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SAND2011-7144C

Evolution of Microstructure in the Deformation of Nanocrystalline Metals

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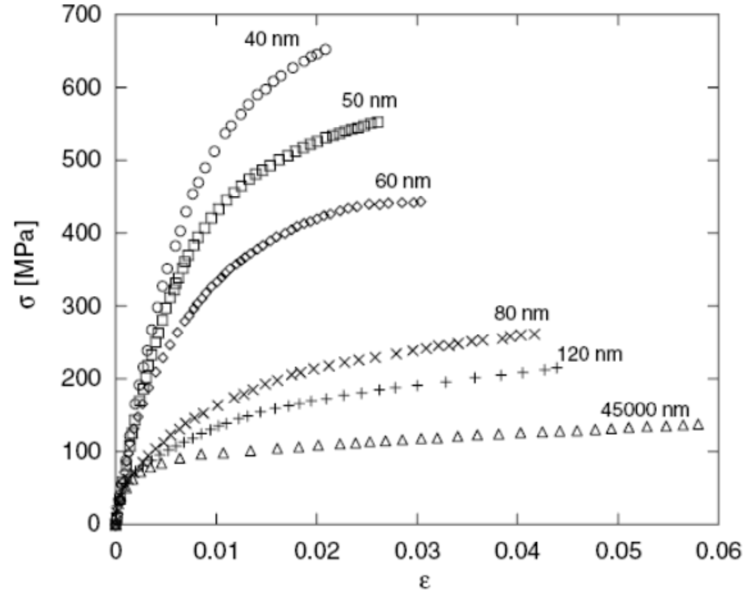
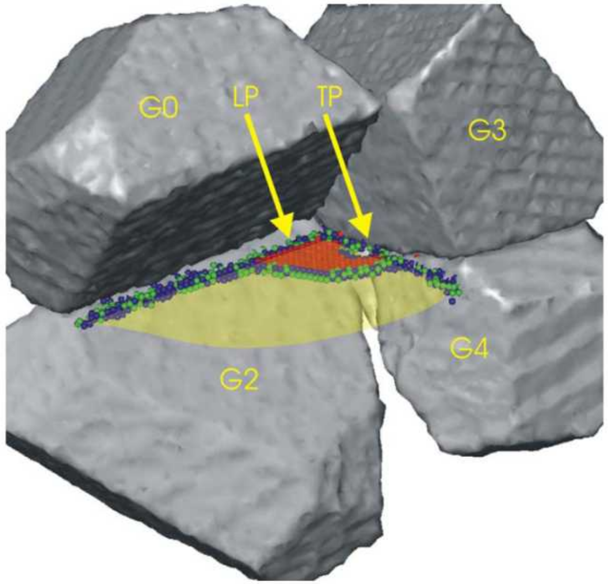
SES 2011, October 12-14, 2011

Introduction

- Mechanical properties of nanocrystalline (NC) materials show potential improvement compared to larger grained polycrystalline materials (e.g., yield strength, fracture/fatigue resistance, and superplasticity).
- In NC materials, a higher number density of atoms are located in grain boundary (GB) regions.
- A deeper understanding of the role of interfaces (e.g., GBs) in NC deformation processes is still needed.

Important to understand influence of GBs and related deformation mechanisms in nanoscale plasticity

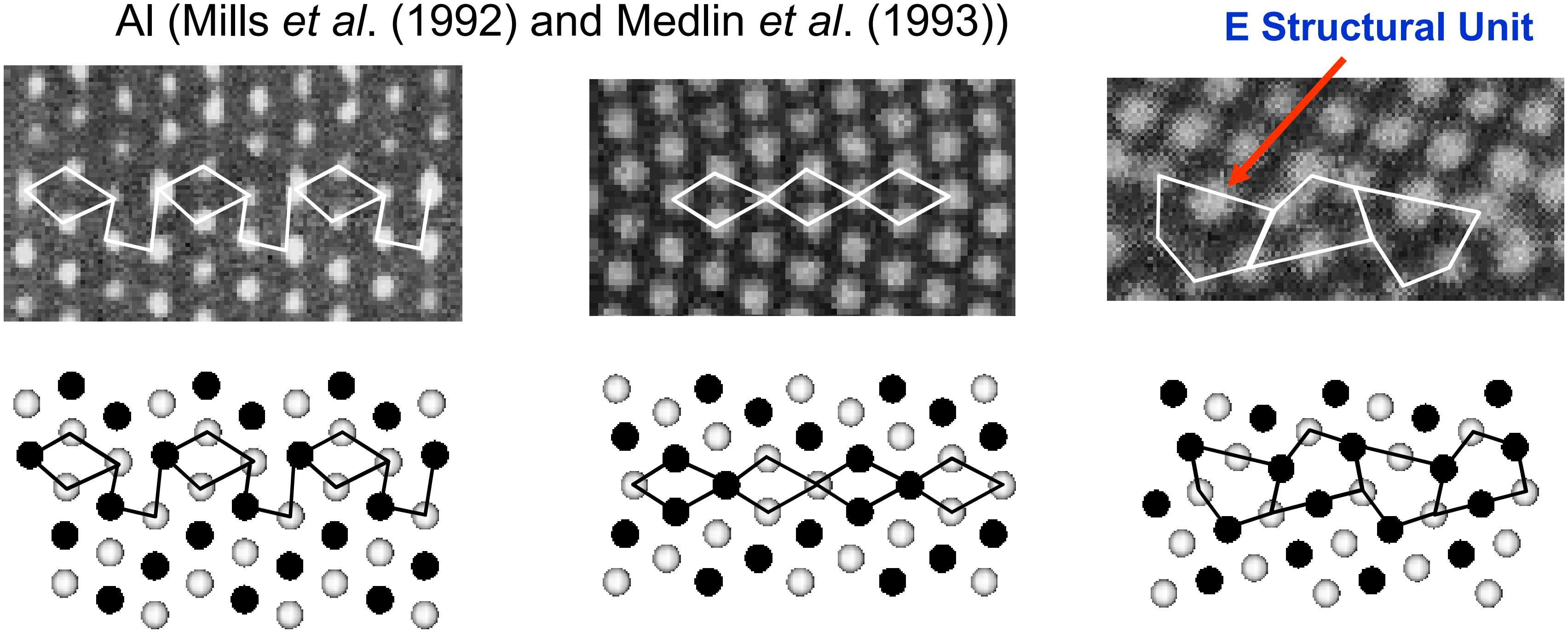




Khan et al., IJP, 22 (2006).
Van Swygenhoven et al., Acta Mat., (2006).

Bicrystal Studies: Preface to NC Materials

- Interface structures are in agreement with published HRTEM data, e.g. Al (Mills *et al*. (1992) and Medlin *et al*. (1993))

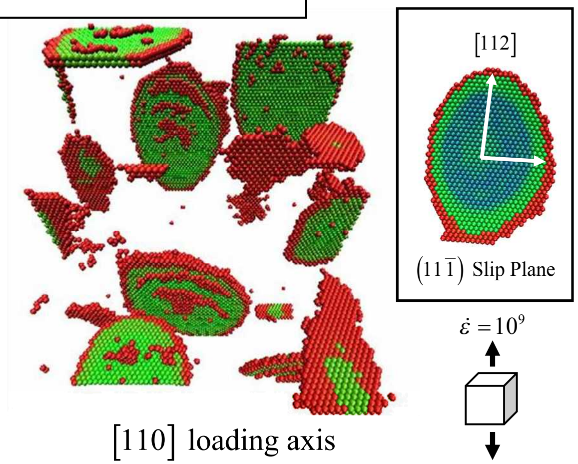


Σ3 (112) 70.5°   Σ11 (113) 50.5°   Σ9 (221) 141.1°

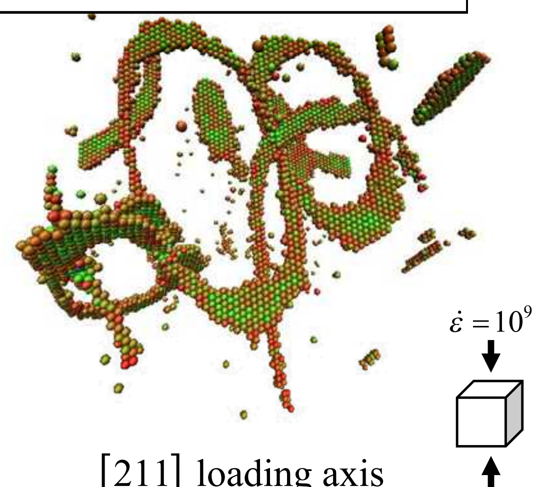
- General (high-angle) interface structure
  - ➢ Structural unit model (SUM) (Sutton and Vitek, 1983)
  - ➢ High-angle grain boundaries are composed of combinations of structural units from 'favored' orientations

