SAND2006-4422C

Capturing Microstructural Scale Effects Through Non-Local Crystal Plasticity

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Acknowledgements:
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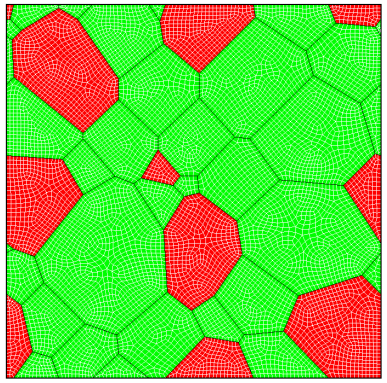
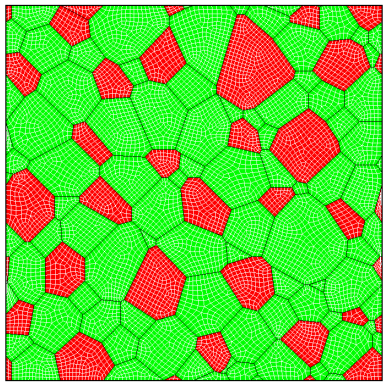
David McDowell, GIT
Ashok Saxena, GIT

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Experimental Observations



150 um



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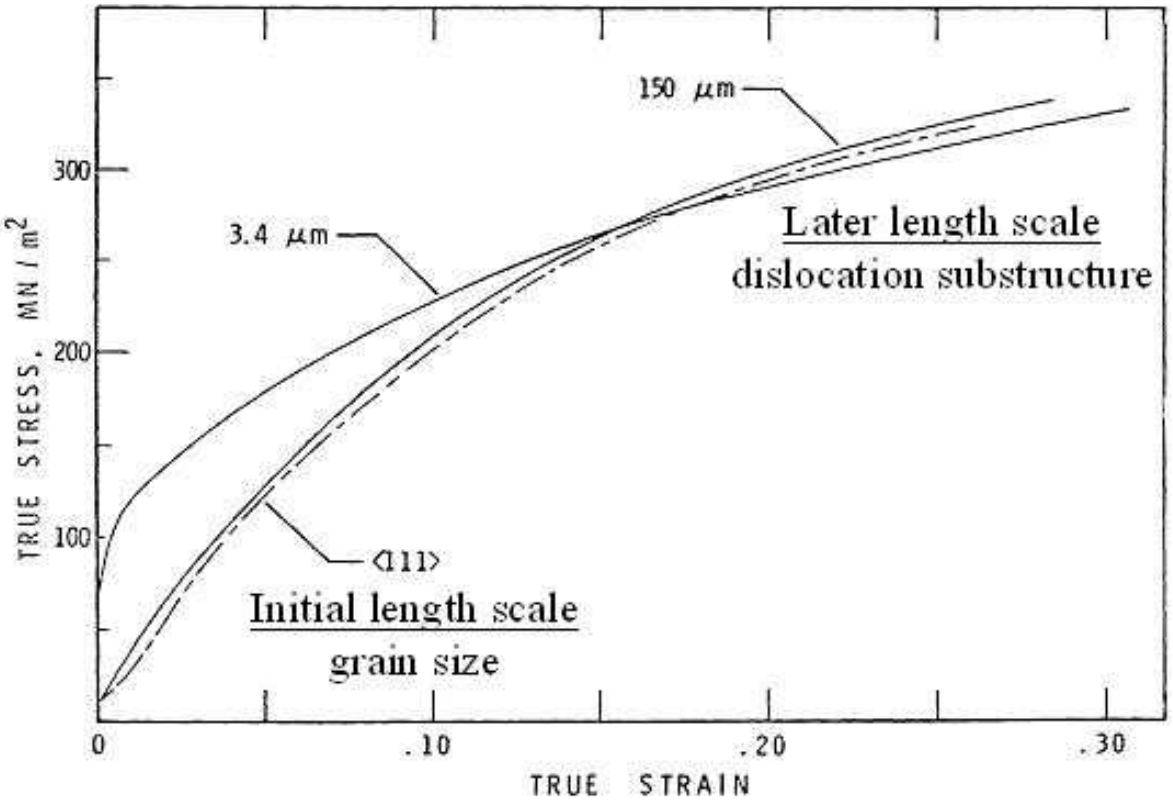


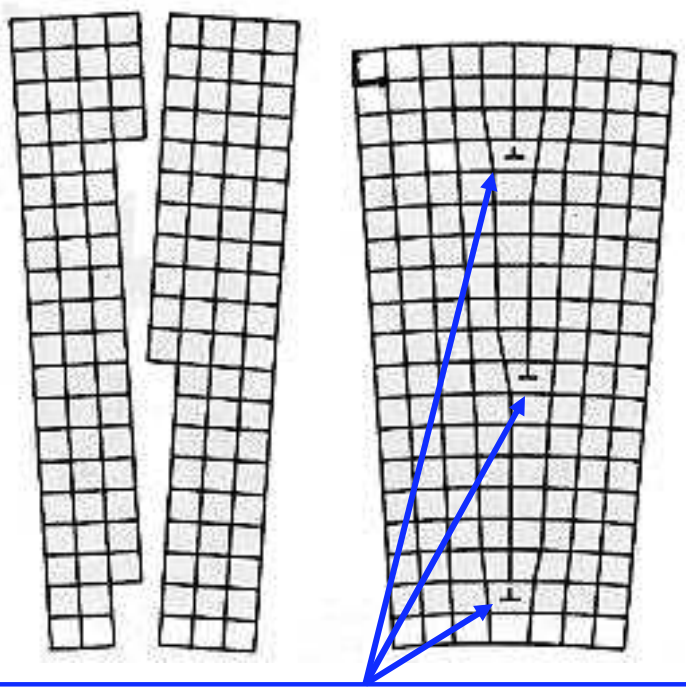
Mechanical response of materials depends on the microstructure of the material

Experimental Observations

- Dominant microstructural features of polycrystals are grain boundaries

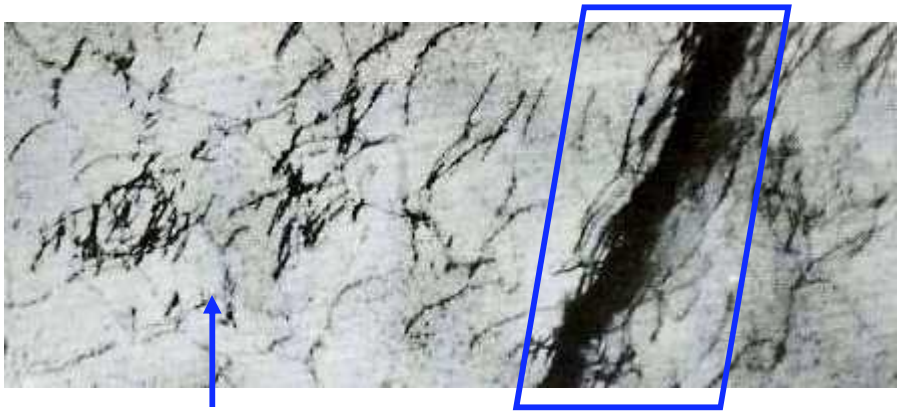
Concept

- Interface between 2 crystals with different orientation



Geometrically Necessary Dislocations (GNDs)

