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Predicting the Hall-Petch effect using non-local crystal plasticity

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Influence of microstructure…

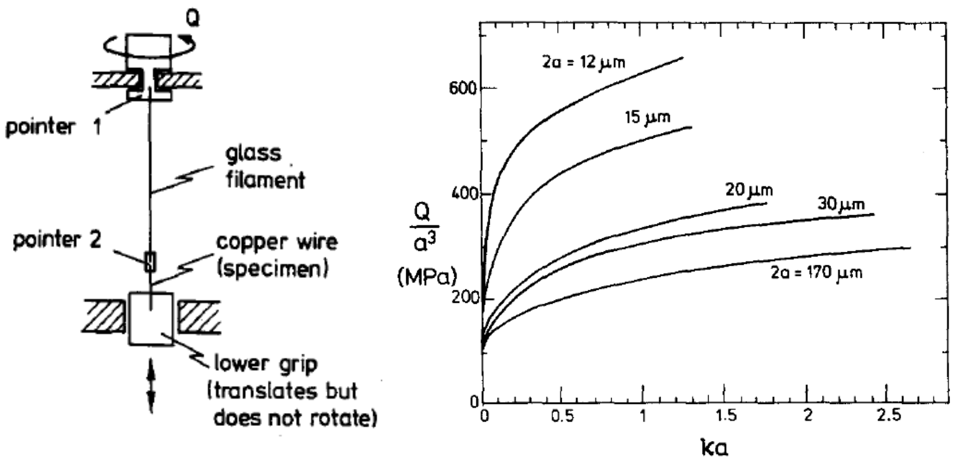
Specimen scale influences hardening

Microstructure scale influences yielding

Microstructure scale influences hardness

Microstructure scale does **not** affect hardening (very much)

Influence of microstructure…



[Fleck, *Acta Metall.*, 1994]

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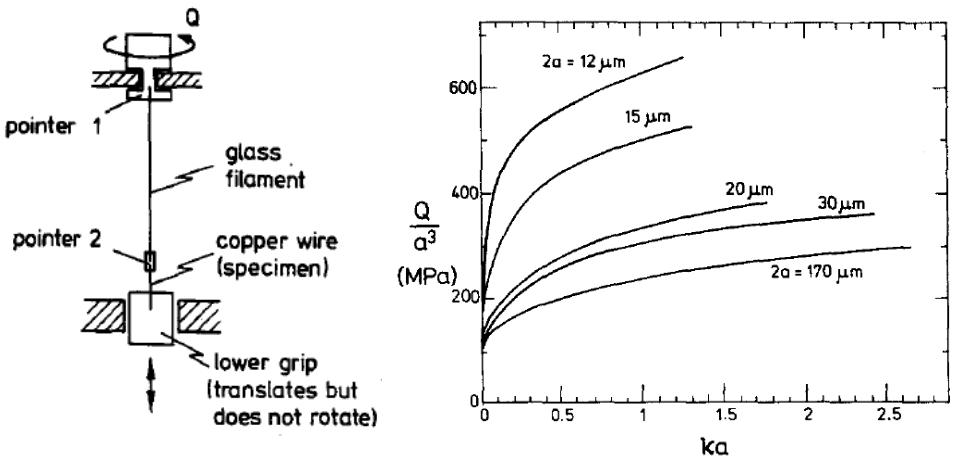
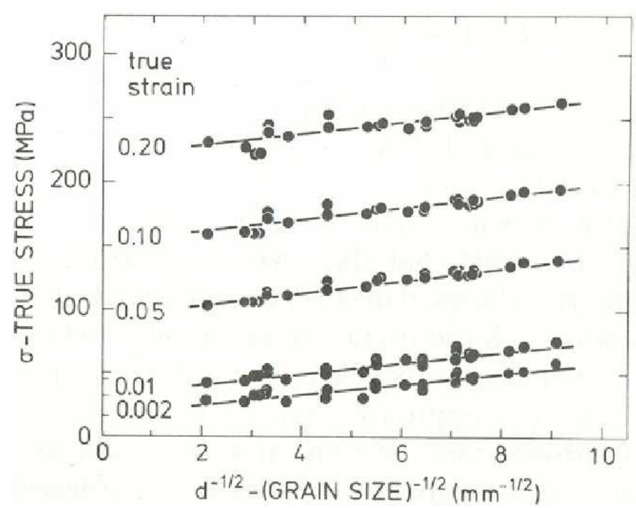
Influence of microstructure…



[Fleck, *Acta Metall.*, 1994]



[Hansen, *Yield Flow and Fracture of Polycrystals*, 1983]

[Hall, *Proc. Phys. Soc. London B*, 1951 ; Petch, *J. Iron and Steel Inst*, 1953]

Microstructure scale influences hardness

Microstructure scale does **not** affect hardening (very much)

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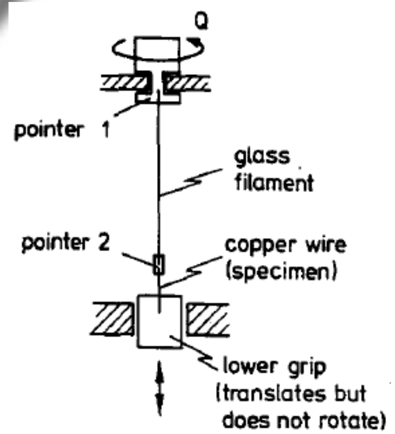
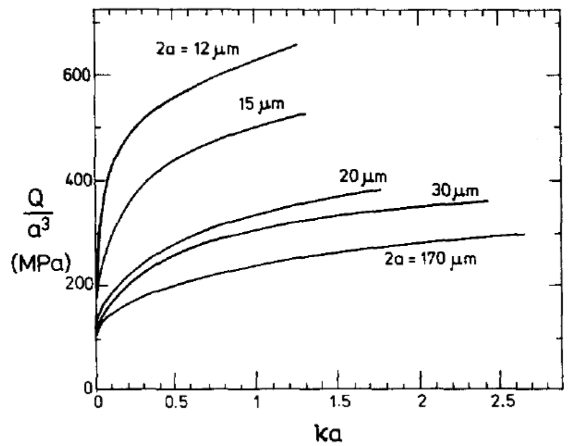
Influence of microstructure…





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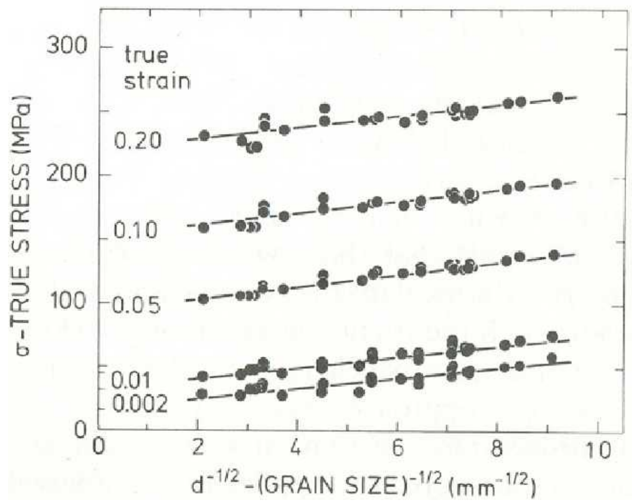