Dislocation Nucleation in Cu: Tension-Compression Asymmetry

TENSION

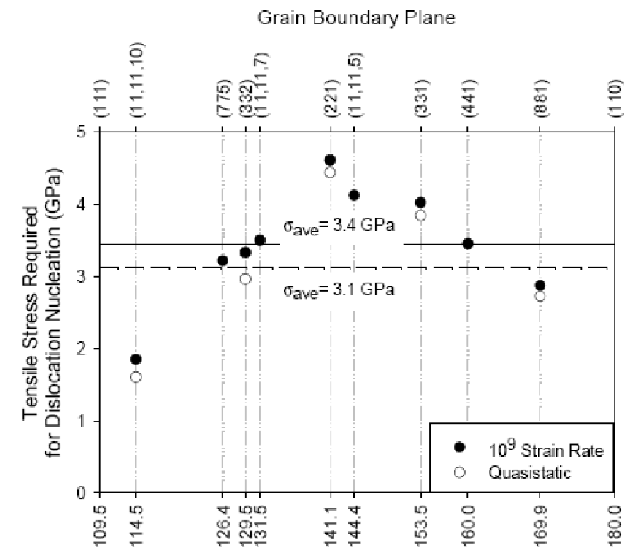


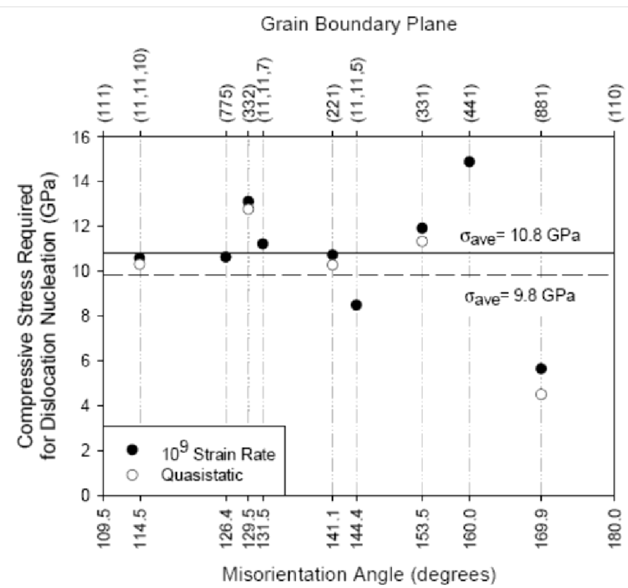
COMPRESSION



<110> GB structures

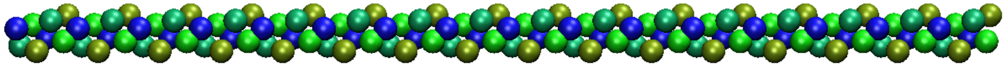
- Tschopp, Tucker, McDowell, Acta Mater. 2008





Tschopp, McDowell, JMPS, 56 (2008) 1806.

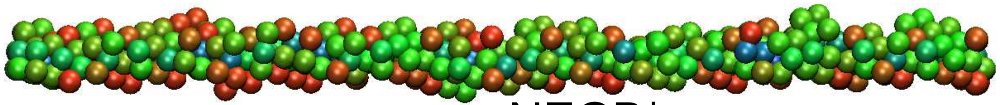
Nonequilibrium GB structures



EGB

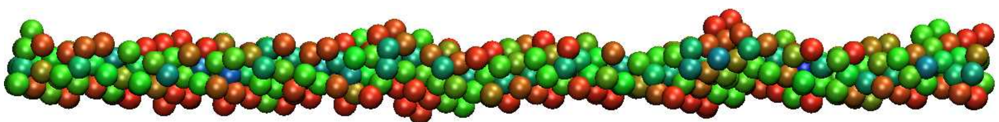
$\Sigma 9$ (221) θ=141.1°

γ_{GB} = 833 mJ/m^2
FV_{GB} = 6.22e-04



NEGB*

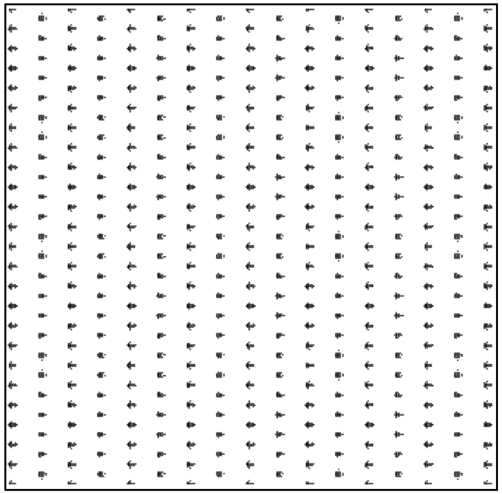
γ_{GB} = 890 mJ/m^2
FV_{GB} = 6.28e-04



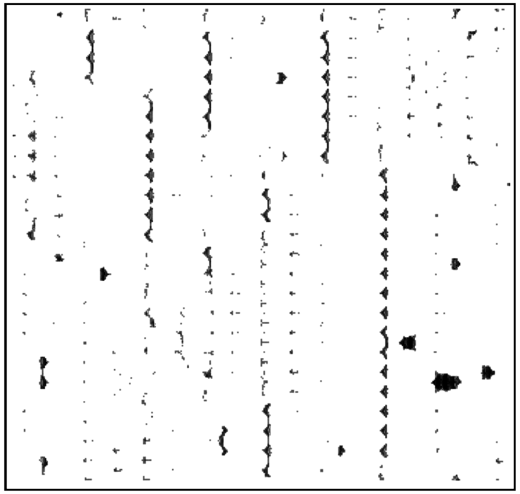
NEGB**

γ_{GB} = 919 mJ/m^2
FV_{GB} = 7.94e-04

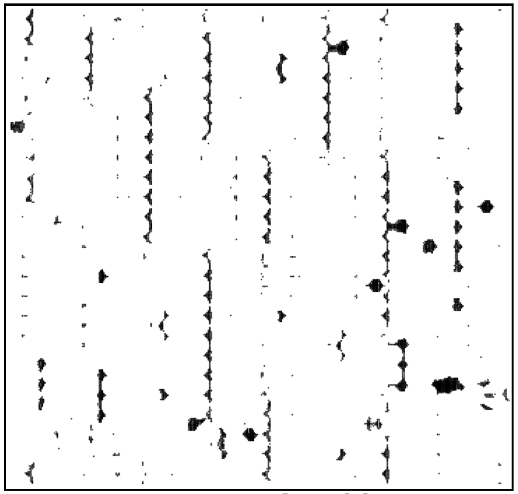
Free Volume (within GB plane)



EGB



NEGB*

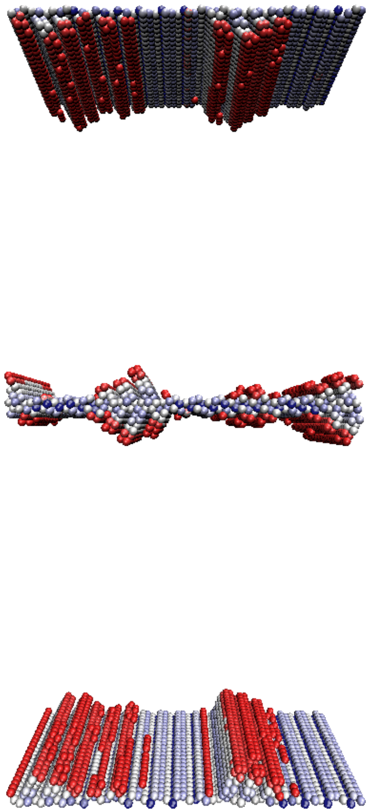


NEGB**

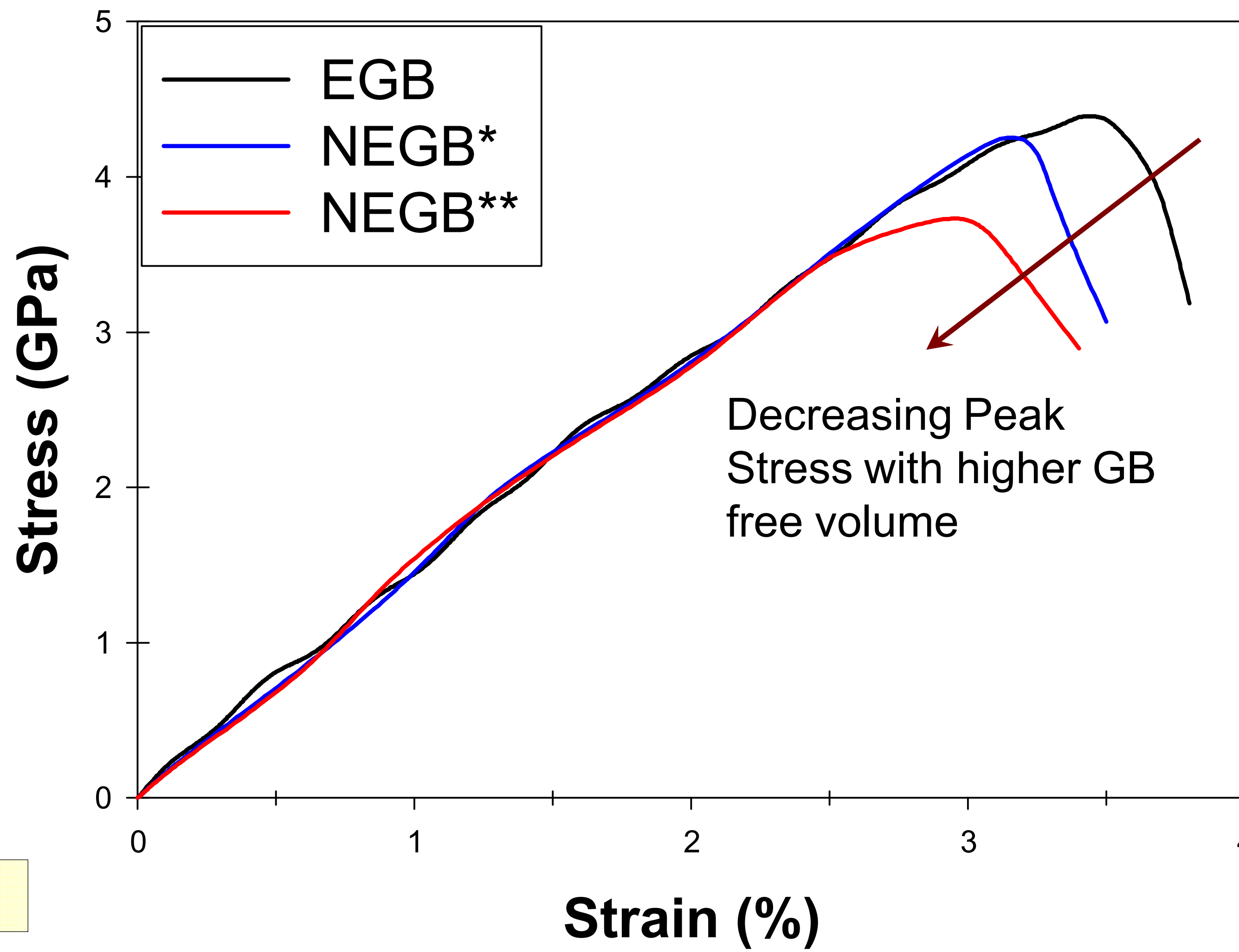
Tucker and McDowell, Int. Journal of Plasticity, 27, 6 (2011).