Reality



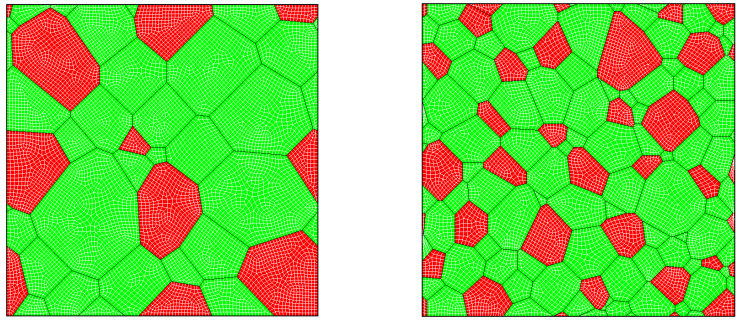
Low density interior

High density boundary

High density boundaries act as barriers to dislocation motion

Classical Continuum Modeling

- Structural finite element codes are continuum based
- Finite element mesh has dimensions but they do not effect the σ–ε result
- Predicted σ–ε results from two different grain sizes are similar



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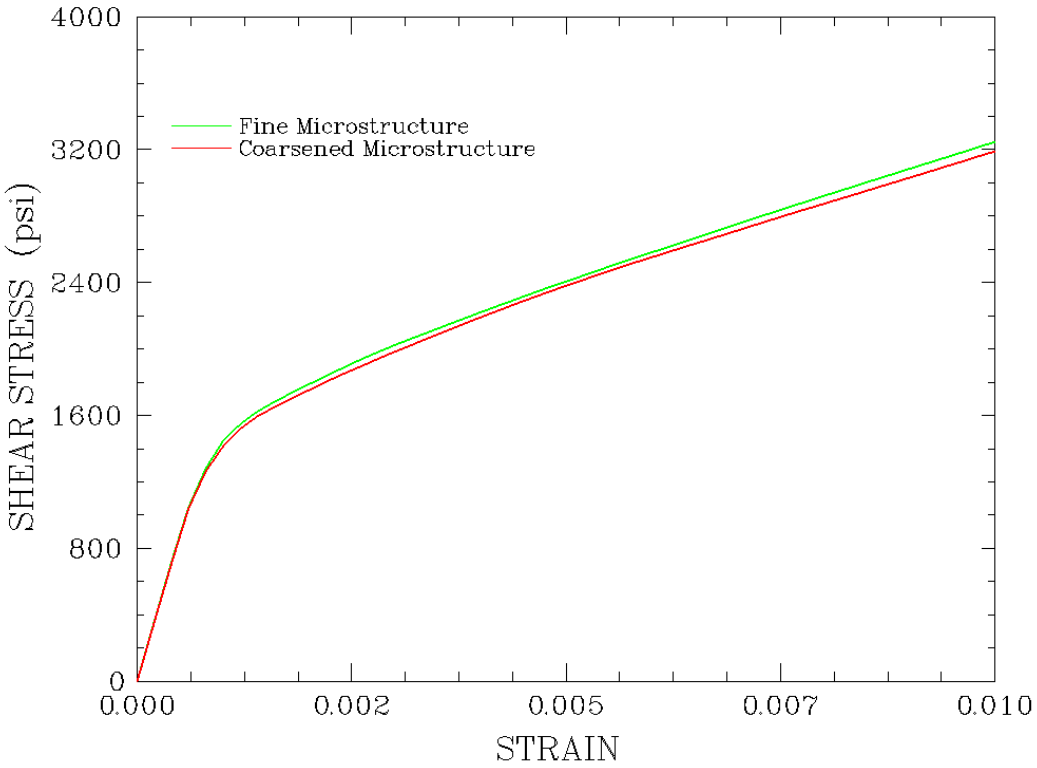
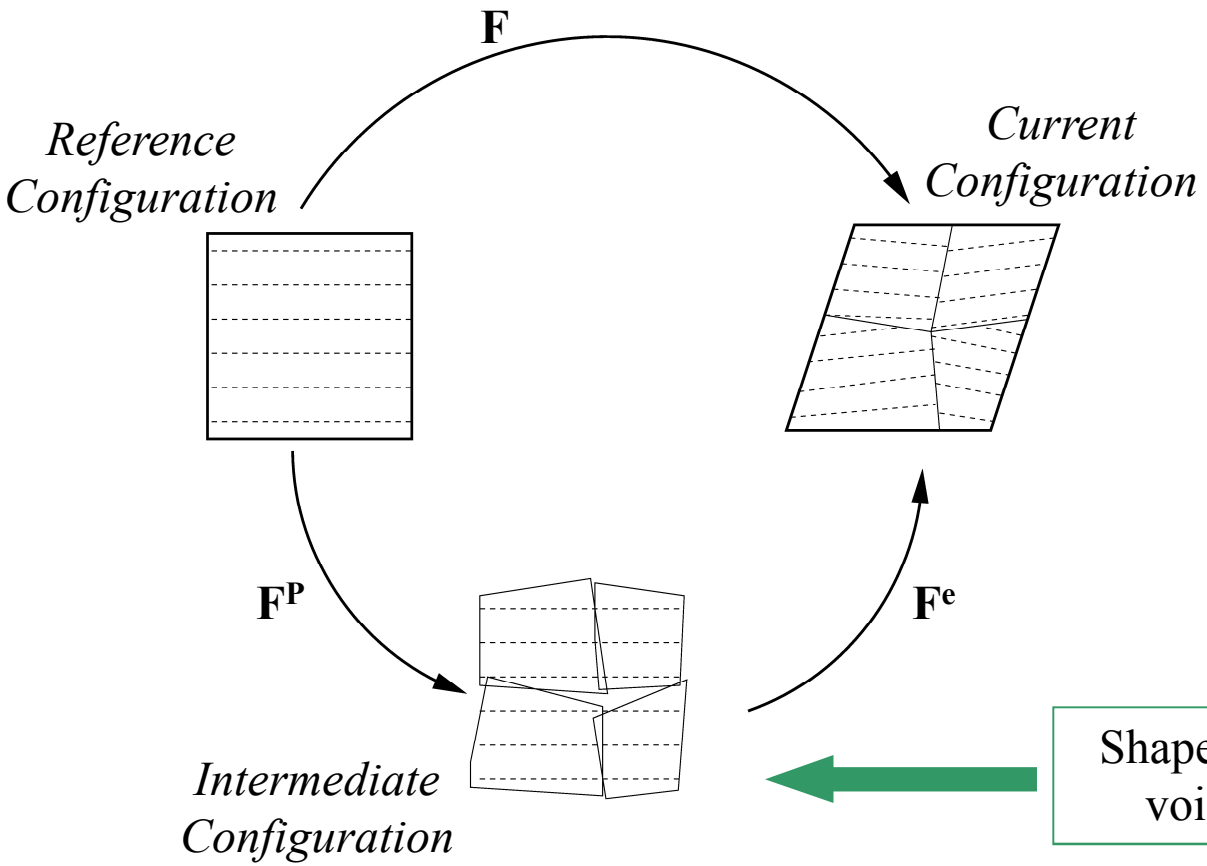