[Hansen, *Yield Flow and Fracture of Polycrystals*, 1983]
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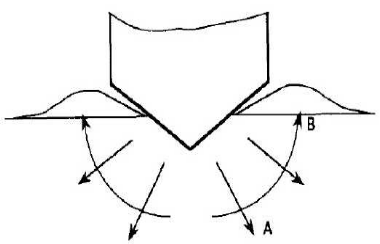
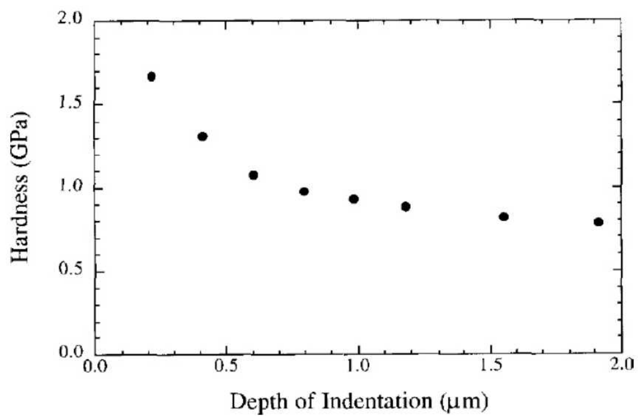
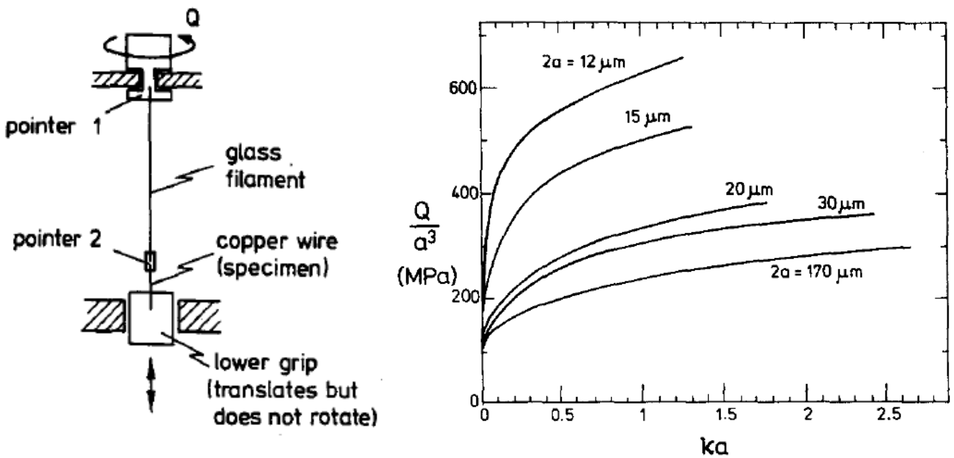




[McElhaney, *JMR*, 1998]

Microstructure scale does **not** affect hardening (very much)

Influence of microstructure…



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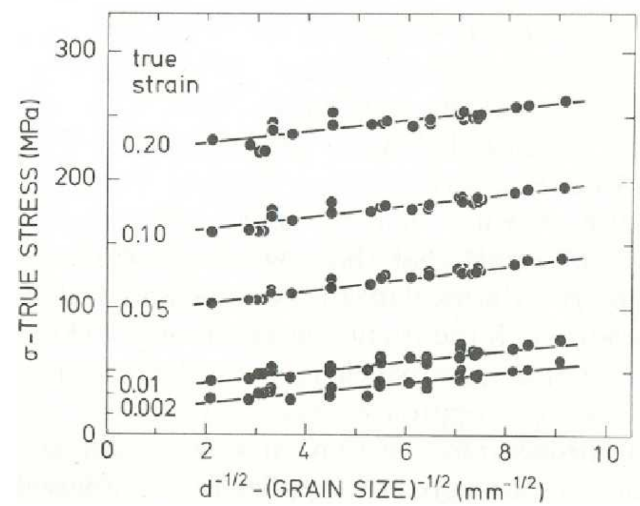
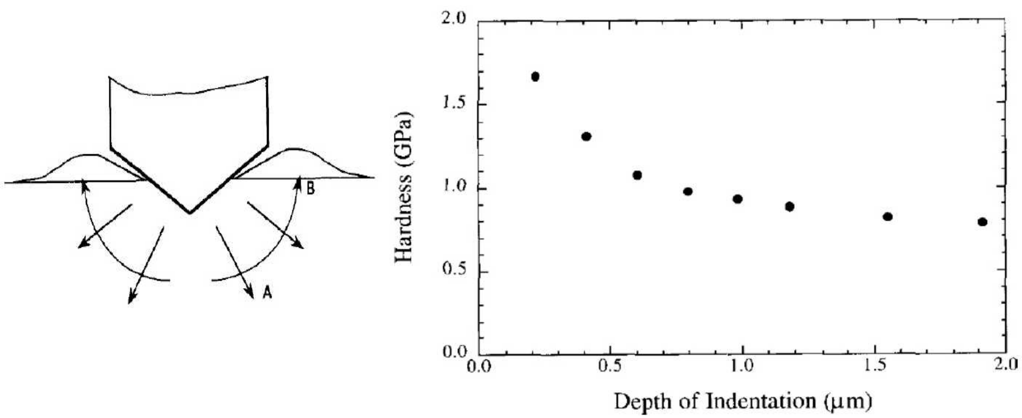


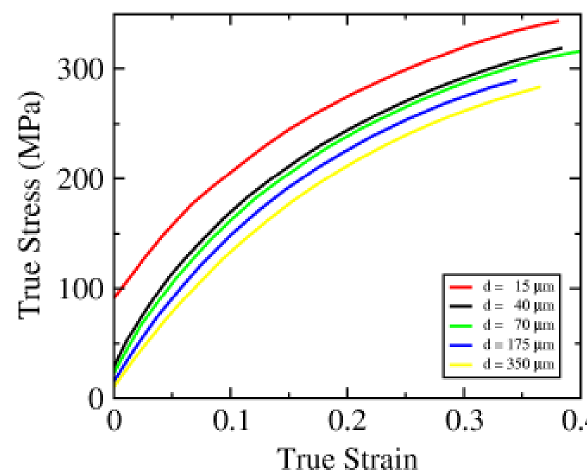
[Hansen, *Yield Flow and Fracture of Polycrystals*, 1983]

[Hall, *Proc. Phys. Soc. London B*, 1951 ; Petch, *J. Iron and Steel Inst*, 1953]

*Mechanical response of materials **depends on the microstructure** of the material*



[McElhaney, *JMR*, 1998]



[Feaugas, *Met. Trans*, 2003]

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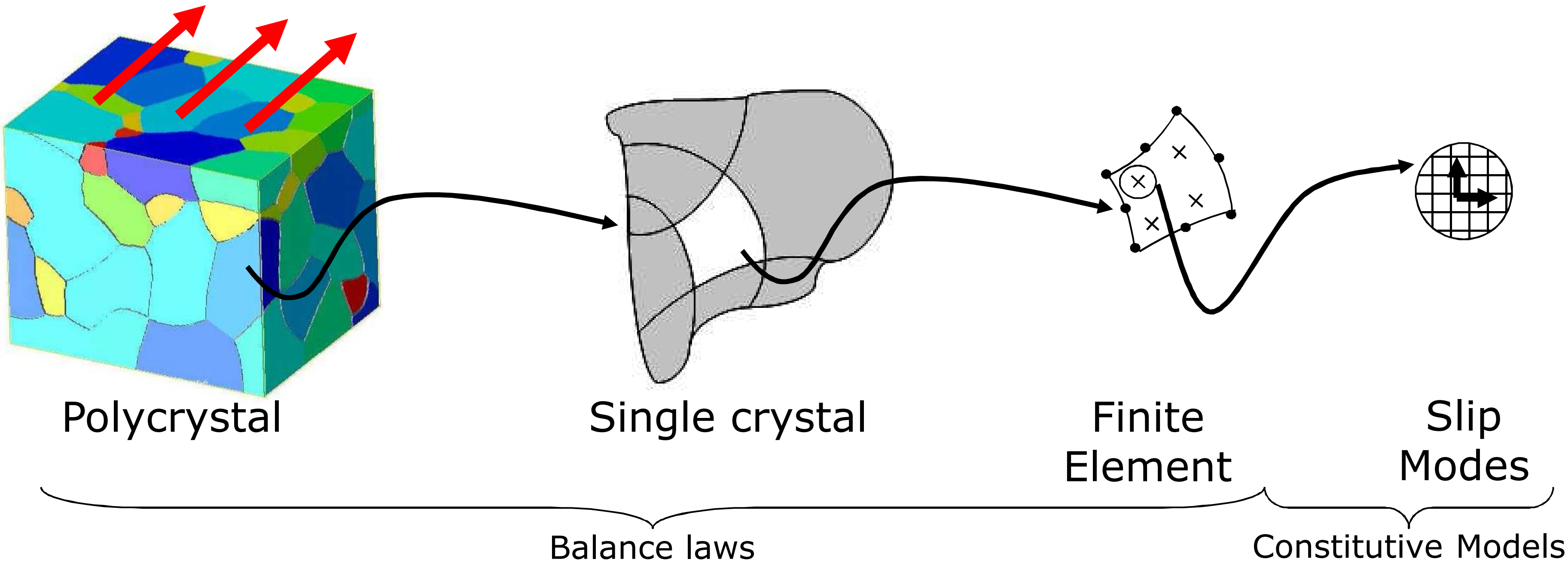
…captured by crystal plasticity…

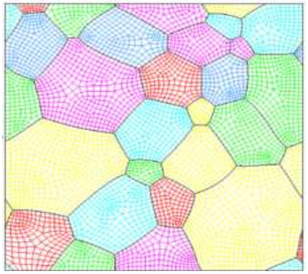
- Crystal plasticity = **Grain-level (mesoscale) approach** to materials modeling using multiscale strategies
- Explicitly model **discrete** grains and slip systems (anisotropy, texture evolution,…)



