}^e$

**Slip system evolution**
(power law viscoplastic flow rule) $\dot{\gamma} = \dot{\gamma}_0 \left| \frac{\tau^a}{\tau^a_{CRSS}} \right|^{1/m} \operatorname{sgn}\left(\tau^a\right)$

**Slip system hardening: Taylor dislocation based**

$$\begin{cases} \tau^\alpha_{CRSS} = C \mu b \sqrt{\rho^\alpha} \\ \dot{\rho}^\alpha = \left( c_1 \sqrt{\rho^\alpha} - c_2 \rho^\alpha \right) \left| \dot{\gamma}^\alpha \right| \end{cases}$$

Multiplicative decomposition




Motion of dislocations
on active slip systems.
(**undistorted** AND **unrotated**)

# What people do elsewhere…

Ecole Polytechnique, FR: **J. Crepin**

**FEM parametric study**

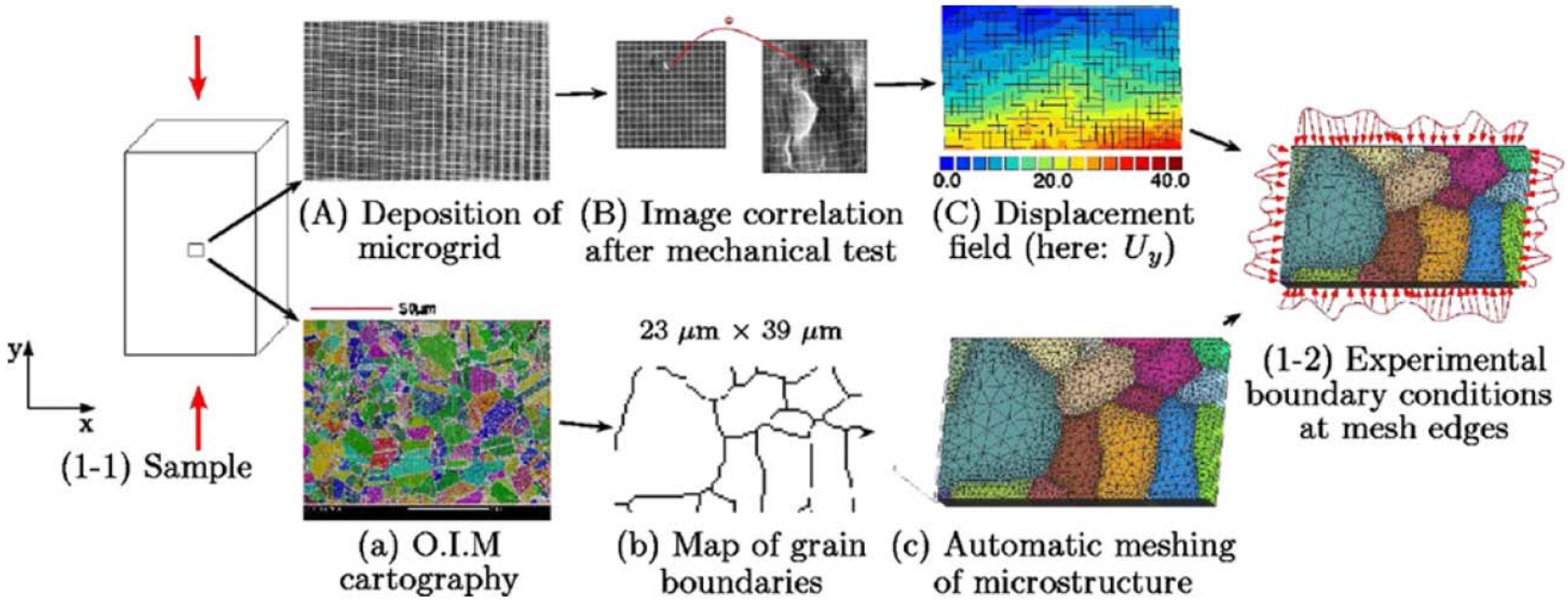
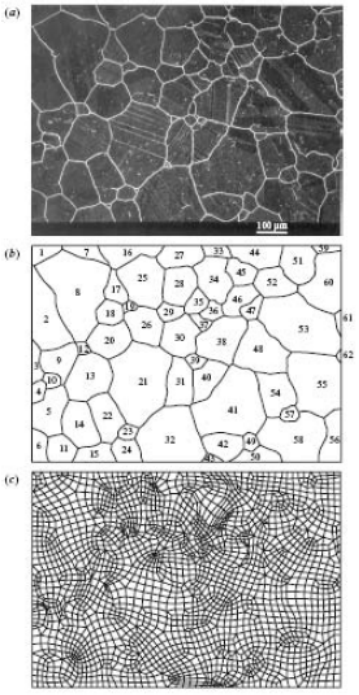