GB Dislocation Nucleation (Tension)

Σ9 (221) θ=141.1°



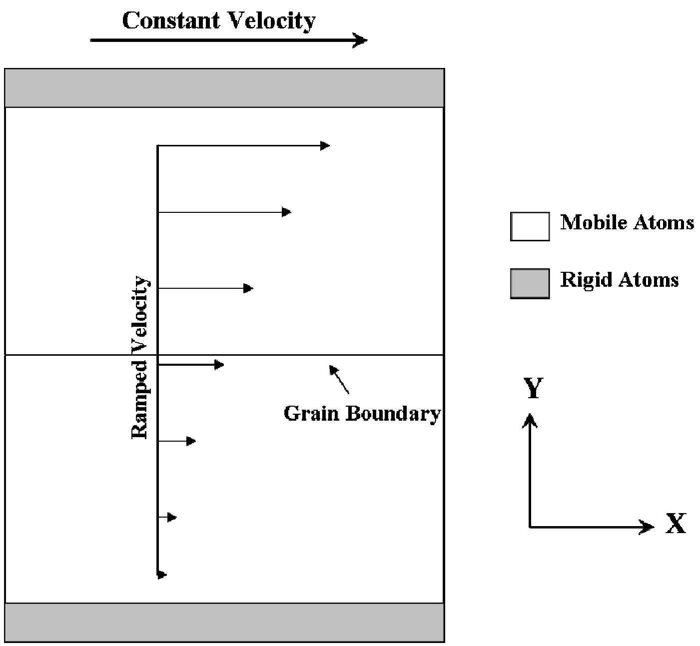
EGB

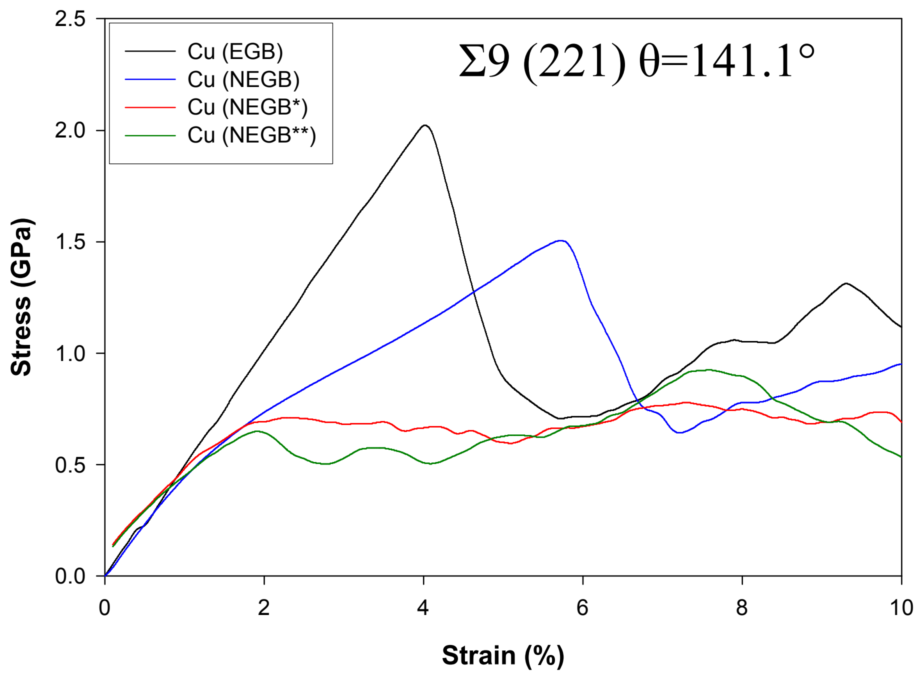


σ_{max} = 4.38 GPa

Tucker and McDowell, Int. Journal of Plasticity, 27, 6 (2011).

Shear Results



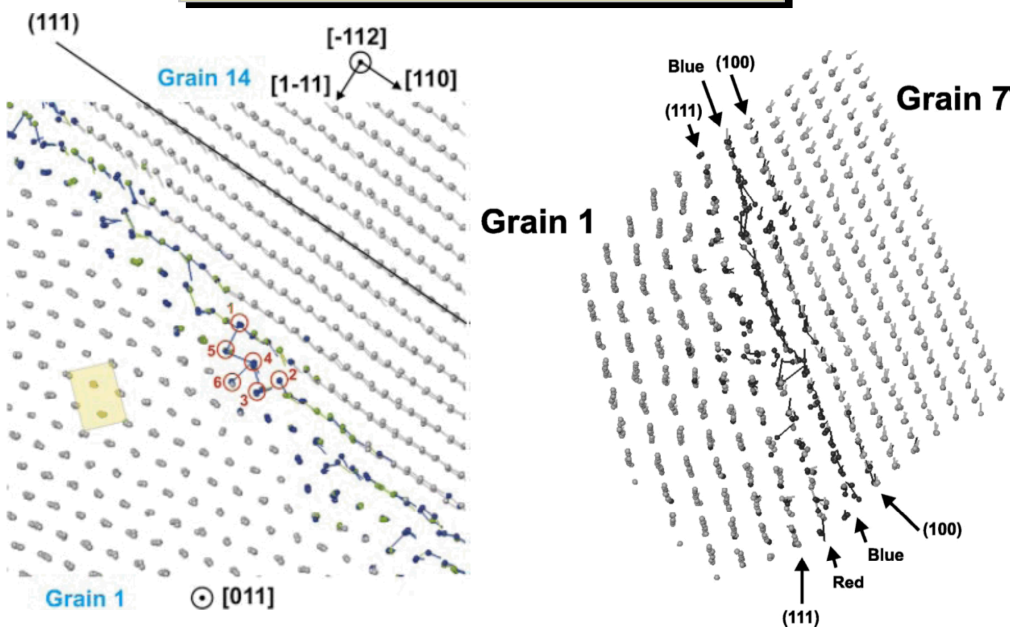


- 2D periodic boundary conditions (parallel to GB plane)
- 'Constrained' free vertical faces
- Constant applied velocity deformation
- 10^9 s^{-1} constant shear strain rate
- NVT at 10 K

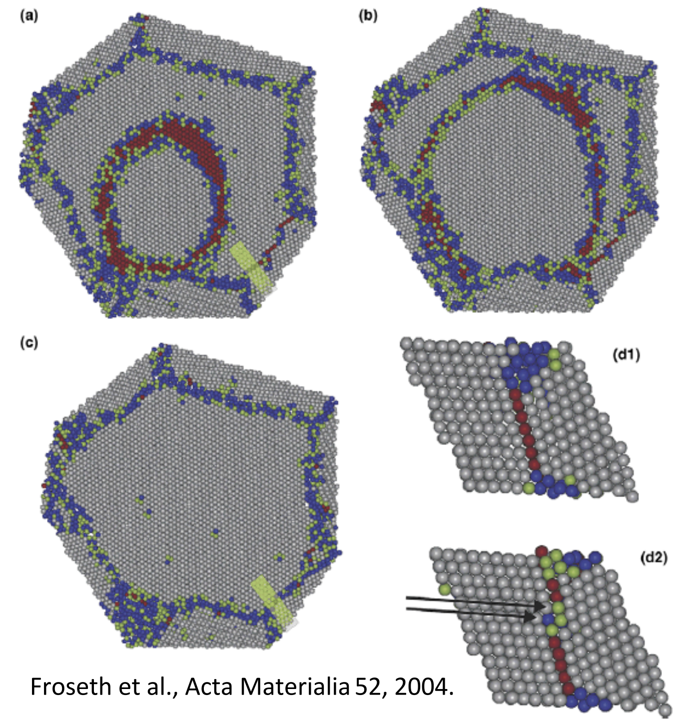
- Grain boundary sliding and significant atomic shuffling occurs in all boundaries
- Behavior is nearly elastic-perfectly plastic
- Reordering and restructuring processes during hardening stage of NEGBs