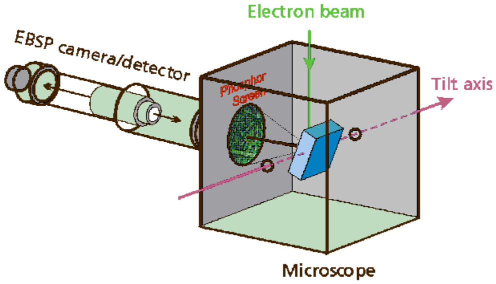
→ **Advantage:** predictive and robust theoretical framework to understand polycrystal behavior

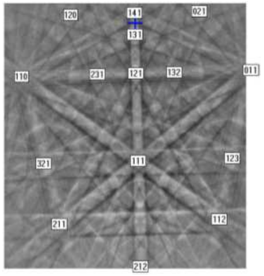
→ **Limitation:** due to high # of ISVs (computational cost) difference in length scale: discrete vs. continuum

…with desired features



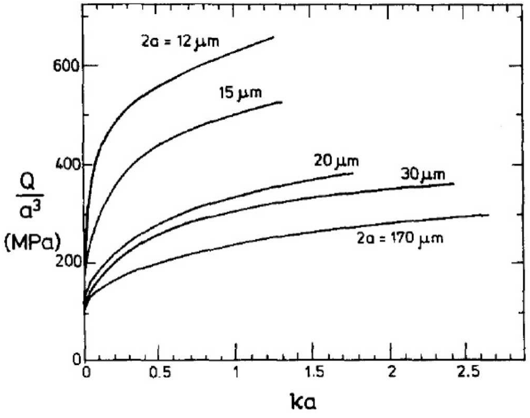
FEM / Crystal Plasticity
(grain level structure)



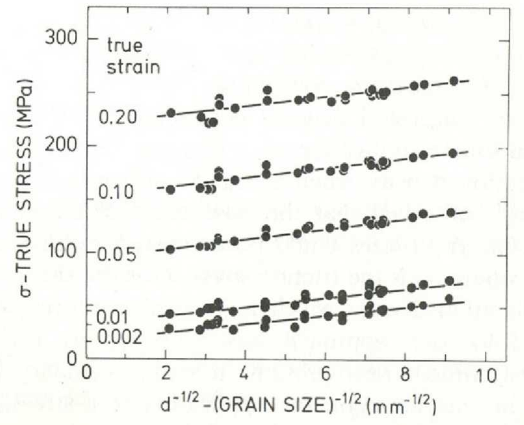


Experimental testing
(continuum mechanics)

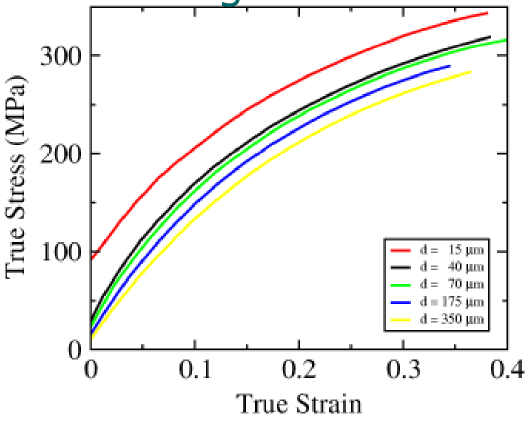
Predicts sensitivity to length scale



Predicts Hall-Petch effect



(Relative) insensitivity of hardening to microstructure



→ Focus on capturing the correct phenomenology
→ Permit extension to existing constitutive foundation
→ Permit implementation into existing finite element codes

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Topic of discussion

- Influence of microstructure…
- …captured by featured crystal plasticity approach
- Crystal Plasticity:
  - An augmented kinematic description
  - Capturing length scale with non-local formulation
- Application:
  - Predicting Hall-Petch effect in FCC metals
  - Crystallographic reorientation and local comparison with EBSD
- Summary and future perspectives…

Crystal Plasticity

A little bit of theory…

Conventional formulation...

Kinematics $\mathbf{L}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p^{-1}} = \sum_{a=1}^{N_{sys}} \dot{\gamma}^a \left(\bar{\mathbf{s}}^a \otimes \bar{\mathbf{m}}^a\right)$

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

Slip evolution $\dot{\gamma}^a = \dot{\gamma}_0 \left|\dfrac{\tau^a}{\tau^{\alpha}_{CRSS}}\right| \mathrm{sgn}\left(\tau^a\right)$

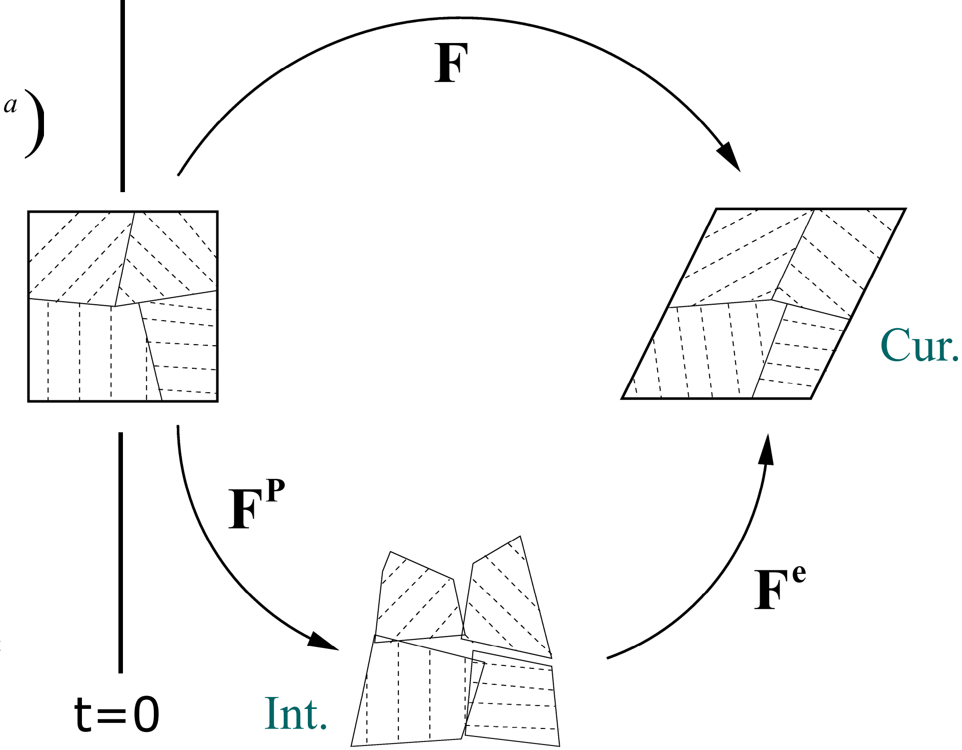
(Power law viscoplastic flow rule)

Hardening law $\tau^a_{CRSS} = C\mu b\sqrt{\rho^a}$
(Anisotropic Taylor hardening)

Dislocation density evolution
(Static and dynamic recovery)

$$\frac{\mathrm{d}\rho^\alpha}{\mathrm{d}\gamma^\alpha} = \mathrm{c}_1\sqrt{\rho^\alpha} - \mathrm{c}_2\, \rho^\alpha$$

Conventional kinematics describe the deformation, starting from a reference polycrystal



[J.W. Hutchinson, (1970) "Elastic-plastic behaviour of polycrystalline metals and composites", Proc. Roy. Soc. Lon., 319 p.247]
[Estrin and Mecking, *Acta Met.* 32 (1984) p.57]