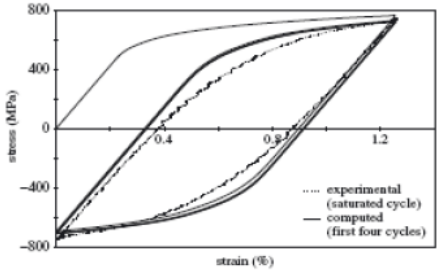

Fig. 1. Coupling between experimental tests and FE simulations.

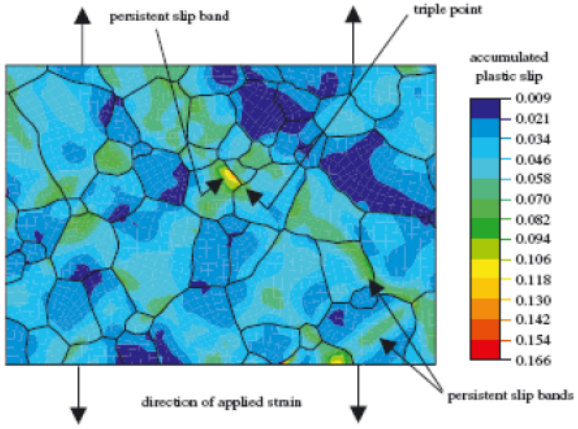
**[E. Heripre et al. "Coupling between experimental measurements and polycrystal finite element calculations for micromechanical study of metallic materials" *IJP* in press]**

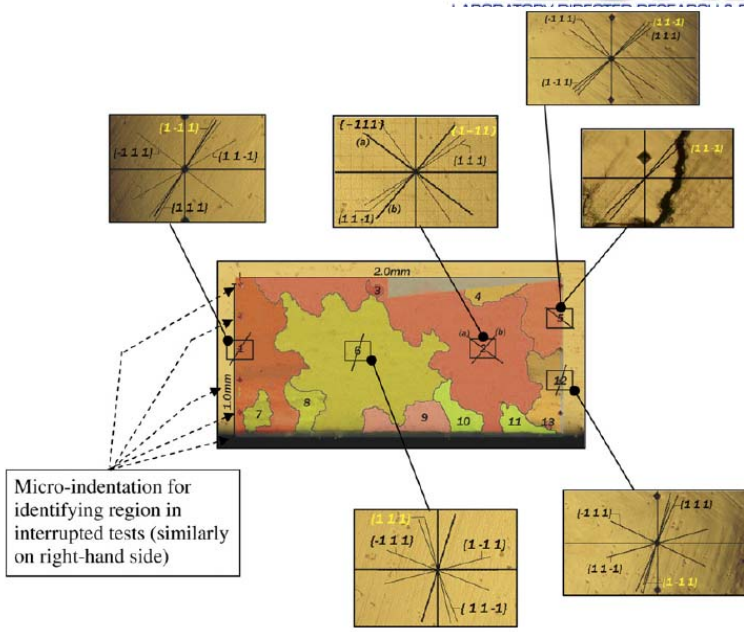
# What people do elsewhere…

Oxford Univ., U.K.: **F.P.E. Dunne**

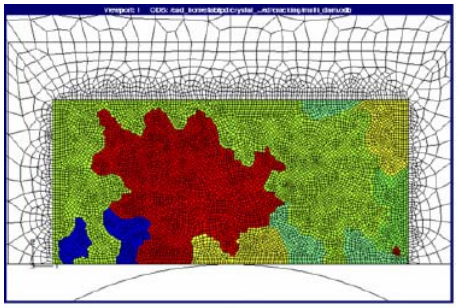


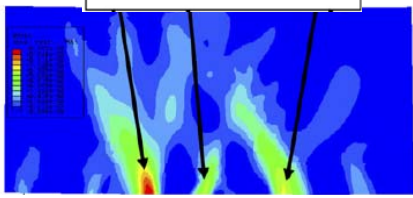




Micro-indentation for identifying region in interrupted tests (similarly on right-hand side)



Locations of Highest Accumulated Plastic Slip and Predicted Crack Initiation in Plane Stress