Single Crystal Kinematics

Total deformation (**F**) is modeled as a two step process:

- Plastic deformation ($\mathbf{F}^P$)
- Elastic deformation ($\mathbf{F}^e$)

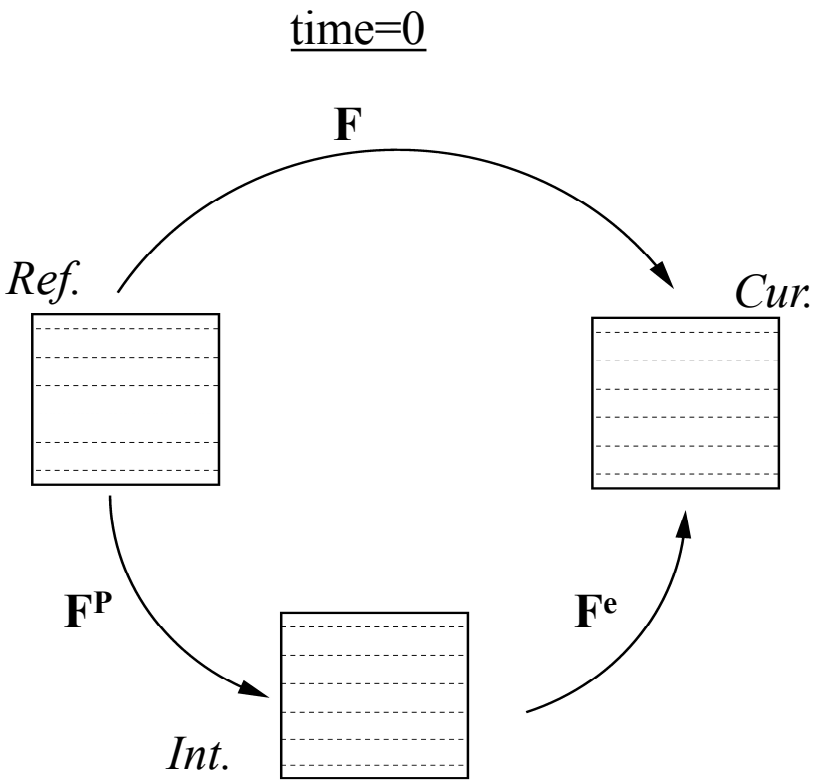
$$\mathbf{F} = \mathbf{F}^e\mathbf{F}^P$$



GNDs are needed to "fix" the voids and overlaps and restore compatibility in current configuration

Shape change produces voids and overlaps

Single Crystal Kinematics



Define a Dislocation Tensor: $\hat{\mathbf{G}}$ [1]

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

$$\mathrm{Det}[\mathbf{F}^e]\,\mathbf{F}^{e^{-1}}\ \mathrm{curl}\ \mathbf{F}^{e^{-1}}$$

At time=t

$$\mathbf{F}^p = \mathbf{F}^p(t),\quad \mathbf{F}^e = \mathbf{F}^e(t) \Rightarrow \hat{\mathbf{G}} = \hat{\mathbf{G}}(t)$$

At time=0

$$\mathbf{F}_0^p = \mathbf{I},\quad \mathbf{F}_0^e = \mathbf{I} \Rightarrow \hat{\mathbf{G}}_0 = 0 \cdot \mathbf{I}$$

How can you account for initial microstructure, specifically GNDs?

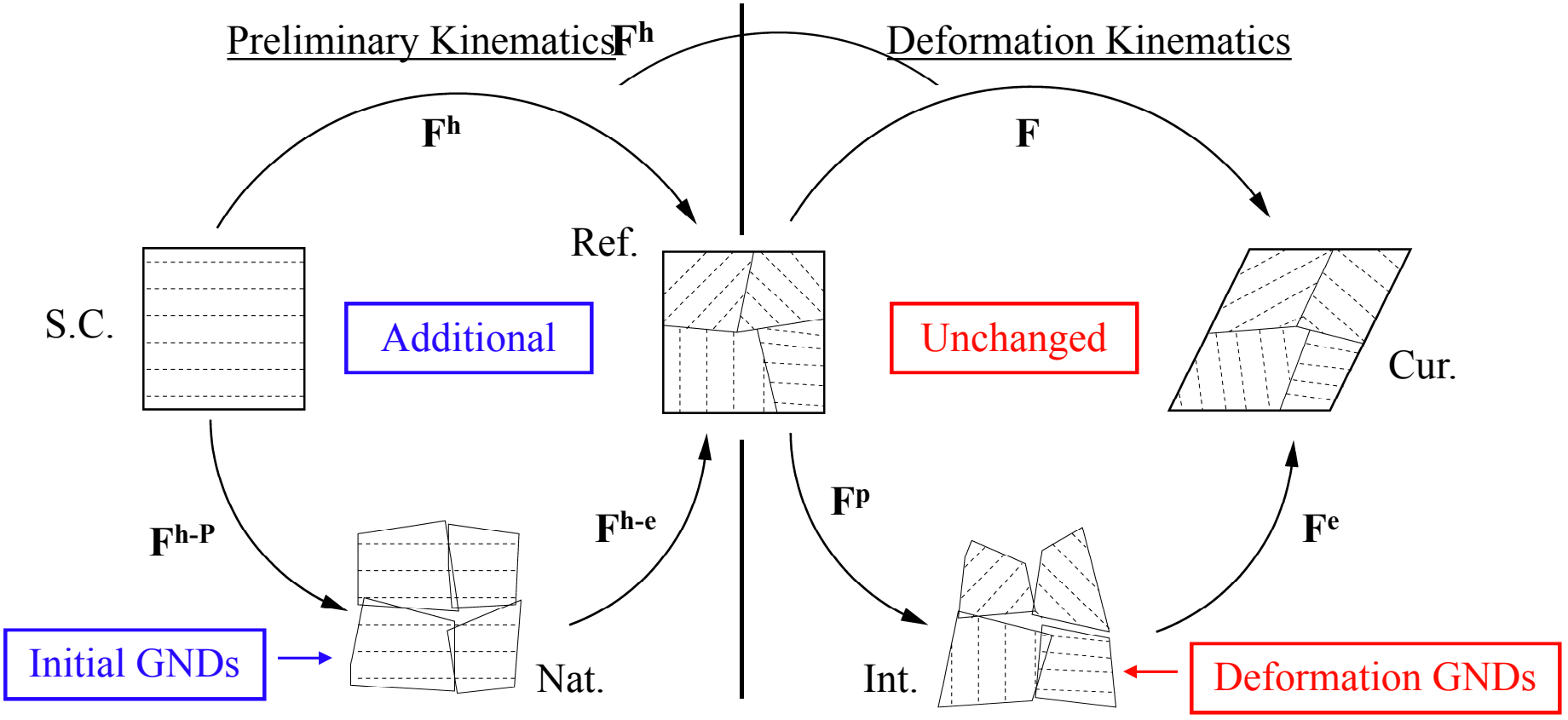
1 Cermelli & Gurtin, (2001)