Relevant NC Phenomena

GB Sliding/Atomic Shuffling

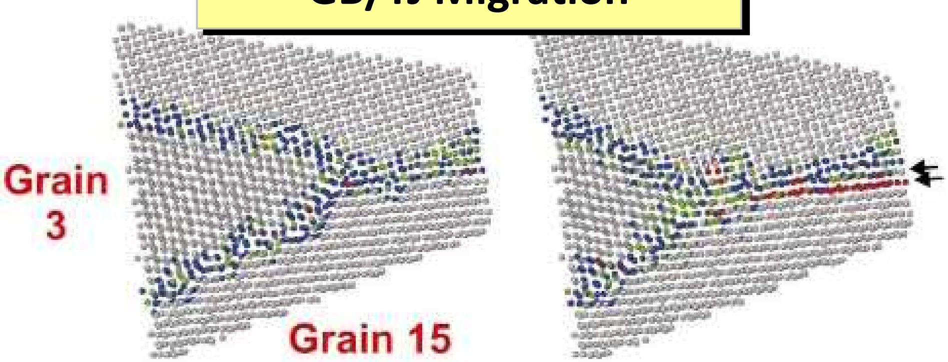


Dislocation Nucleation

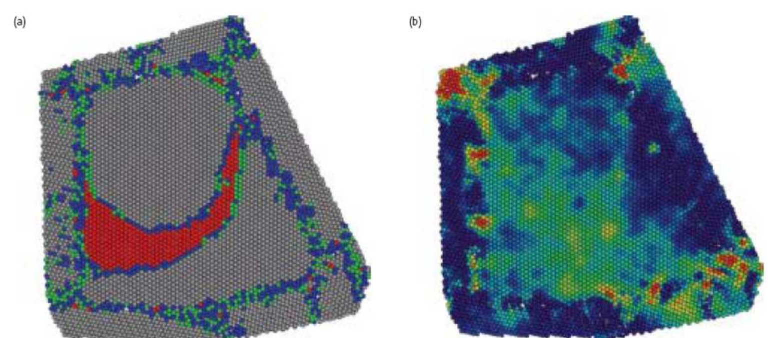


Froseth et al., Acta Materialia 52, 2004.

GB/TJ Migration



Van Swygenhoven and Derlet., PRB 64, 2001.



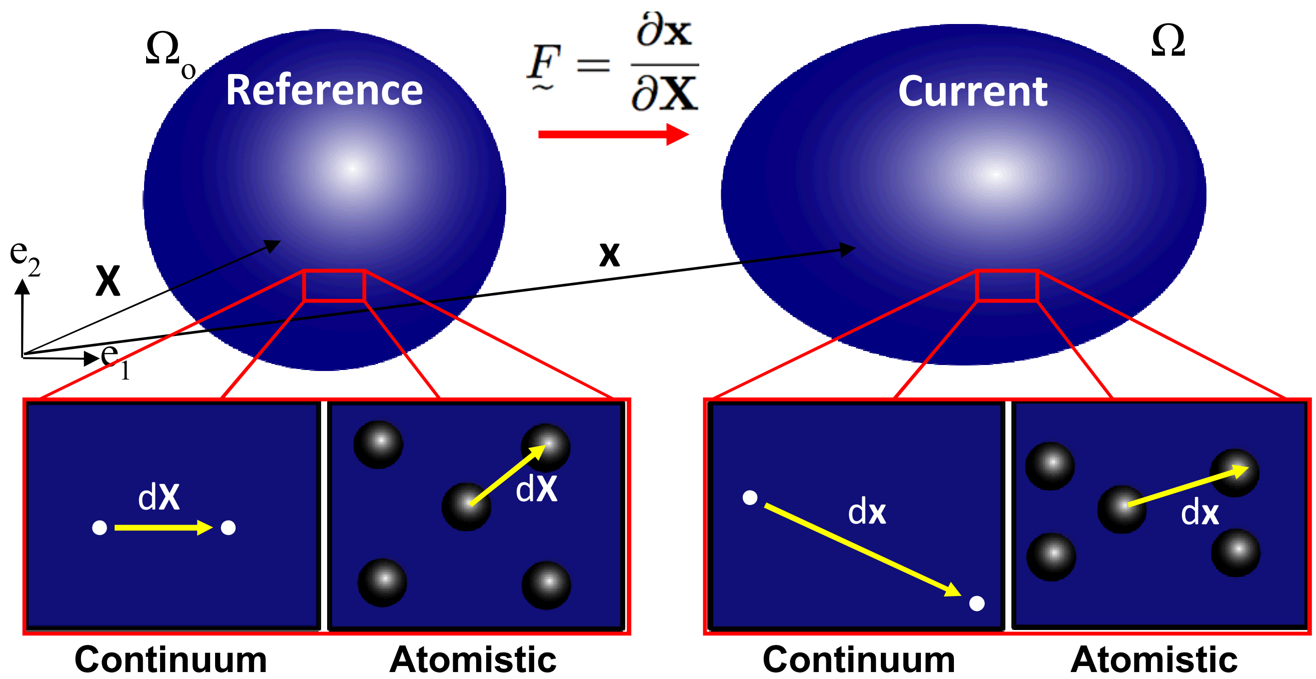
Van Swygenhoven, Materials Today 9, 2006.

Some Implications for NC Metal Plasticity

- ✓ Non-Schmid effects
- ✓ Tension-compression asymmetry
- ✓ Competing/combined effects of
  - GB reordering, shuffling/sliding, and/or migration
  - dislocation nucleation/desorption/absorption

- ➢ Sensitive to GB network
- ➢ Affected by excess free volume – NEGB structures

Visual Tools: Kinematics



Deformation Gradient $F_{iI} = \dfrac{\partial x_i}{\partial X_I} \rightarrow \quad dx_i = F_{iI} dX_I$

Atomistic Formulation

$$\sum_{\beta=1}^{n} (x_i^{\alpha\beta} X_M^{\alpha\beta} - F_{iI}^{\alpha} X_I^{\alpha\beta} X_M^{\alpha\beta}) = 0$$

where

$$\omega_{iM}^{\alpha} = \sum_{\beta=1}^{n} x_i^{\alpha\beta} X_M^{\alpha\beta} \quad \text{and} \quad \eta_{IM}^{\alpha} = \sum_{\beta=1}^{n} X_I^{\alpha\beta} X_M^{\alpha\beta}$$

$$\longrightarrow \boxed{F_{iI}^{\alpha} = \omega_{iM}^{\alpha} (\eta^{\alpha})_{MI}^{-1}}$$

Deformation Gradient

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*** Zimmerman *et al.*, IJSS (2009)**

See also Gullett *et al.* MSMSE (2008), Hartley and Mishin (2005)

- $\underset{\sim}{F} = \underset{\sim}{R}\underset{\sim}{U}$ where $\underset{\sim}{R} = \underset{\sim}{R}_{sym} + \underset{\sim}{R}_{skew}$

$$\longrightarrow \underset{\sim}{R}_{skew} = \frac{1}{2}(\underset{\sim}{R} - \underset{\sim}{R}^T) \longrightarrow \boxed{\phi_k} = -\frac{1}{2}\epsilon_{ijk}(R_{skew})_{ij}$$

microrotation vector

- $\underset{\sim}{L} = \underset{\sim}{D} + \underset{\sim}{W}$

$$\longrightarrow \underset{\sim}{W} = \frac{1}{2}(\underset{\sim}{L} - \underset{\sim}{L}^T) \longrightarrow \boxed{\omega_k} = -\frac{1}{2}\epsilon_{ijk}W_{ij}$$

vorticity vector

• Tucker, G.J., Zimmerman, J.A., and McDowell, D.L., MSMSE 18(1) 2010, 015002.
• Tucker, G.J., Zimmerman, J.A., and McDowell, D.L., Int. J. Engineering Science in memoriam to C. Eringen, in press.

Why Continuum Metrics?