**[F. P. E. Dunne et al. (2004) "High- and low-cycle fatigue crack initiation using polycrystal plasticity", *Proc. R. Soc. Lond.* A460, p. 1881–1903]**

**[F.P.E. Dunne (2007) "Experimental and computational studies of low cycle fatigue crack nucleation in a polycrystal", *IJP* 23 p. 273–295]**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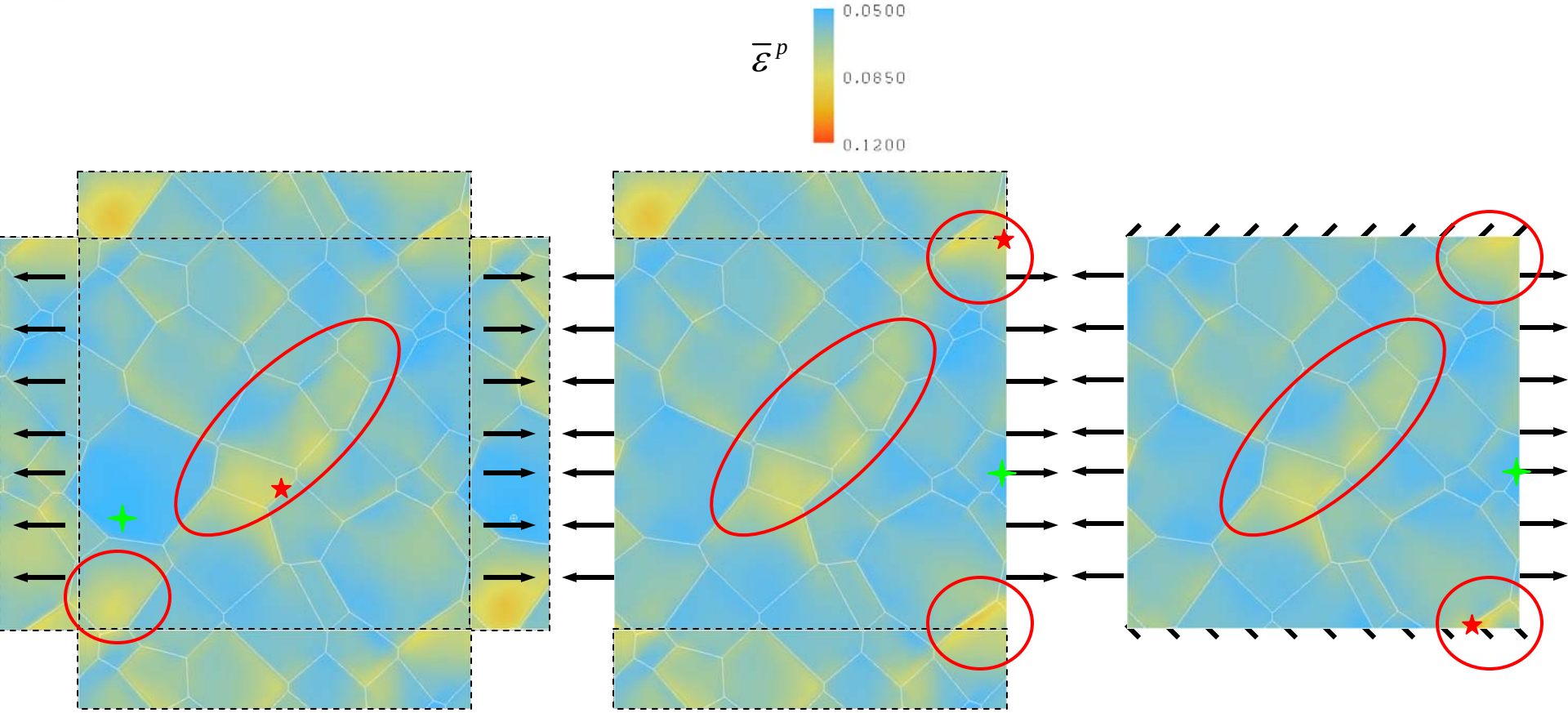
# Microstructural level information: Equivalent Plastic Strain

## Uniform displacement control

5% deformation




X dir.: Periodic BC
Y dir.: Periodic BC

$\overline{\varepsilon}^p_{\max}$ ★ 0.084

$\overline{\varepsilon}^p_{\min}$ ✦ 0.050

X dir.: Uniform strain
Y dir.: Periodic BC

$\overline{\varepsilon}^p_{\max}$ ★ 0.104

$\overline{\varepsilon}^p_{\min}$ ✦ 0.051

X dir.: Uniform strain
Y dir.: No Displ.