Polycrystal Kinematics

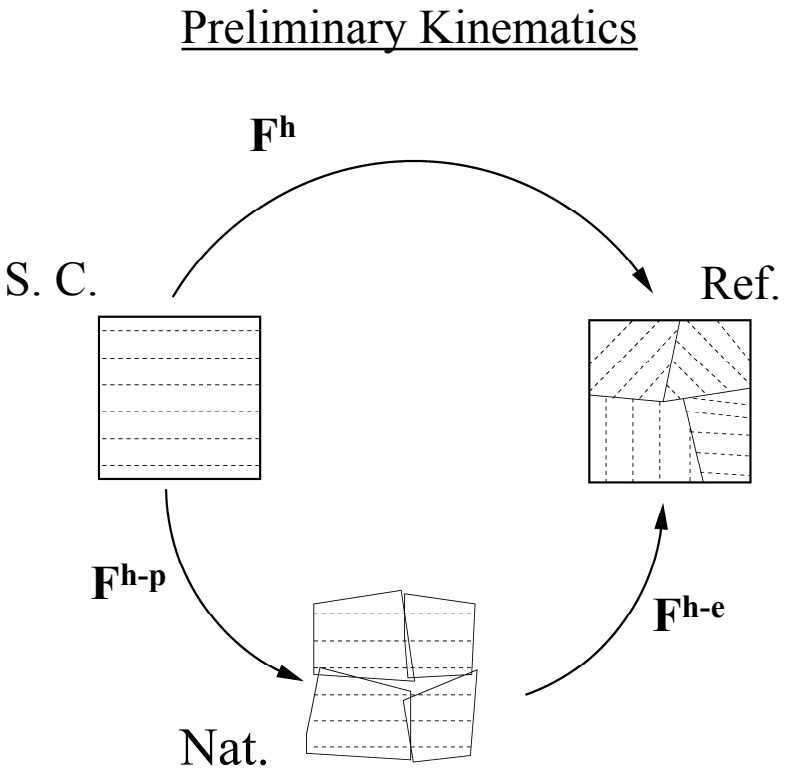
- Based on a geometric argument
- Introduce a *fictitious* deformation
- Establish Preliminary Kinematics

$$\mathbf{F}^{h} = \mathbf{F}^{h\text{-}e}\,\mathbf{F}^{h\text{-}P}$$

Purpose: Provide a consistent framework to determine the *initial* and *evolving* GND state.



Polycrystal Kinematics



- Define an Initial Dislocation Tensor

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

$\tilde{\mathbf{G}}_0$

- $\mathbf{F}^{h-e} = \mathbf{R}^{h-e}\ \mathbf{U}^{h-e}$

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

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

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

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

- Define a Deformation Dislocation Tensor

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

- Define a Total Dislocation Tensor

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

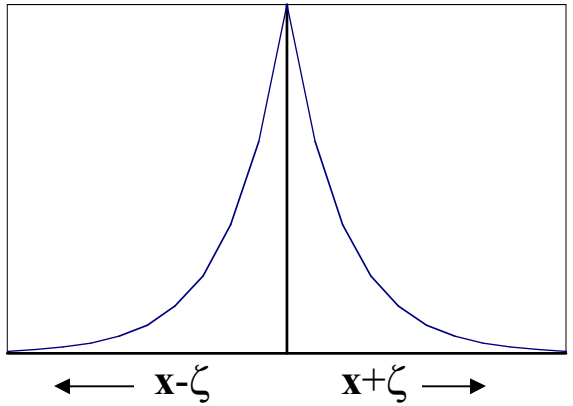
Non-Local Integral Method

Define a non-local curl

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

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

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



The Non-Local Integral Based Dislocation Tensors

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

Crystal Plasticity Model

- Standard Crystal Plasticity

$$\hat{\mathbf{L}}^{\mathbf{P}} = \dot{\mathbf{F}}^{\mathbf{P}}\mathbf{F}^{\mathbf{P}-1} = \sum_{\alpha=1}^{N} \dot{\gamma}^{\alpha} \left(\hat{\mathbf{s}}^{\alpha} \otimes \hat{\mathbf{m}}^{\alpha}\right)$$

$\hat{\mathbf{s}}^{\alpha} \otimes \hat{\mathbf{m}}^{\alpha}$ = schmid tensor

$\dot{\gamma}^{\alpha}$ = slip rate

- Anisotropic Taylor Hardening

$$\tau^{\alpha}_{CRSS} = C\, G_{110}\, b \sqrt{\rho^{\alpha}_{GND} + \rho^{\alpha}_{SSD}}$$

Scalarization of $\hat{\mathbf{G}}^{\mathbf{Tot}}$

$$\rho^{\alpha}_{GND} = J^{\mathbf{F^e}} \frac{\left| \hat{\mathbf{G}}^{\mathbf{Tot}} : \left(\hat{\mathbf{s}}^{\alpha} \otimes \hat{\mathbf{m}}^{\alpha}\right) \right|}{b}$$

b = burgers vector

SSD Evolution Equation [3]

$$\frac{d\rho^{\alpha}_{SSD}}{d\gamma^{\alpha}} = c_1 \sqrt{\rho^{\alpha}_{SSD} + \rho^{\alpha}_{GND}} - c_2 \left(\rho^{\alpha}_{SSD} + \rho^{\alpha}_{GND}\right)$$