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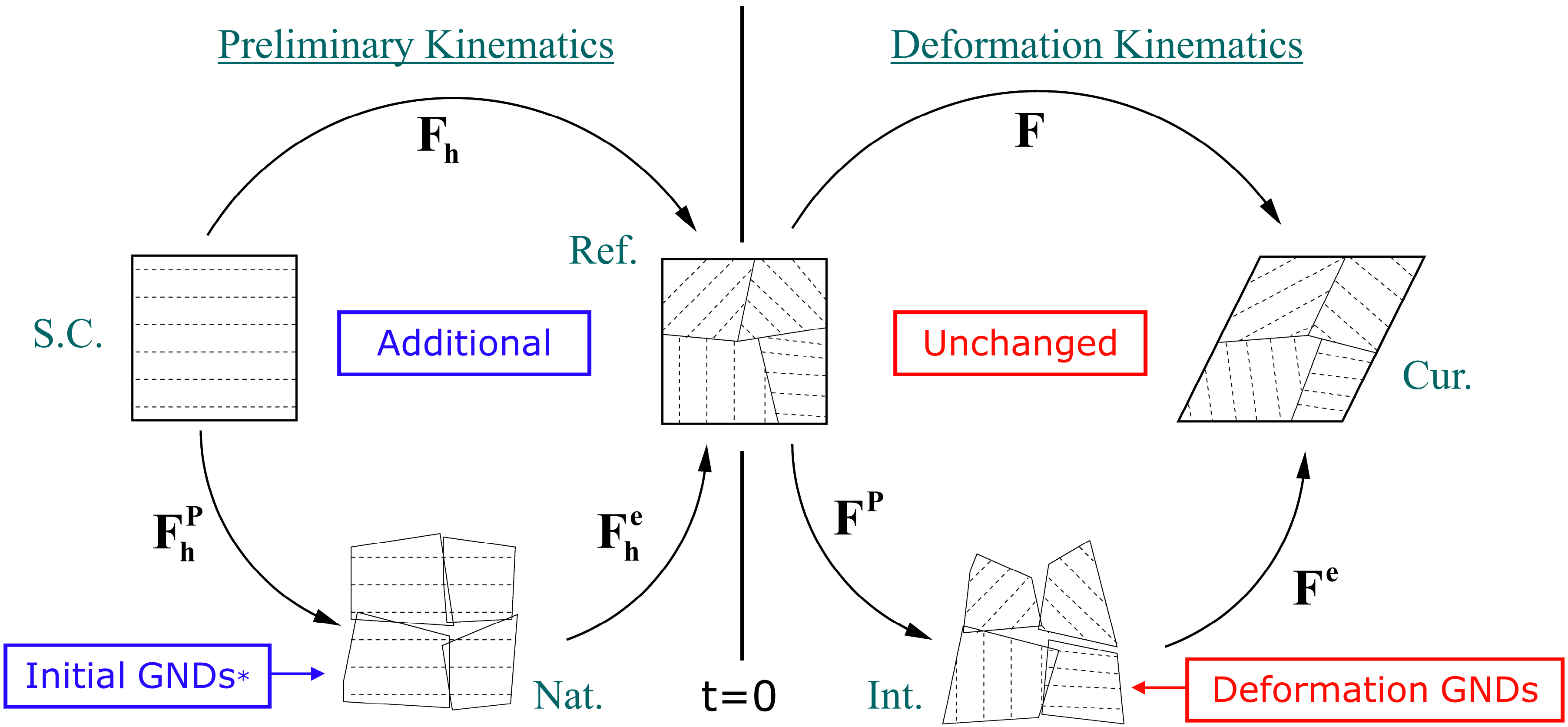
… with an augmented kinematics

Accounting for initial microstructure

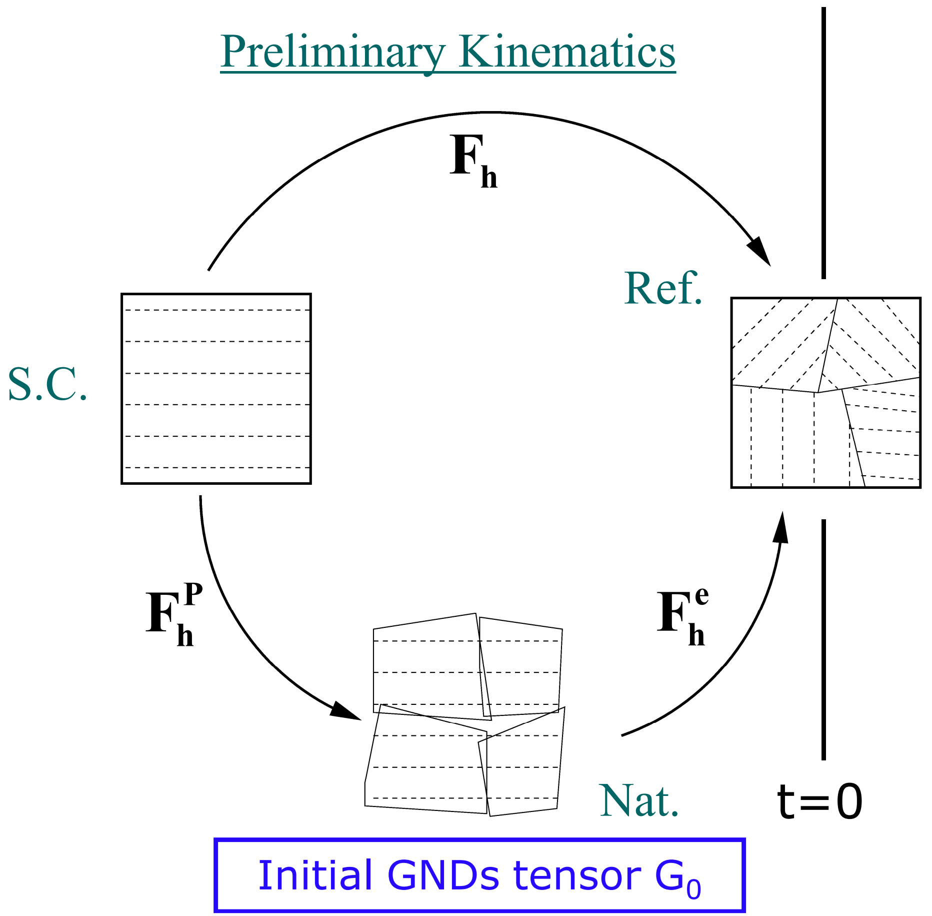
→ Based on a **geometric argument**
→ Introduce a ***fictitious* deformation** relative to a hypothetical single crystal
→ Establish crystal rotations necessary to produce grain boundaries (GBs)