$\overline{\varepsilon}^p_{\max}$ ★ 0.117

$\overline{\varepsilon}^p_{\min}$ ✦ 0.050

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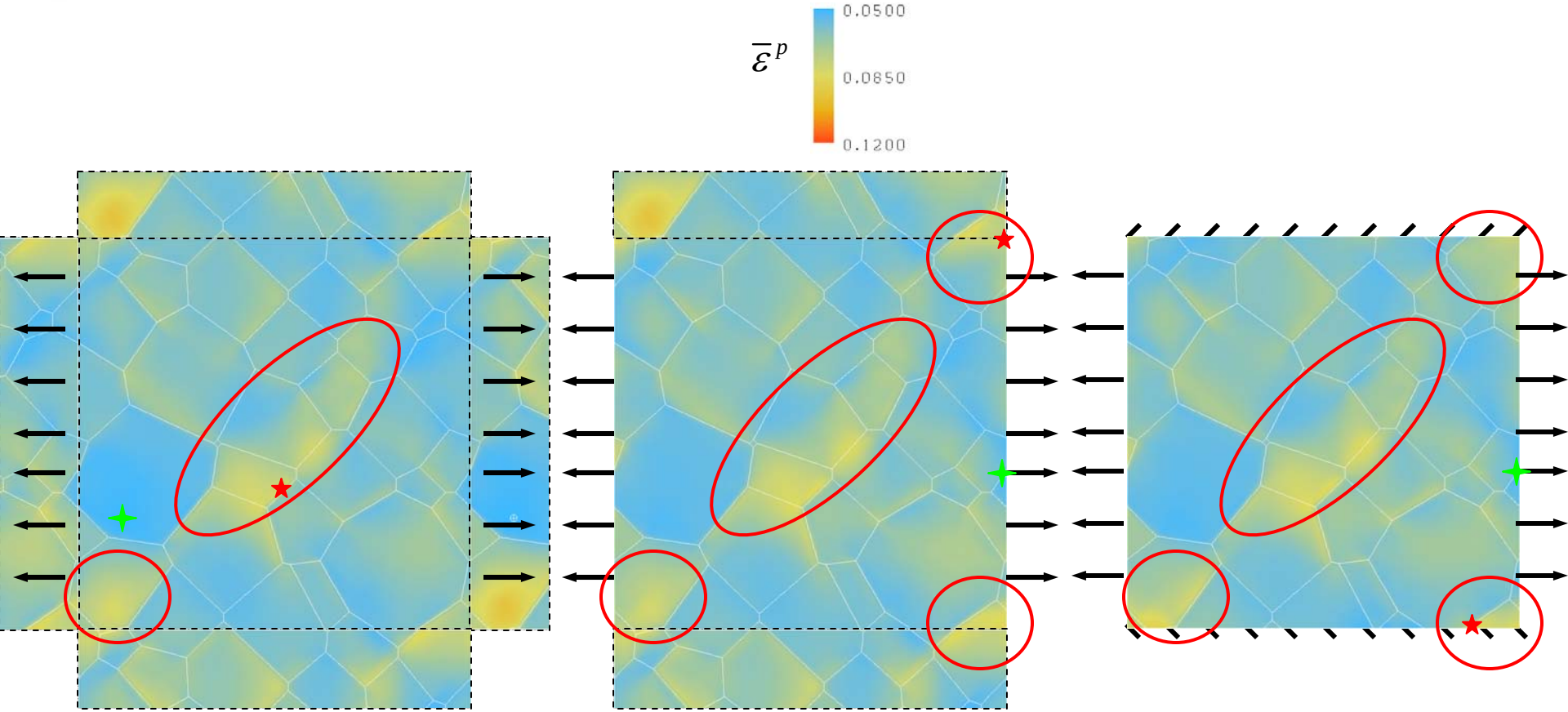
# Microstructural level information: Equivalent Plastic Strain

Load control

5% deformation




X dir.: Periodic BC
Y dir.: Periodic BC

$\overline{\varepsilon}^p_{\max}$ ★ 0.084

$\overline{\varepsilon}^p_{\min}$ ✦ 0.051

X dir.: Uniform strain
Y dir.: Periodic BC

$\overline{\varepsilon}^p_{\max}$ ★ 0.089

$\overline{\varepsilon}^p_{\min}$ ✦ 0.052

X dir.: Uniform strain
Y dir.: No Displ.