Metal plasticity at the nanoscale is complex

- Use of centrosymmetry, CN, slip vector, etc. is complicated in terms of characterization and visualization of high density of evolving line defects
- These continuum metrics can address either history of process or current configuration – useful for understanding mechanisms

Informing continuum models

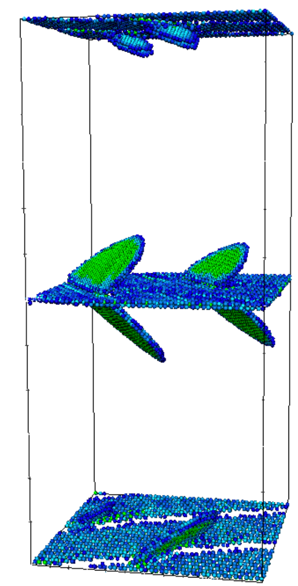
- Kinematics of continuum description can perhaps be bridged in terms of understanding based on statistical fields from atomistic simulations
- Check assumptions, trends from proposed continuum constitutive models (e.g., Khan et al. (2006), Capolungo et al. (2007), Wei and Anand (2004) and Wei et al.(2006))

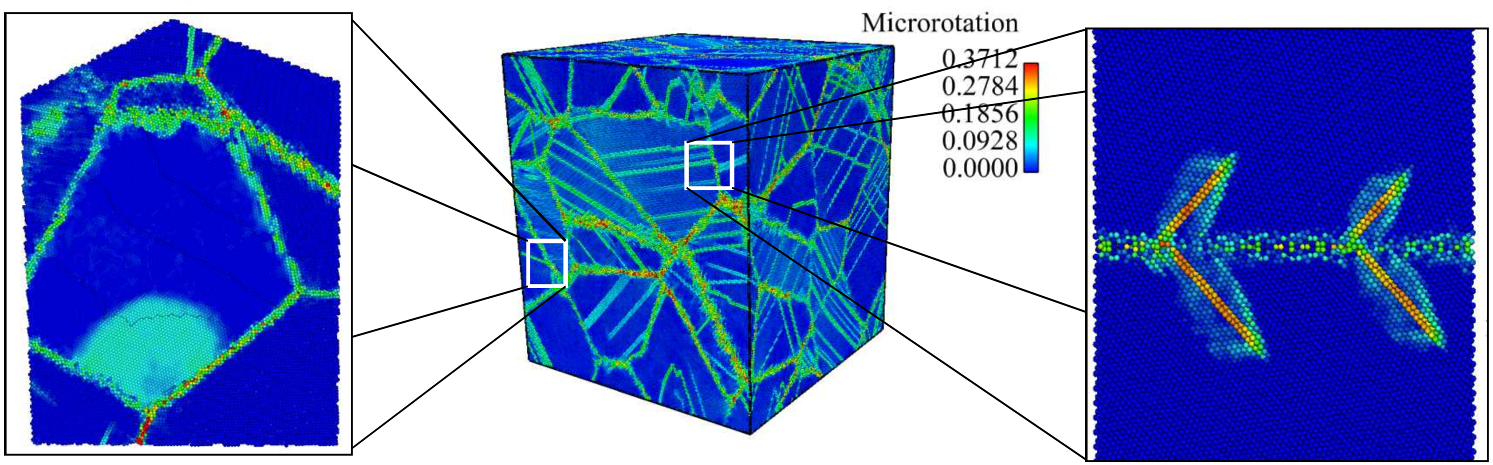
Some connections

- microrotation (ϕ) gradient [Atomistics]
- torsion-flexure tensor [Continuum]

Objectives

- Formulate nonlocal metrics from continuum mechanics for use in atomistic simulation analysis
- Investigate the evolution of kinematic metrics for various deformation mechanisms in NC metals
- Resolve the contribution of different deformation mechanisms during uniaxial deformation of NC copper
  - Dislocation Nucleation
  - GB Sliding/Atomic Shuffling





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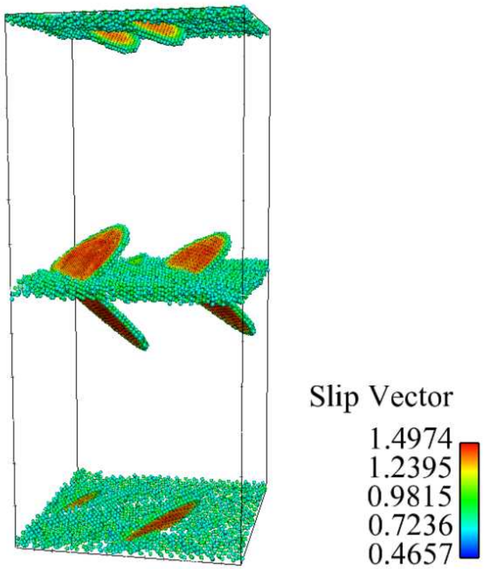
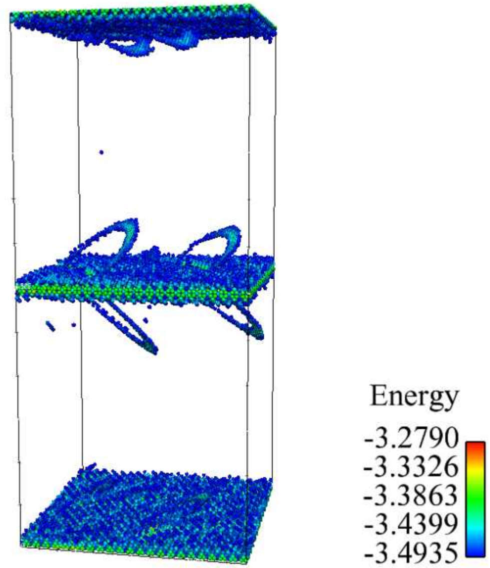
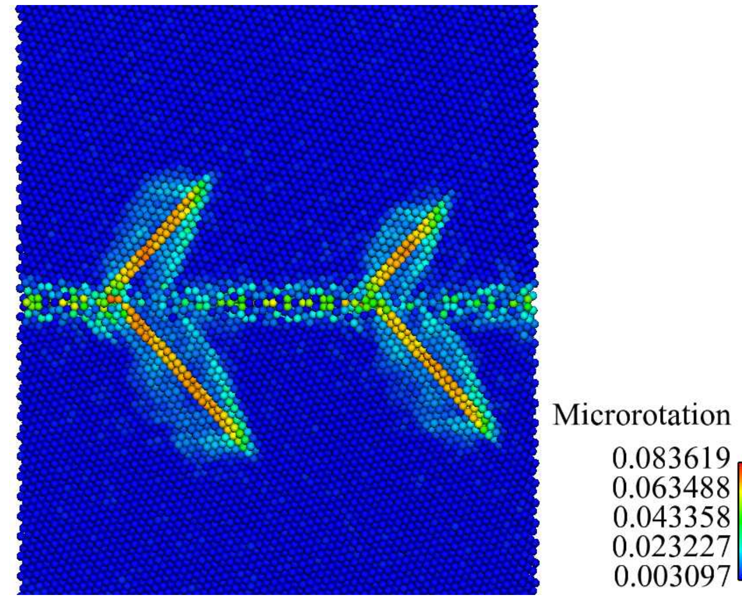
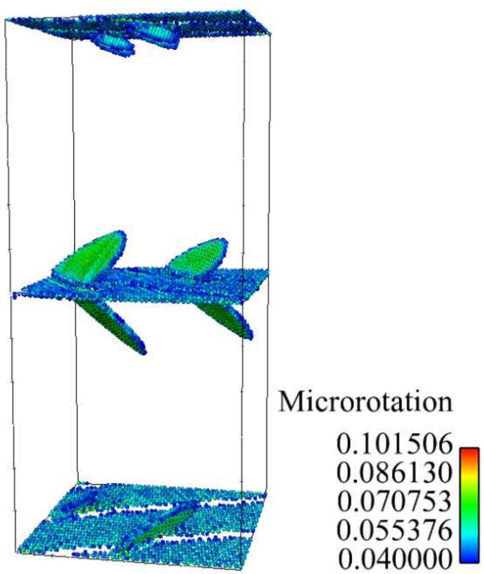
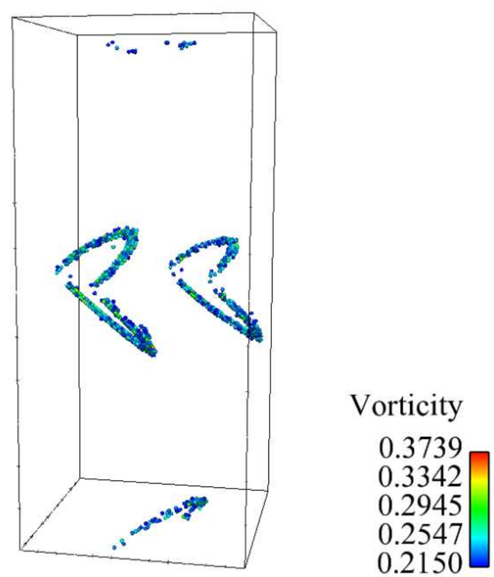
Information gained from Metrics