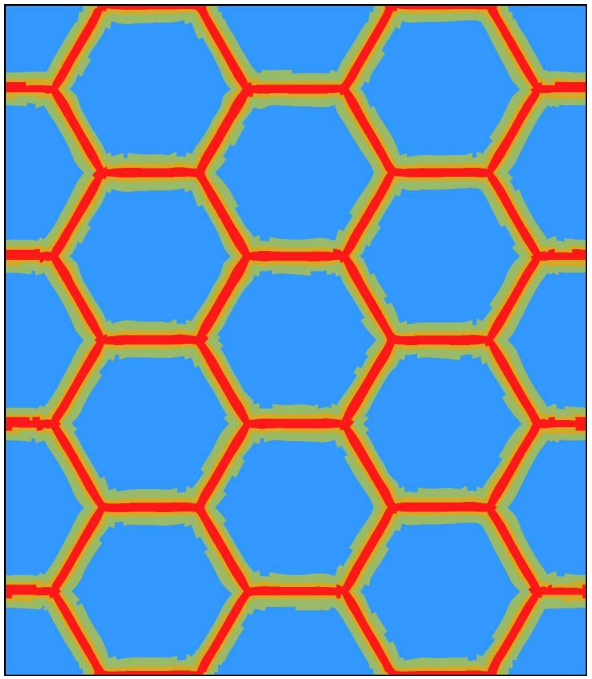
γ = slip

c_1, c_2 = material constants

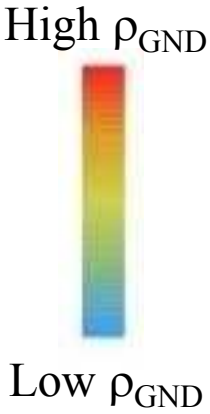
3 Kocks & Mecking, (1981)

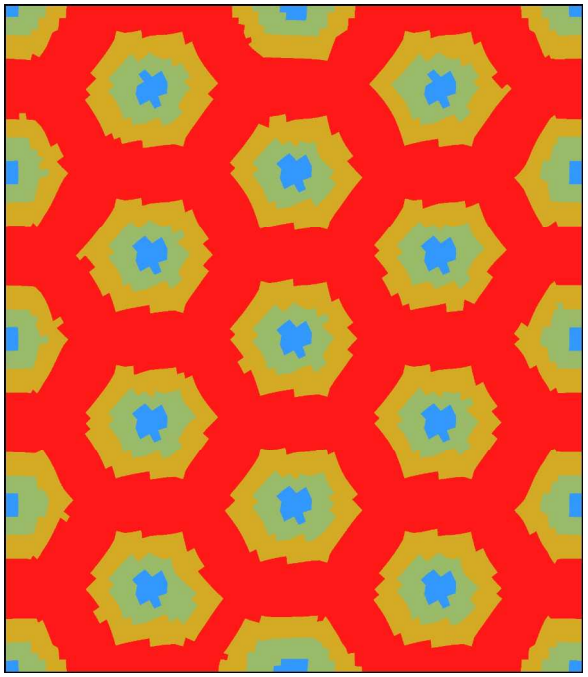
General Results

GND Density @ time=0



125μm

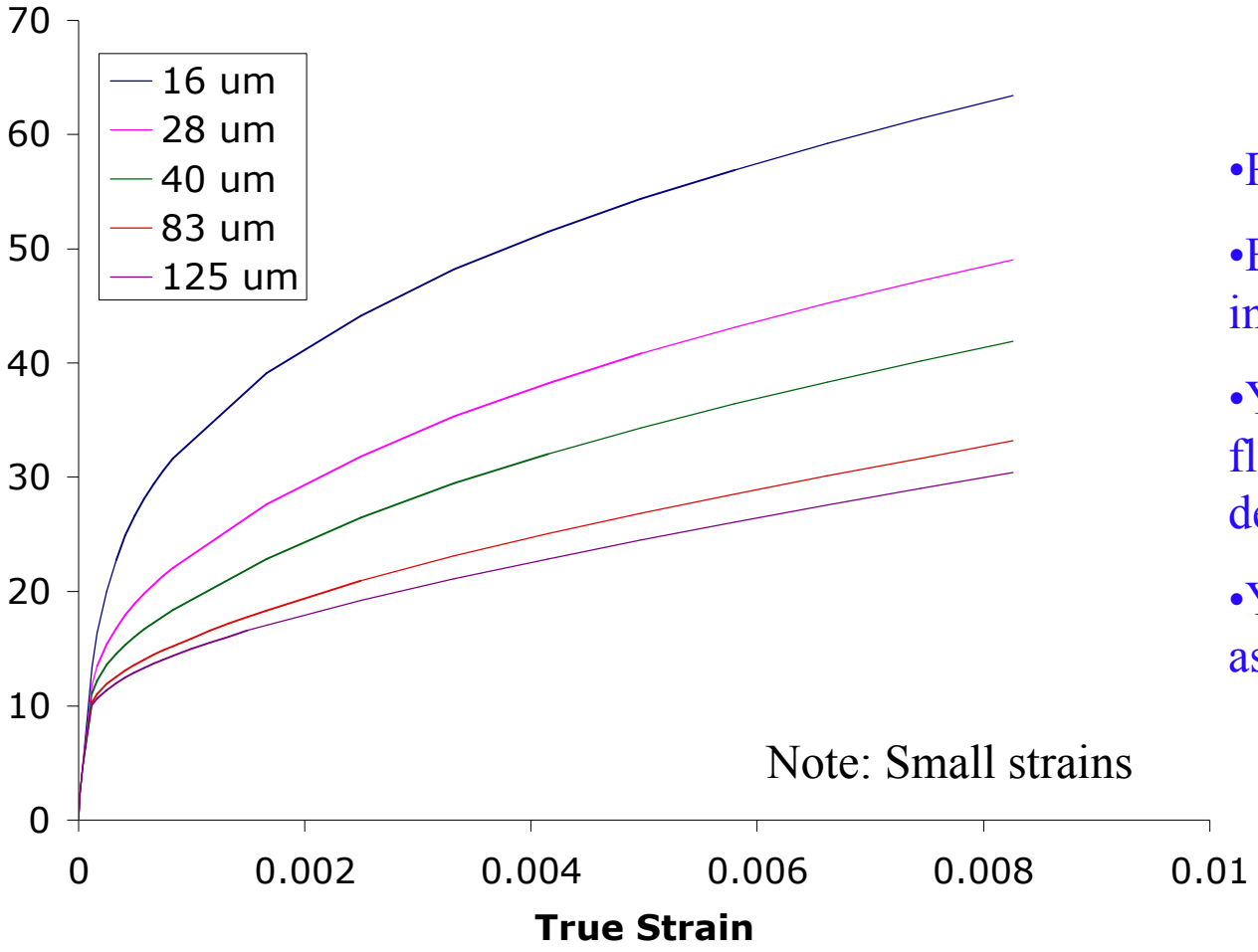




20μm

- Kinematics behind $\tilde{\mathbf{G}}_0^{\mathbf{NL}}$ ➡ initialize microstructure
  - Non-local approach ➡ length scale

General Results



- Realistic curve shapes.
- Elastic behavior is independent of grain size.
- Yield strength and plastic flow are grain size dependent.
- Yield strength increases as grain size decreases.