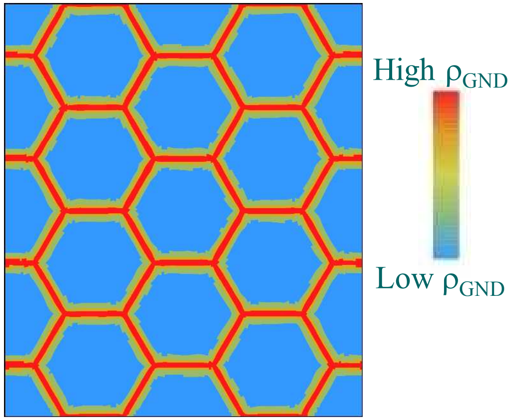


*Geometrically Necessary Dislocations

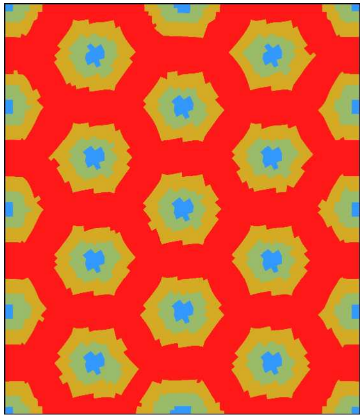
Initial microstructure

Smaller grains generate a higher fraction of "hard" material nearby





125μm



20μm

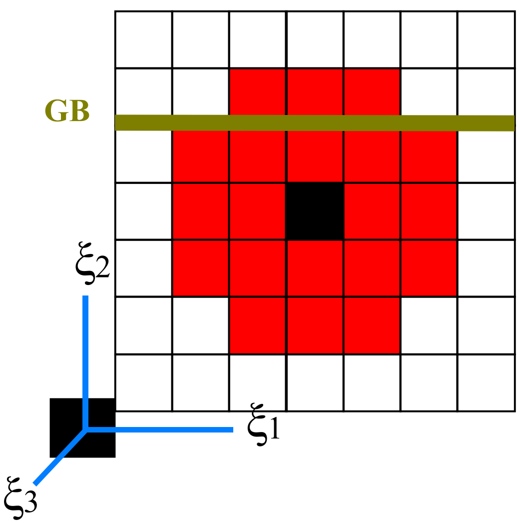
Non-local formulation

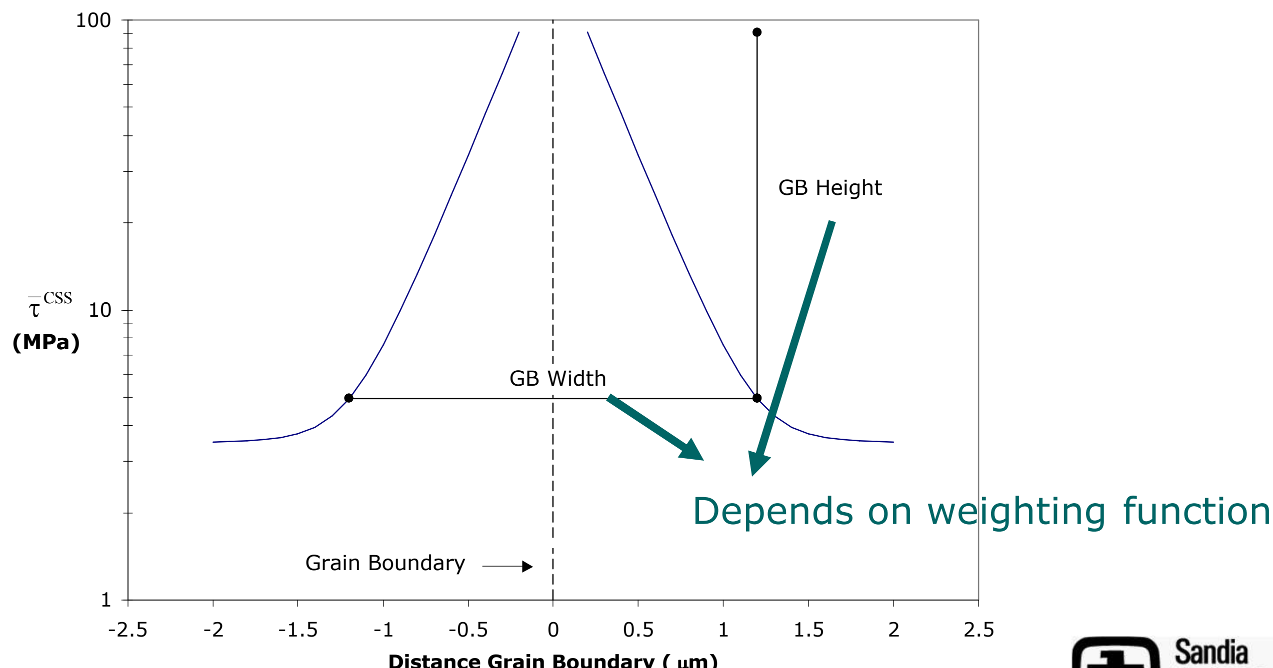
Modeling length scale phenomena with non-local integral method

→ Weighted average integral formulation for GND tensor

$$\{\mathbf{G}\}(\mathbf{x}) = \frac{1}{V_{cell}} \int \Theta(\mathbf{x},\xi)\mathbf{G}(\xi)\,d\xi$$

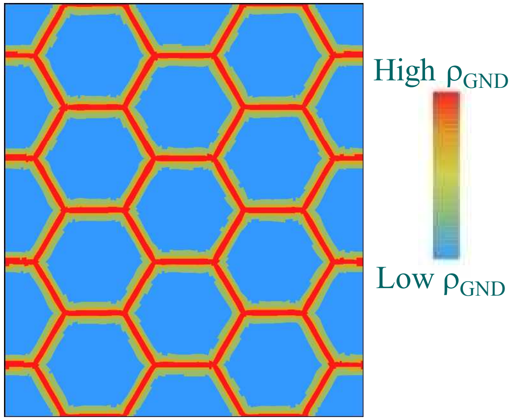
→ Length scale enters as a material parameter (defines weighting function)





Capturing a length scale effect

Preliminary kinematics



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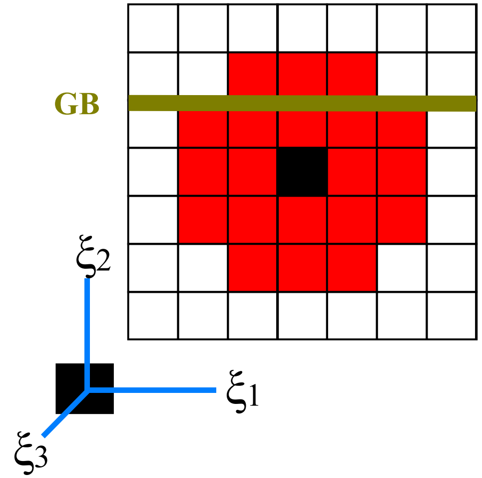
Non-local integral method



Kinematics behind $\mathbf{G}_0$ → Initialize microstructure

Non-local approach → Length scale

Impact hardening law → $\tau^{a}_{CSS} = CG_{110} b \sqrt{\rho^{a}_{GND} + \rho^{a}_{SSD}}$

<u>Non-local formulation of GND evolution</u>

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

(Harder strength as one approaches the GB)

<u>SSD evolution equation</u>

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

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Application

Predicting the Hall-Petch effect in FCC metals

[W.A. Counts (2006) "Predicting the Hall-Petch effect in FCC metals using non-local crystal plasticity", ***PhD Dissertation,*** **GIT]**

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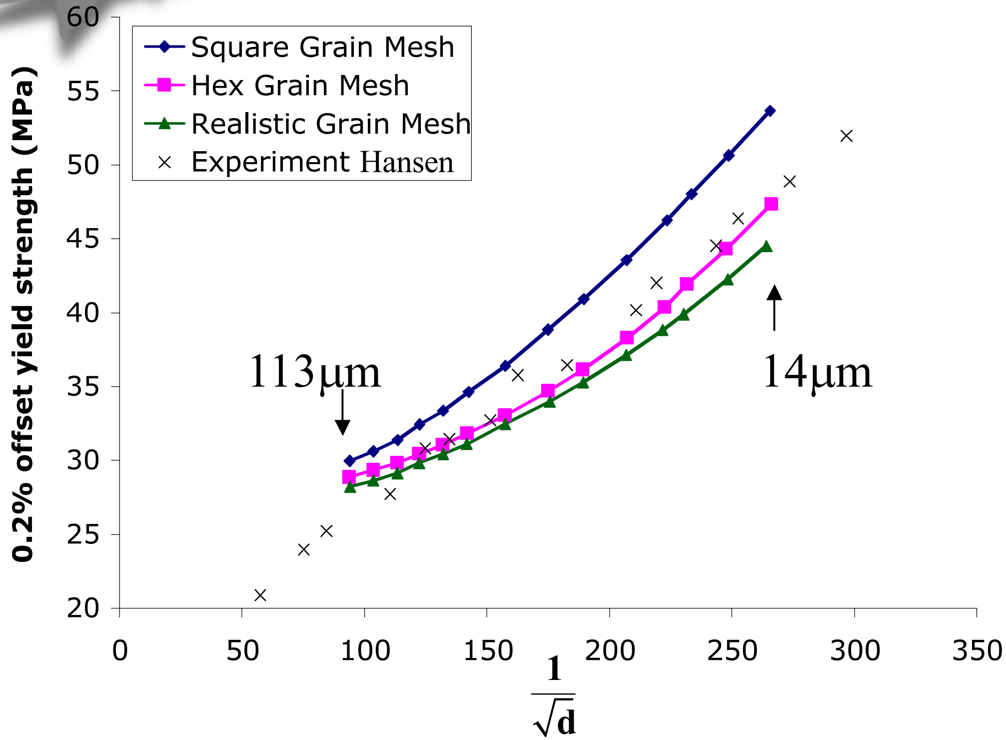
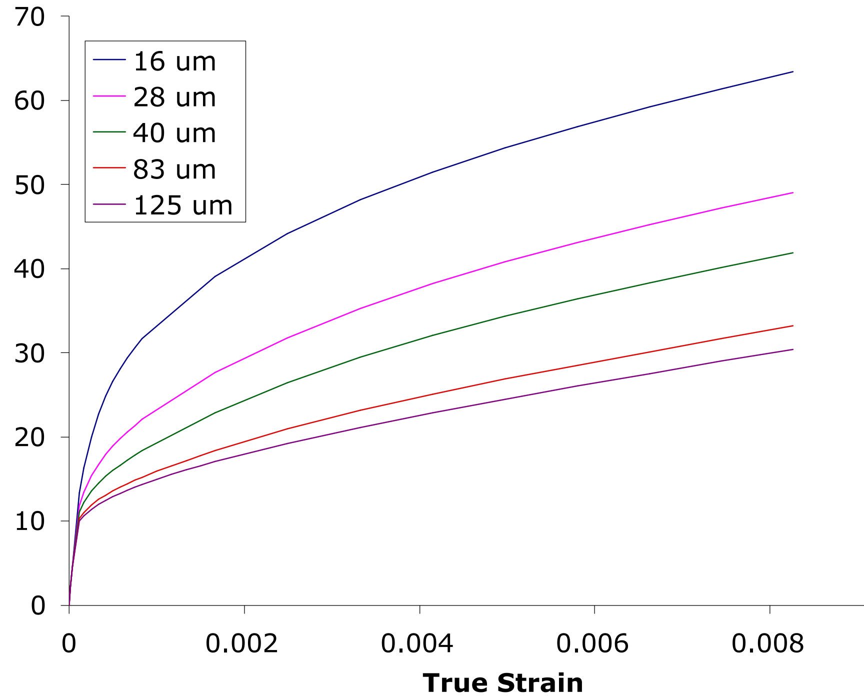
Predicting the Hall-Petch effect