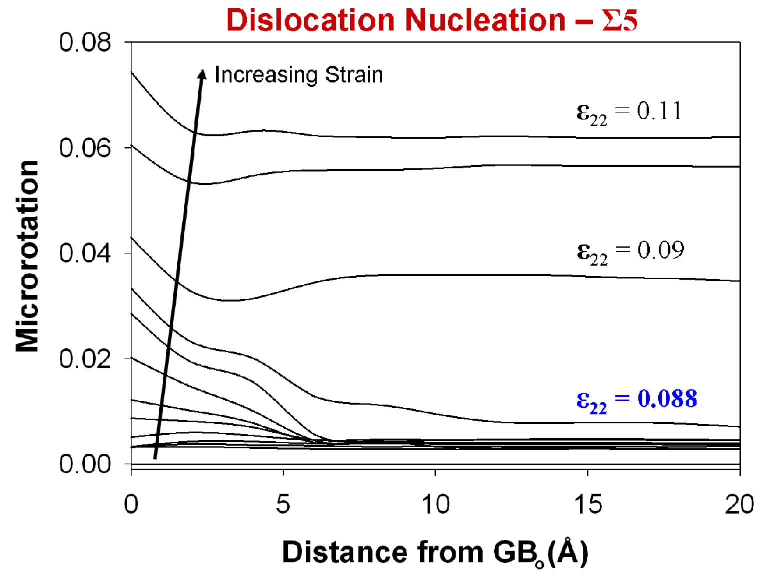






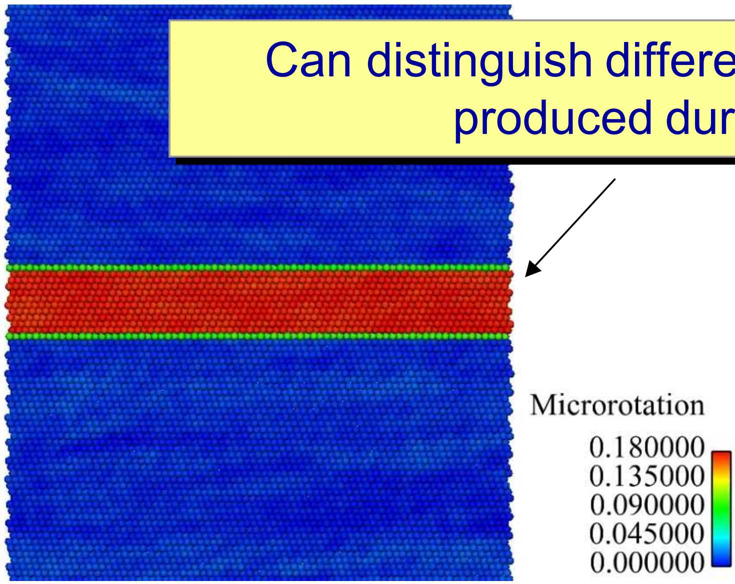


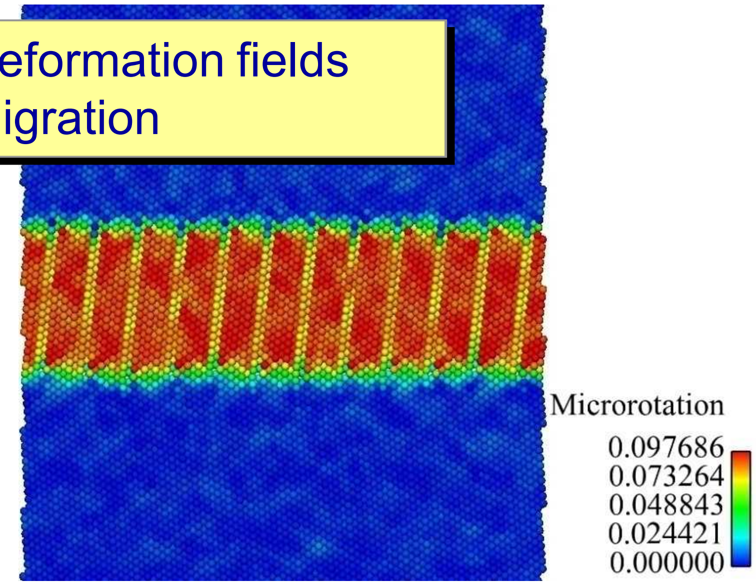


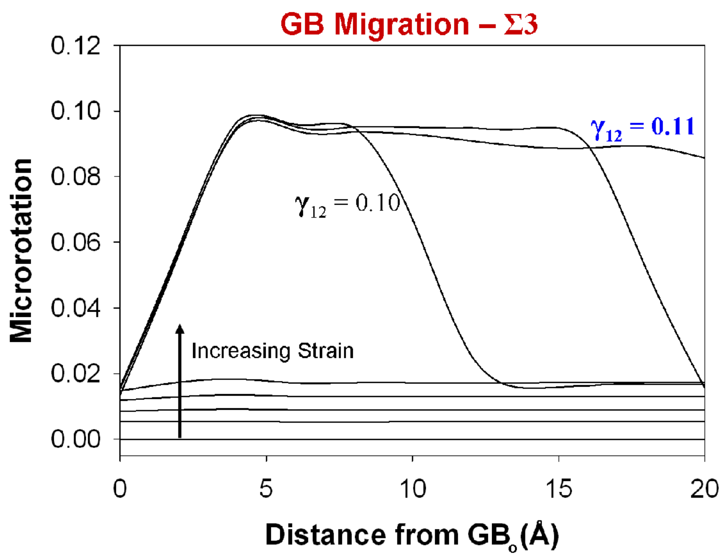


Information gained from Metrics

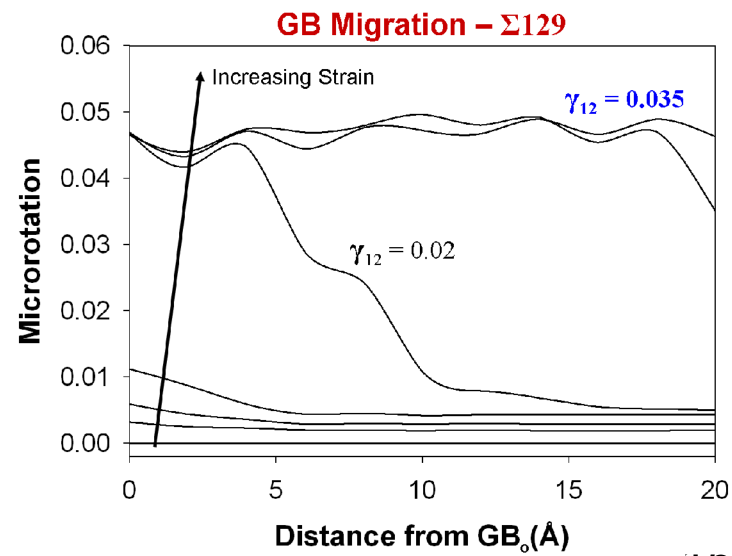
Can distinguish differences in deformation fields produced during GB migration