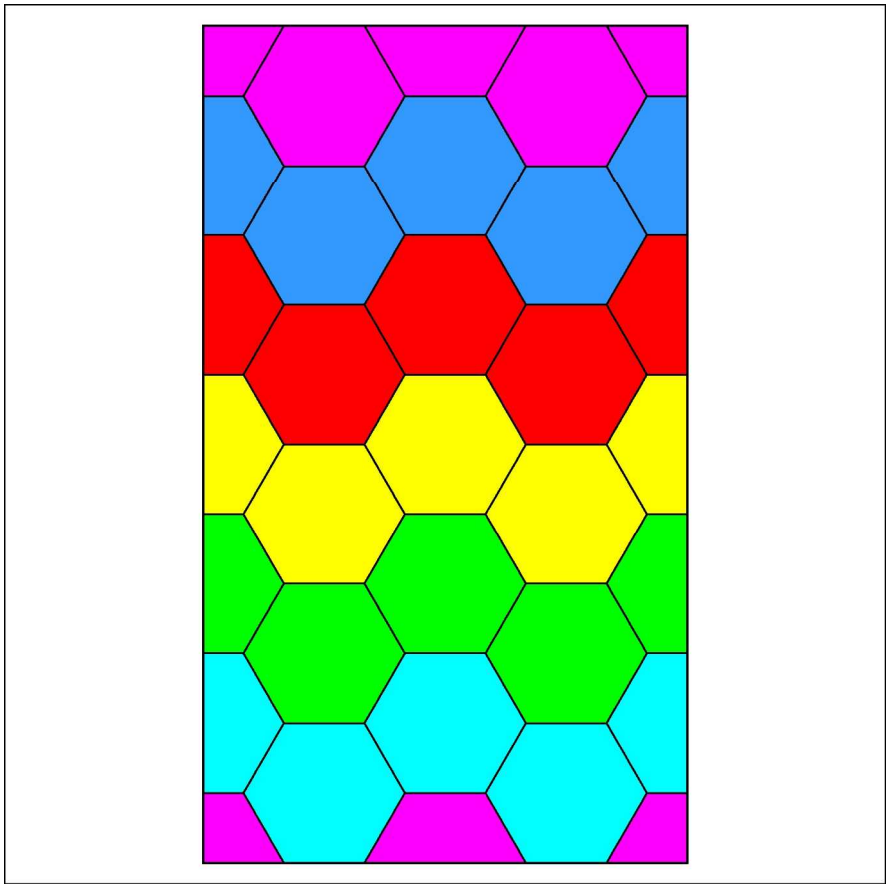
Results: Grain size effect

- 3 Different Grain Shapes
- Random Texture
  - 100 runs; data shows average
- Periodic BC in all directions

- Material ➡ Copper

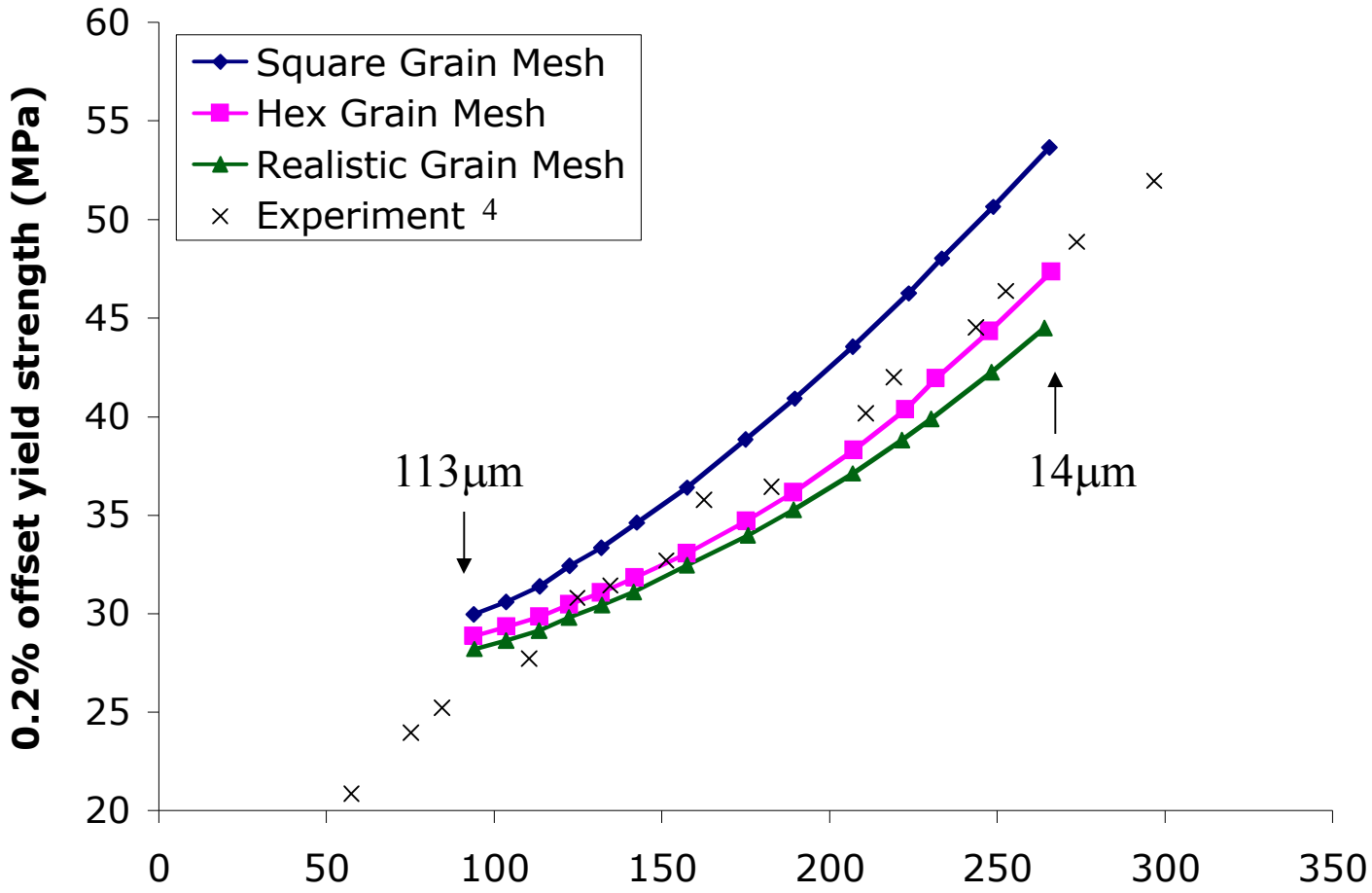
- 4 different mesh resolutions
  - 7000 - 34000 elements
- Convergence criteria
  - $\Delta\sigma_{ys} < 1\%$