$\overline{\varepsilon}^p_{\max}$ ★ 0.100

$\overline{\varepsilon}^p_{\min}$ ✦ 0.052

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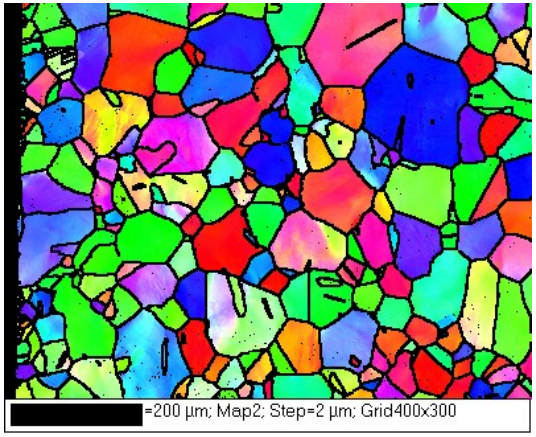
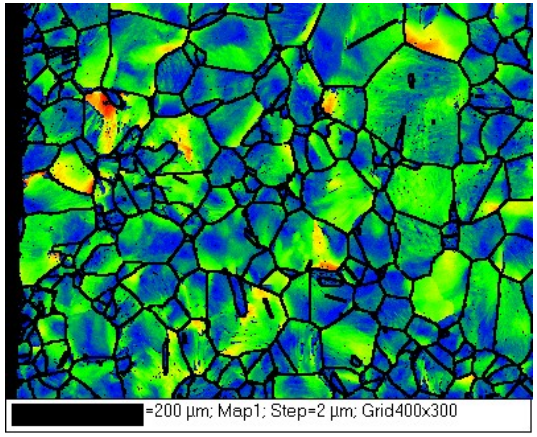
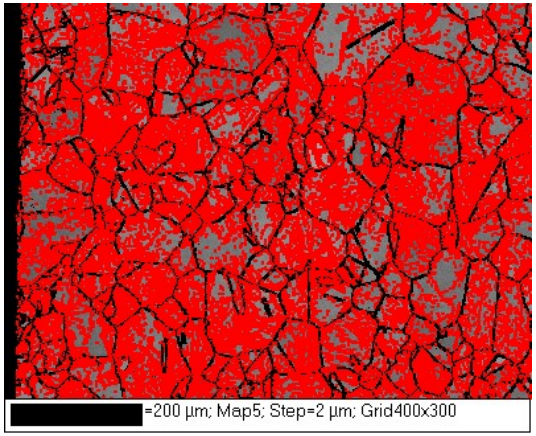
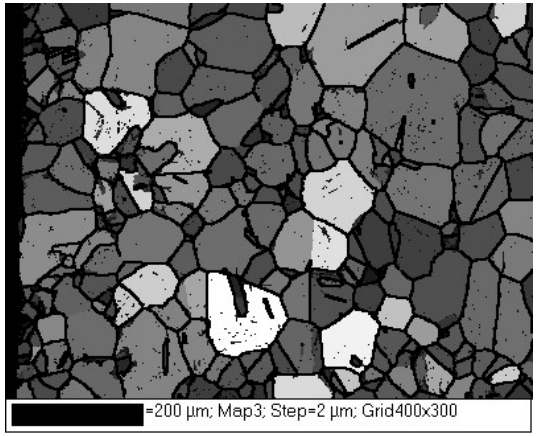
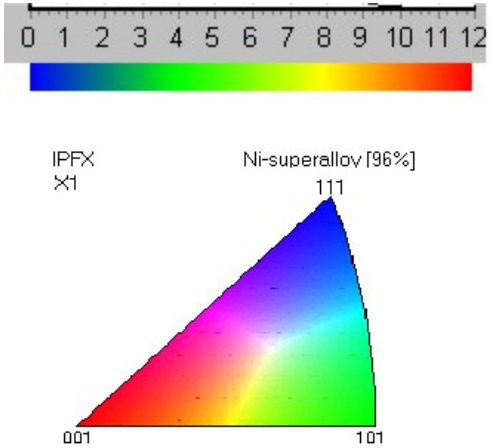
## EBSD maps from cross section of gage section of tensile bar (10% applied macro strain)




- **Really no strong gradient in rotation from surface (on left) to mid-plane of sample**