- Implemented with GND initialization (Accounts for initial microstructure)
- Integral (Non-local formulation) of GND densities provides length scale
- Elastic behavior is independent of grain size
- σ-ε curves stacked on top of each other
- Yield strength increases as grain size decreases
- Predicts Hall-Petch behavior with dependence 1/*d*

[Hansen, *Yield Flow and Fracture of Polycrystals*, 1983]

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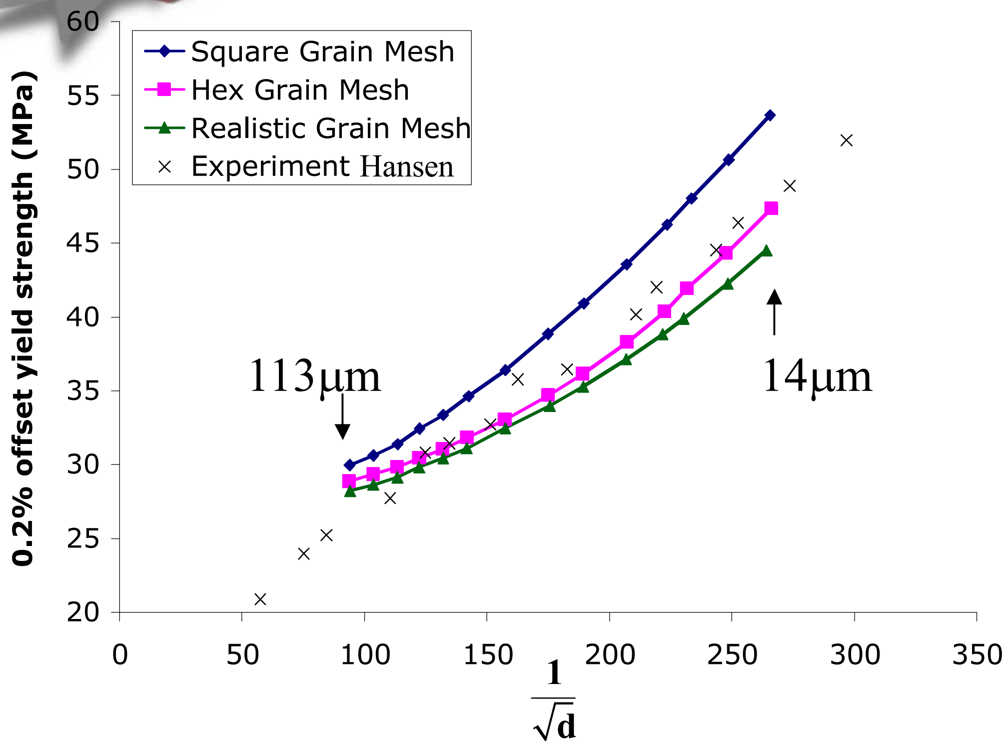
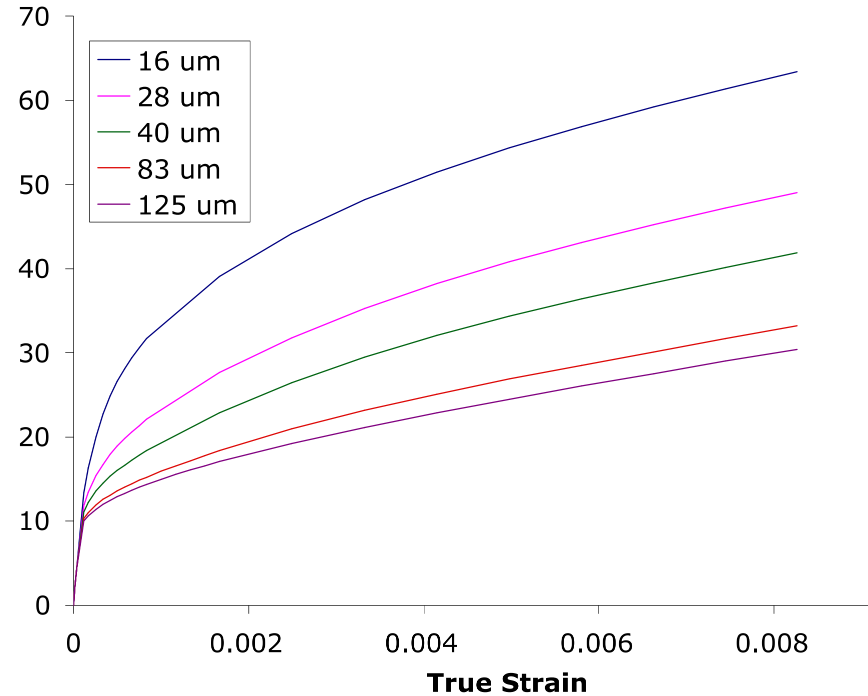
Predicting the Hall-Petch effect





Non-local model produces **continuum** level results that resemble experiments

…but what about the **micro-scale**??

[Hansen, *Yield Flow and Fracture of Polycrystals*, 1983]

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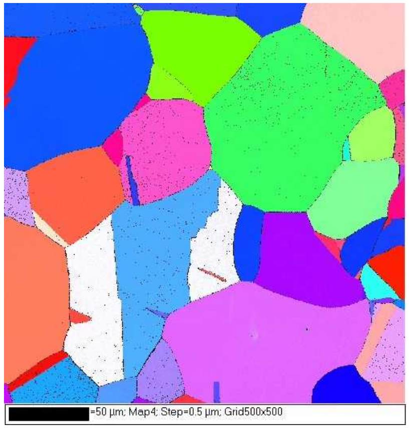
Microstructural Plasticity Evolution

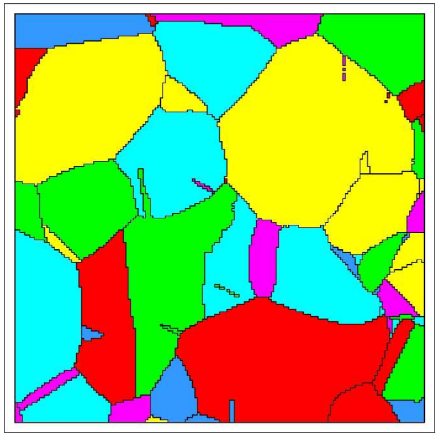
Experimental

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



Numerical simulation

- Initial microstructure meshed from EBSD map
- Local / Non-local models to 10% strain
- Periodic boundary conditions
  : columnar structure



Comparison

→ Local microstructural distribution of misorientation (LIMIS)
→ Overall average intra-grain misorientation (AMIS)