- Fit experimental stress-strain curve with Hex mesh



- 24 Grain Polycrystal
- Equiaxed Grains

Results: Grain size effect



- Not a $d^{-1/2}$ dependence. Closer to a d^{-1} dependence.
- Grain morphology affects the grain size behavior

4. Hansen, 1982

Results: Misorientation

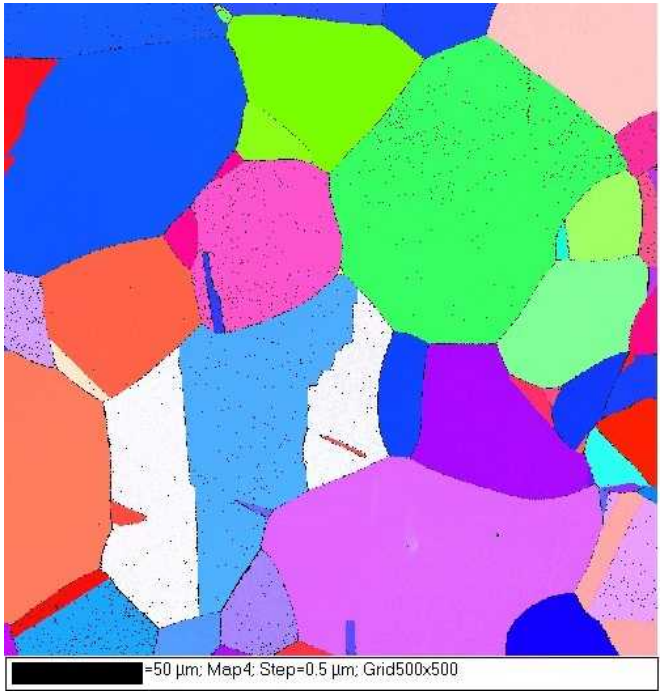
Experimental

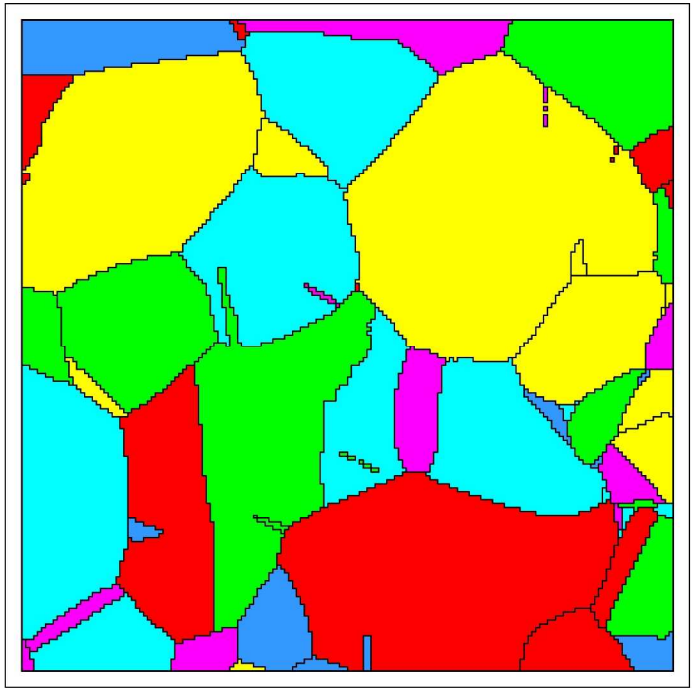
- Ni polycrystal
- Interrupted Tensile Test
- EBSD data @ same location
  - 0%, 1%, 5%, 10% Strain

Simulation

- Meshed the initial microstructure
- Ran both the local and non-local models to 10% strain

Initial Microstructure





Results: Misorientation

- Local Model: 0-10% Strain

QuickTime™ and a
MPEG-4 Video decompressor
are needed to see this picture.

Local Misorientation

- Within each grain
  - Calculate misorientation from 8 surrounding elements
  - Find the minimum misorientation in each grain
  - Re-calculate the misorientation from this minimum at each point

Results: Misorientation

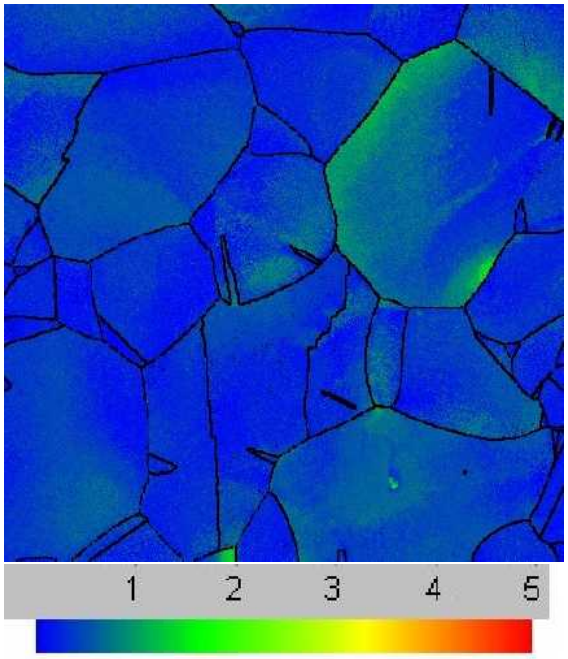
- Non-Local Model: 0-10% Strain

QuickTime™ and a
MPEG-4 Video decompressor
are needed to see this picture.