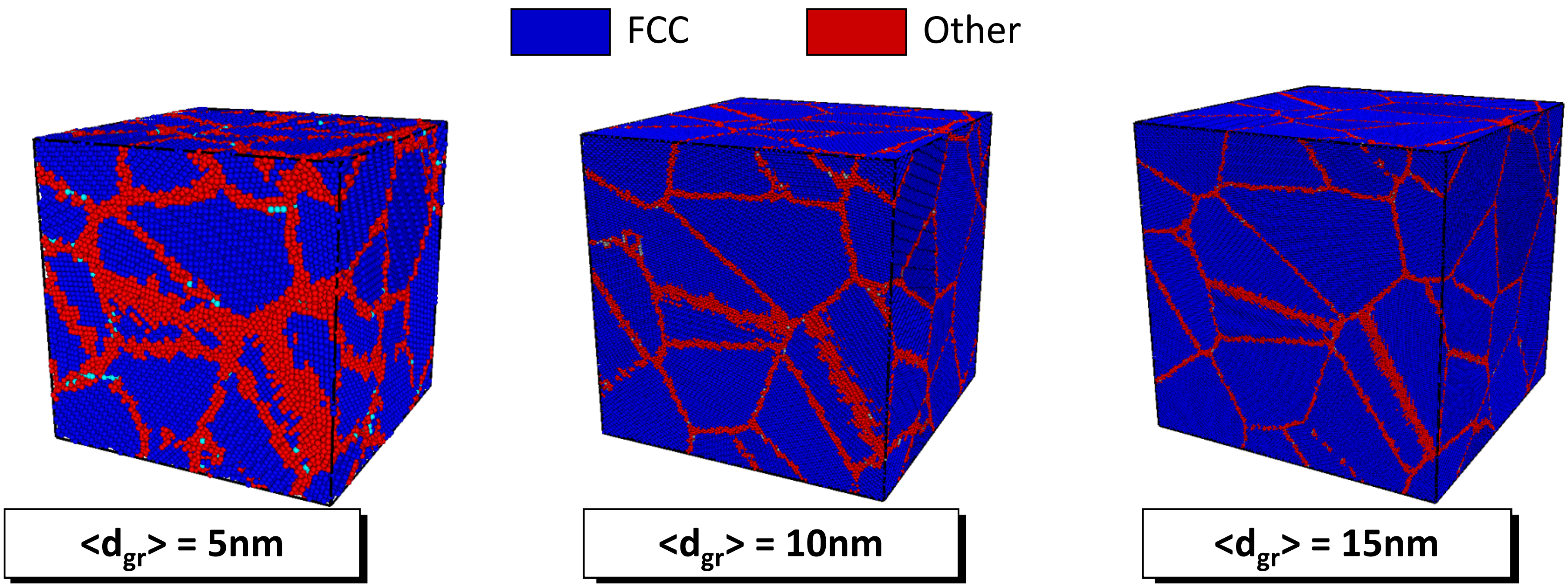


Average microrotation over slices || to boundary



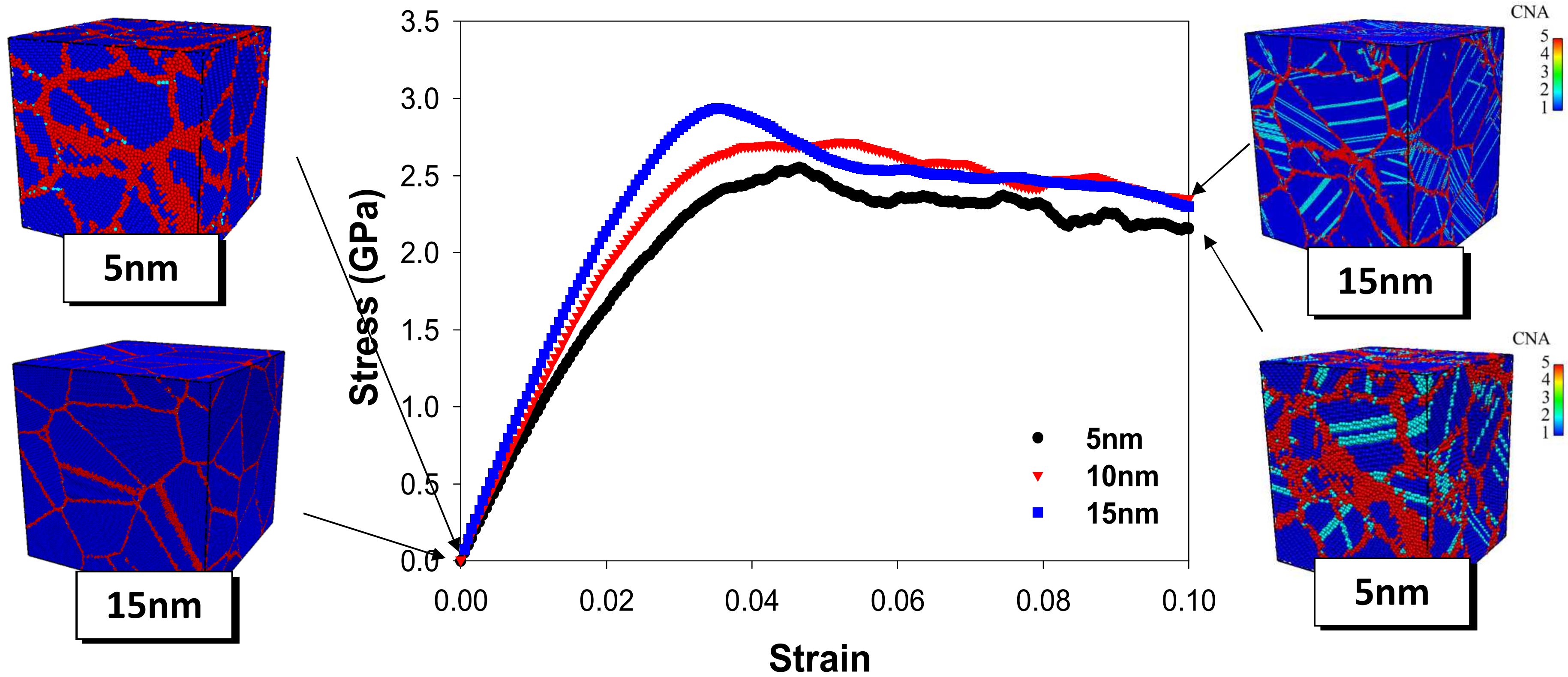
Tucker, G.J., Zimmerman, J.A., and McDowell, D.L., MSMSE 18(1) 2010, 015002.

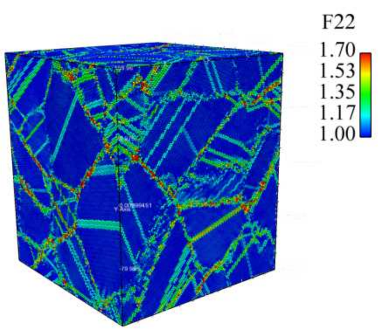
3D Nanocrystalline Structures



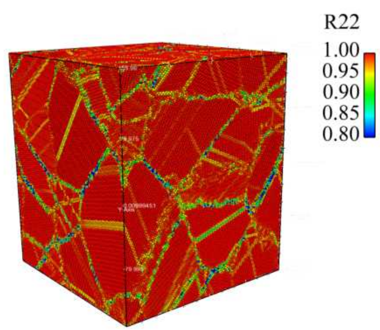
- Full 3D nanocrystalline structure (Voronoi Tessellation, random lattice orientations)
- 3D periodic BCs
- Atom overlap deletion and equilibration for 50 ps at 10K
- Uniaxial tension at 10K under NPT, constant strain rate of 10^9 s^{-1}
- Analysis of deformation mechanisms using microscale continuum metrics