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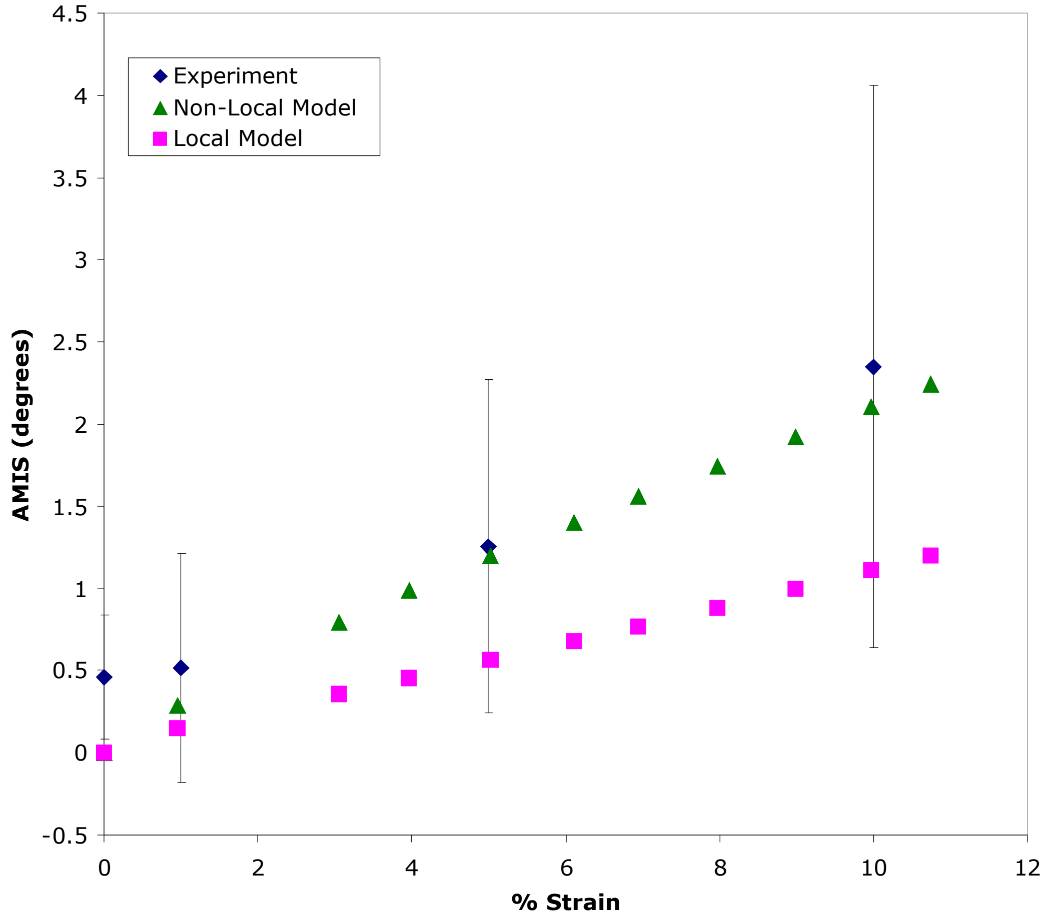
*Electron backscattered diffraction

Average misorientations



→ Average misorientations are predicted well by the non-local formulation

→ Large experimental error bars due to the relatively small number of grains samples (<100)

→ AMIS values for local model lower than experimental value

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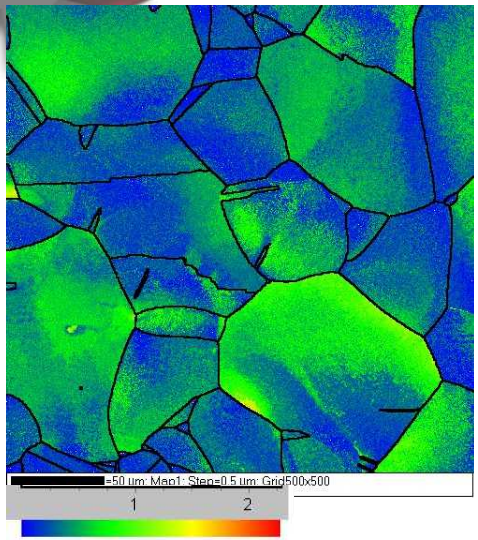
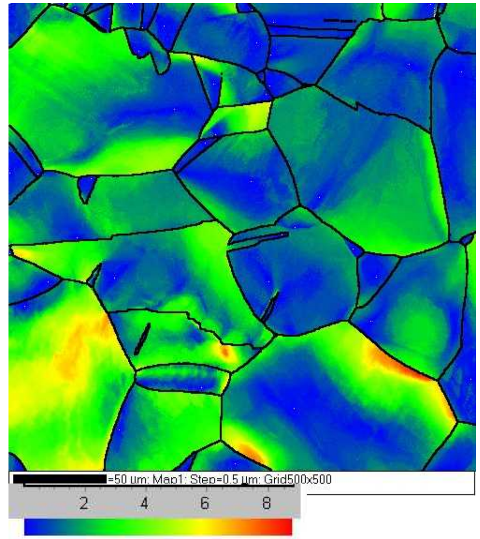
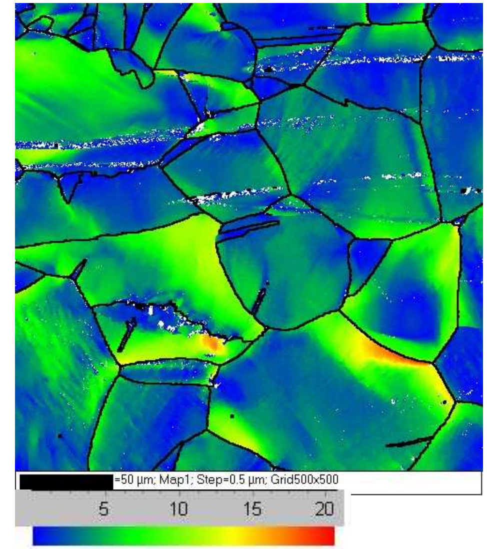
Local intra-grain misorientation

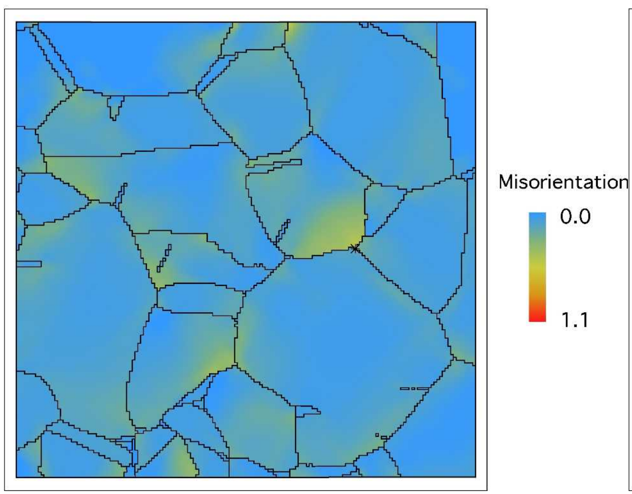




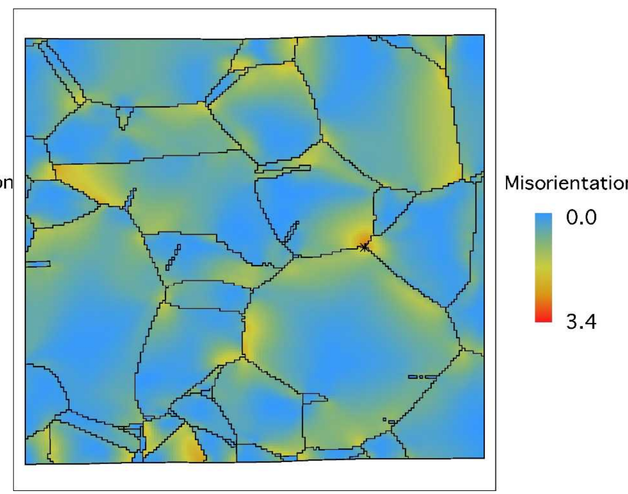


Local formulation → <u>Underestimate</u> local misorientation

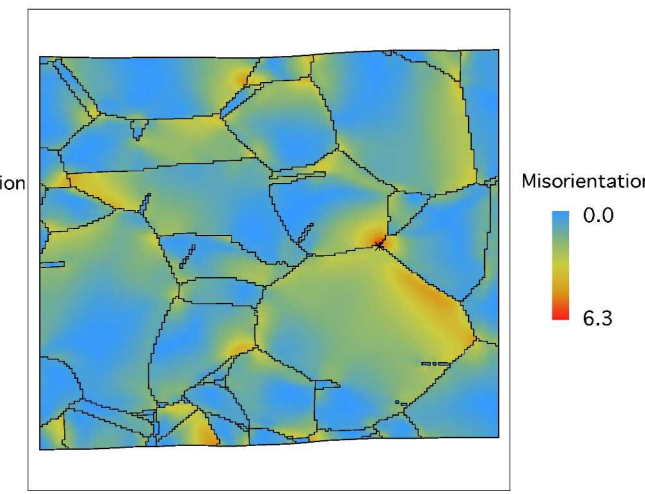
1% Strain



5% Strain



10% Strain



[units in degrees]