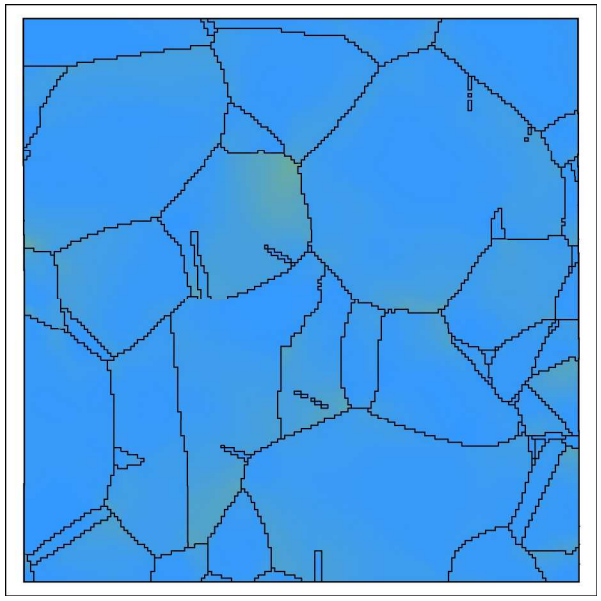
Hardened grain boundaries causes misorientation to accumulate

Results: Misorientation

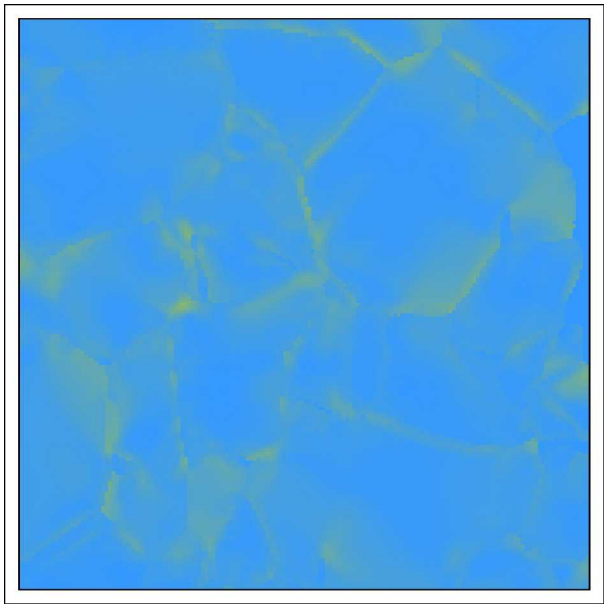
Comparison with experiment - 1%



Local Model

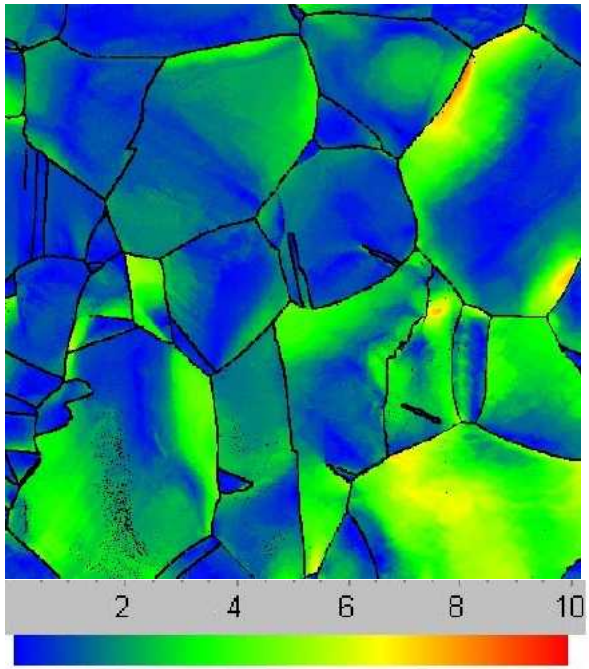


Non-Local Model



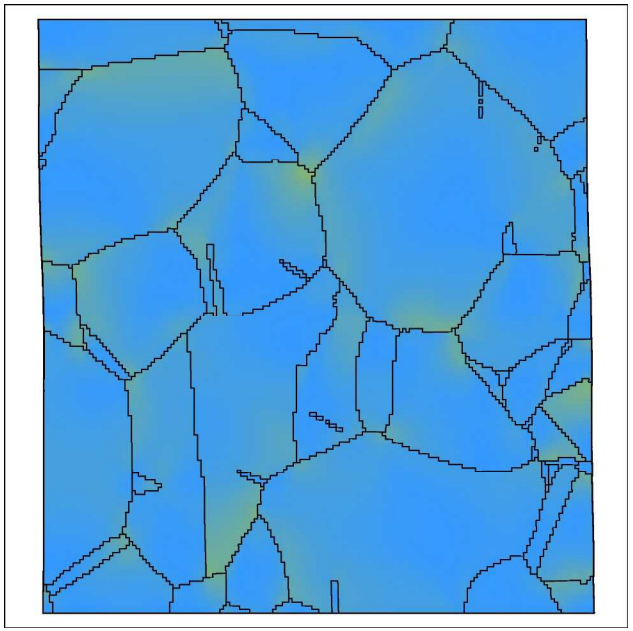
Results: Misorientation

Comparison with experiment - 5%



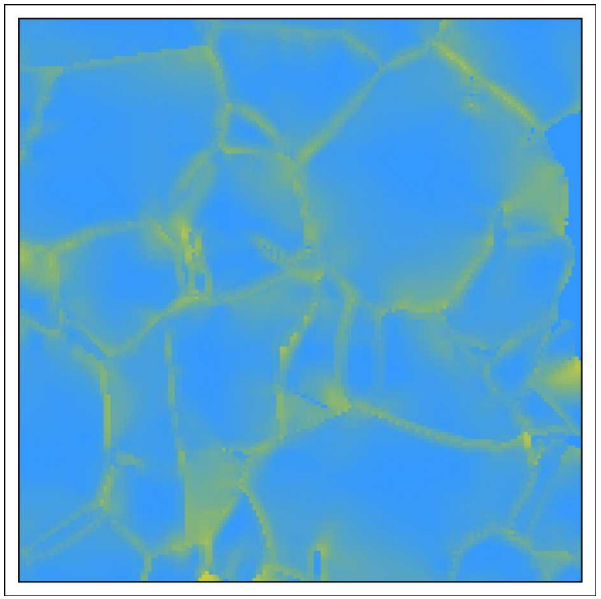
Local Model

- Underestimates



Non-local Model

- Too localized



Conclusions

- Shown that polycrystal kinematics provide a consistent approach to initializing grain boundary microstructure.
- Developed a non-local integral based model that predicts a grain size dependence of yield stress.
- Grain size dependence is closer to a d^{-1} than $d^{-0.5}$.
- Grain morphology affects the Hall-Petch behavior.
- Hardened grain boundaries causes misorientation accumulation.
- Local crystal plasticity model underestimates misorientation development, while the spatial distribution of misorientation is too localized in the non-local model.