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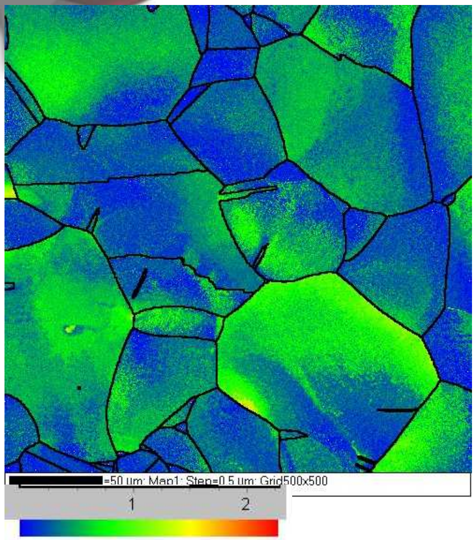
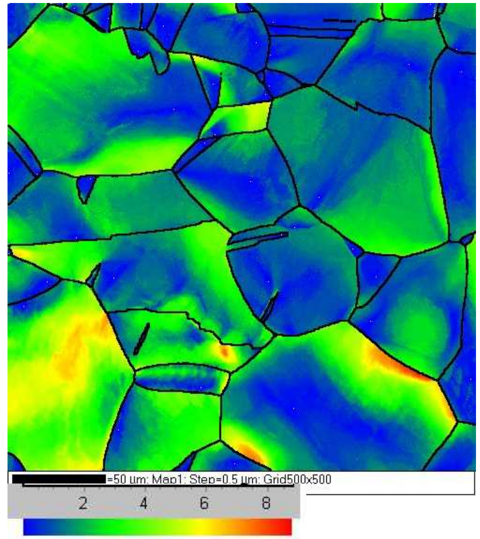
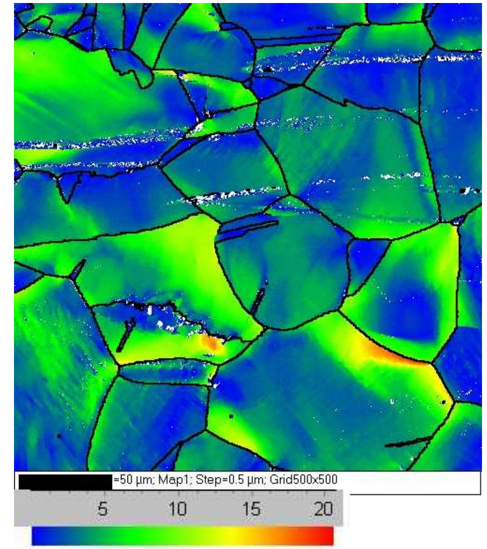
Local intra-grain misorientation

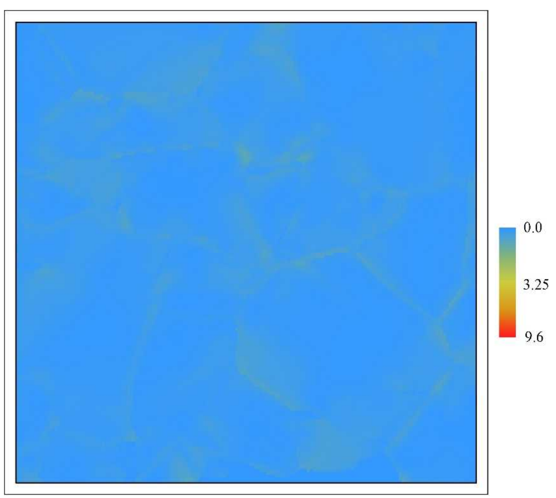




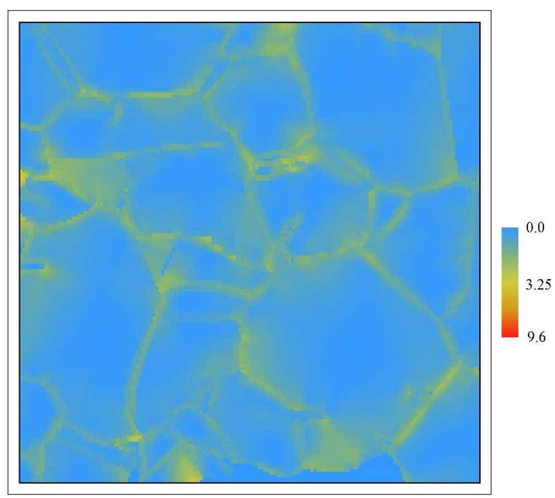


Non-Local formulation → Misorientation <u>too localized</u>

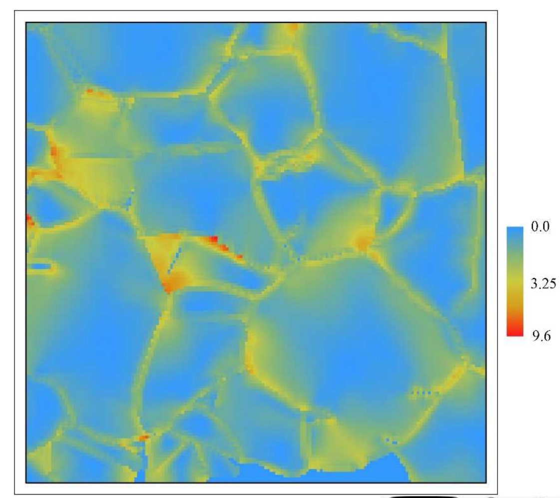
1% Strain



5% Strain



10% Strain



[units in degrees]

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Summary and recommendations

What we’ve learned…
What can be done…

What we learned…what's next?

• **Take away**

- Polycrystal kinematics provide a **consistent approach to initializing grain boundary microstructure**

- Non-local formulation predicts a **grain size dependence of yield stress**

- Grain morphology affects the Hall-Petch behavior

- Hardened grain boundaries causes misorientation accumulation

- Non-local model **reproduces**, with reasonable accuracy, **macroscale quantities** (s-e curves, AMIS)

- **Limited agreement locally**: Local crystal plasticity model underestimates local misorientation development, while the spatial distribution of misorientation is too localized in the non-local formulation

• **Future perspective**

- Grain boundary behavior

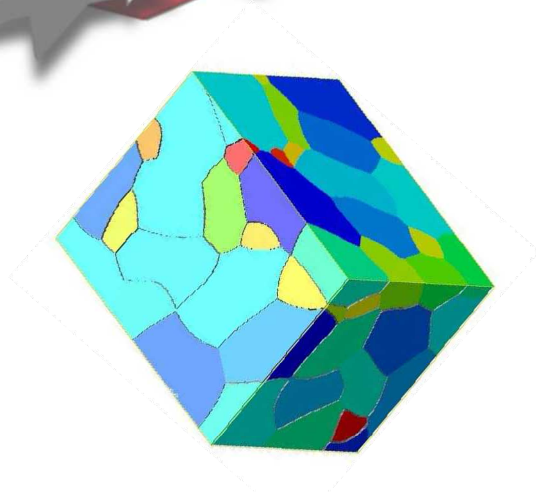
- Flow rule (power law vs. thermally activated for example)

- Hardening law (phenomenological vs. micromechanics)

- Boundary conditions (homogeneous vs. experimental)

- RVE (statistically representative vs. columnar structure)

Thank you for your attention



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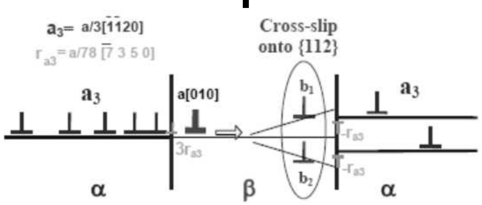

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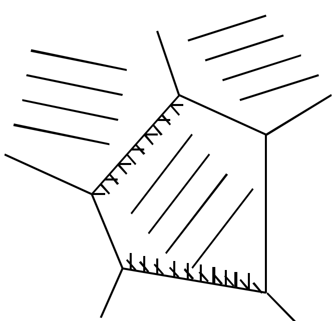

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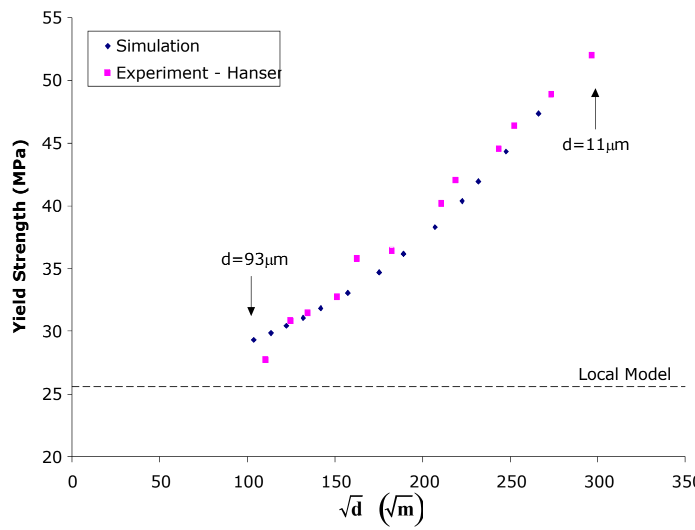

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