Nanocrystalline Copper

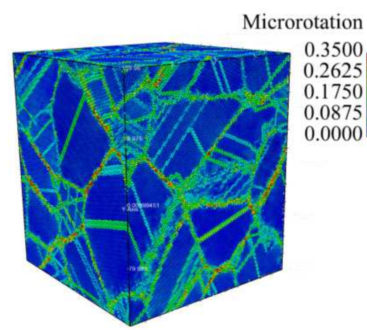




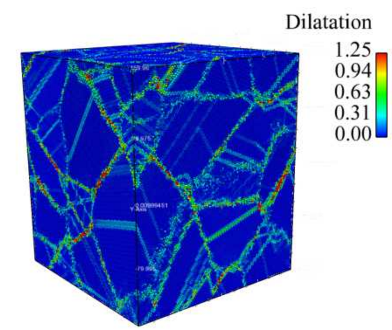
Deformation Gradient



Rotation Metric

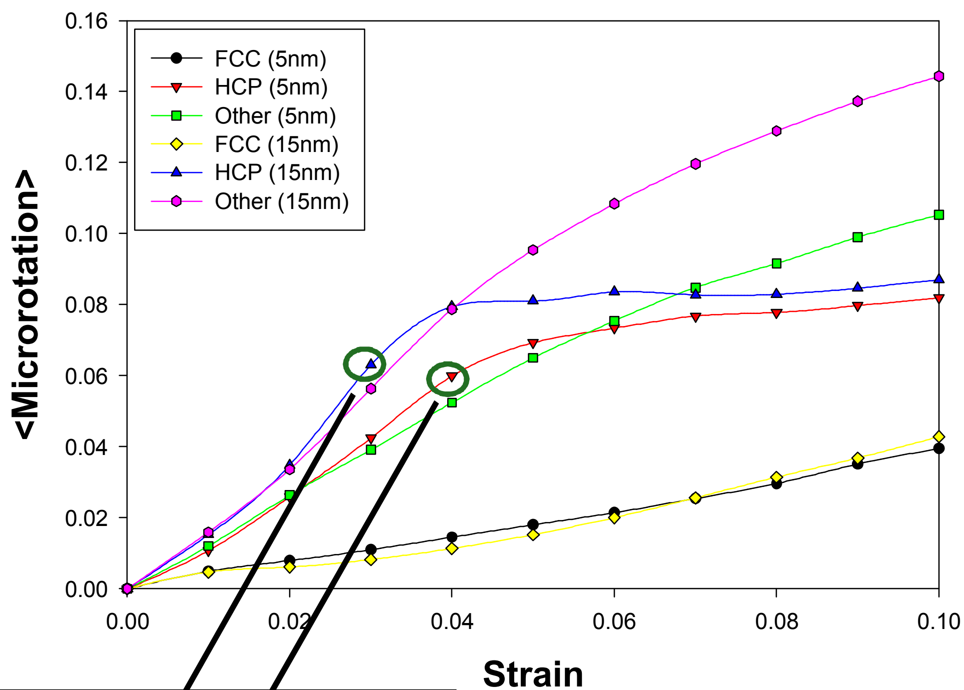


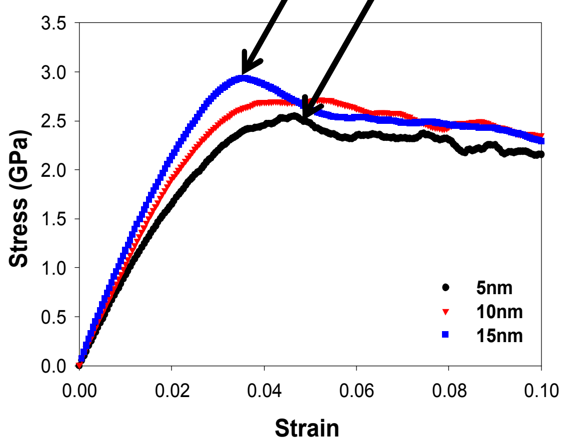
Microrotation

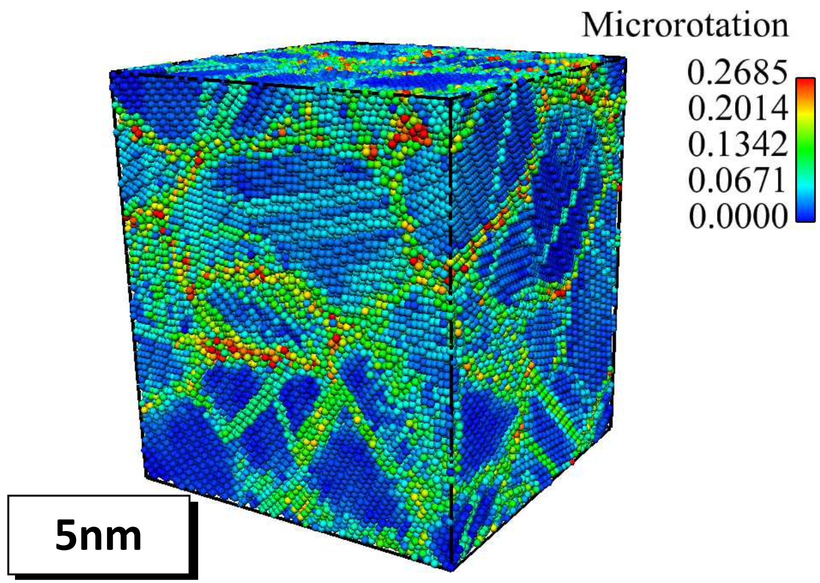


Dilatation

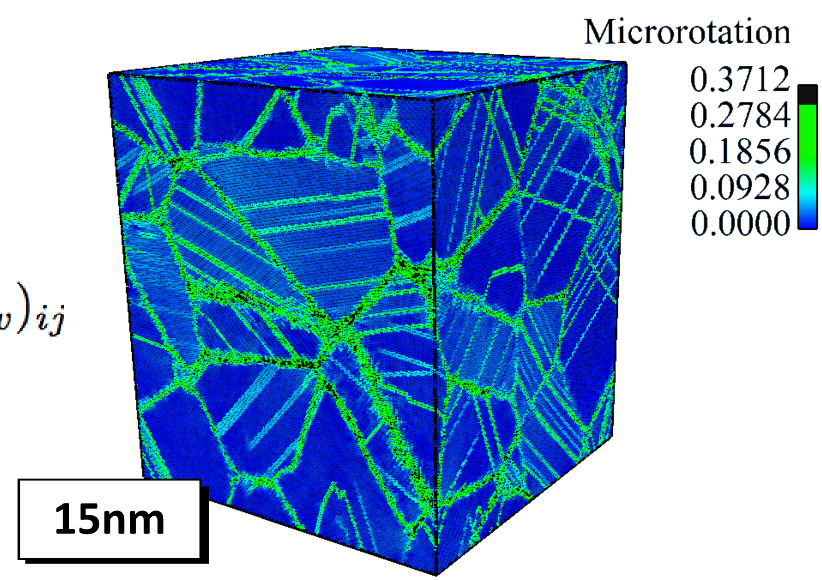
Nanocrystalline Copper



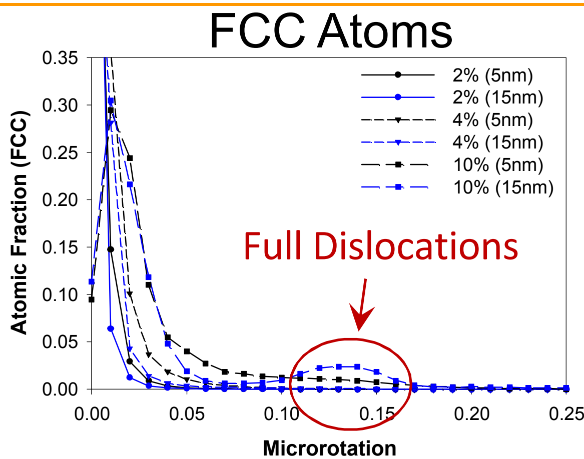


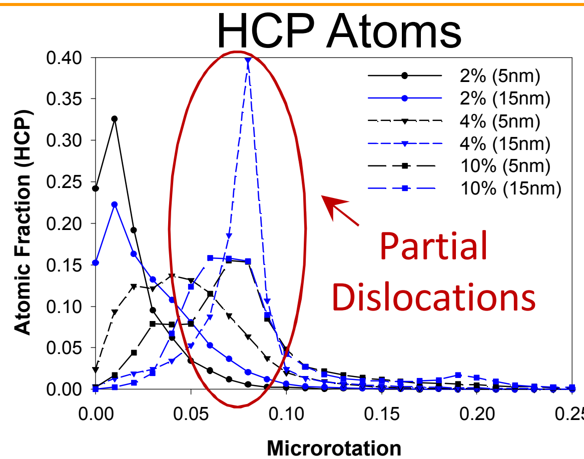


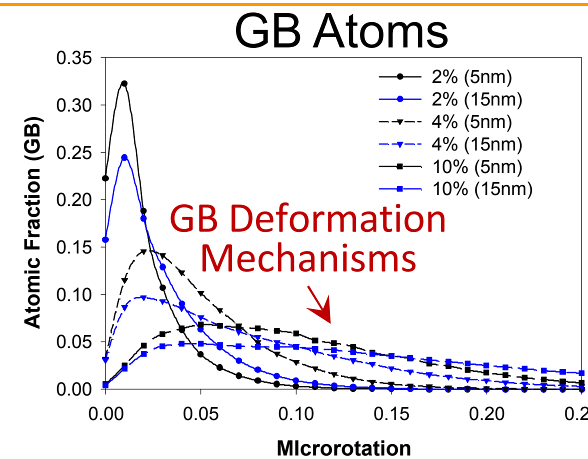
$$\phi_k = -\frac{1}{2}\epsilon_{ijk}(R_{skew})_{ij}$$

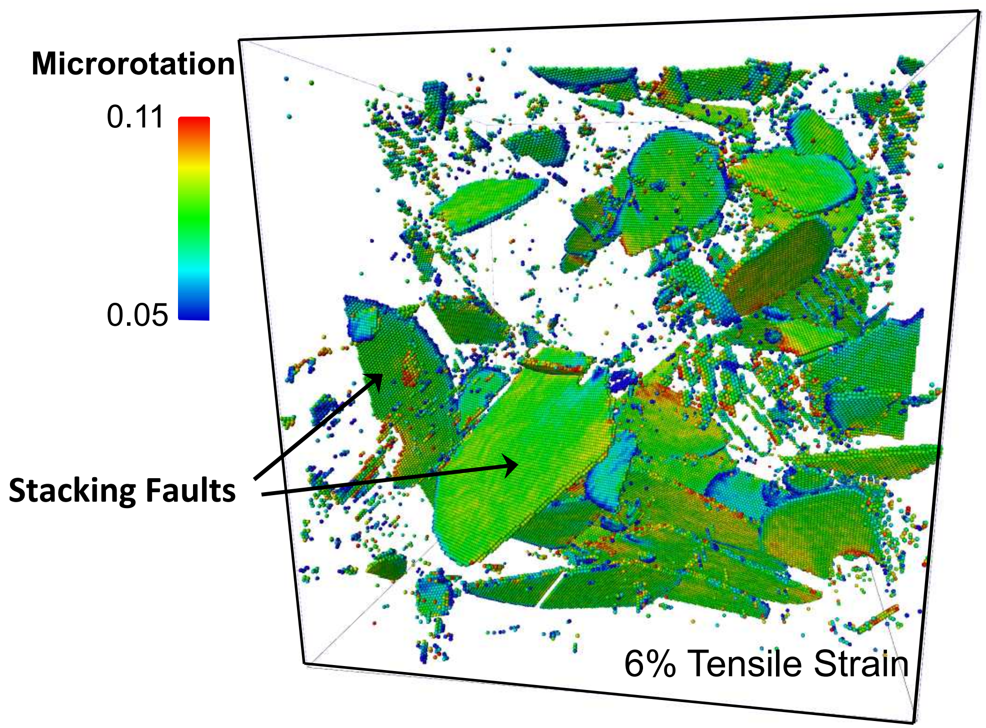


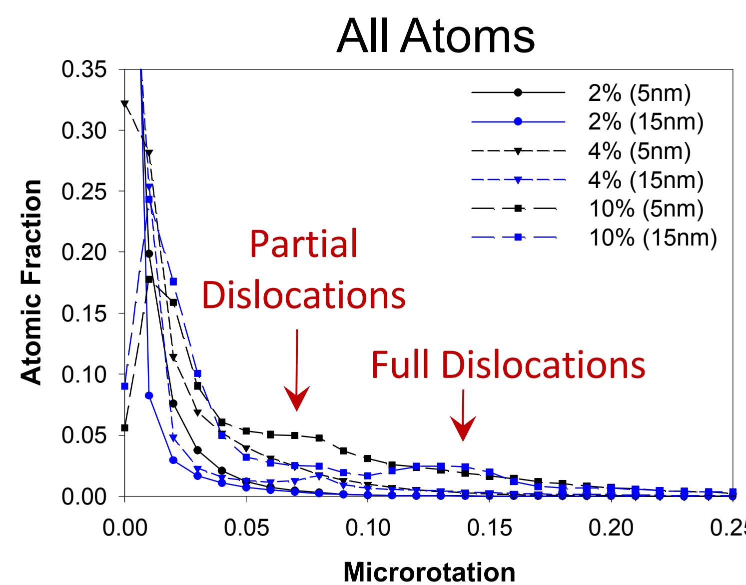
Microrotation Distribution



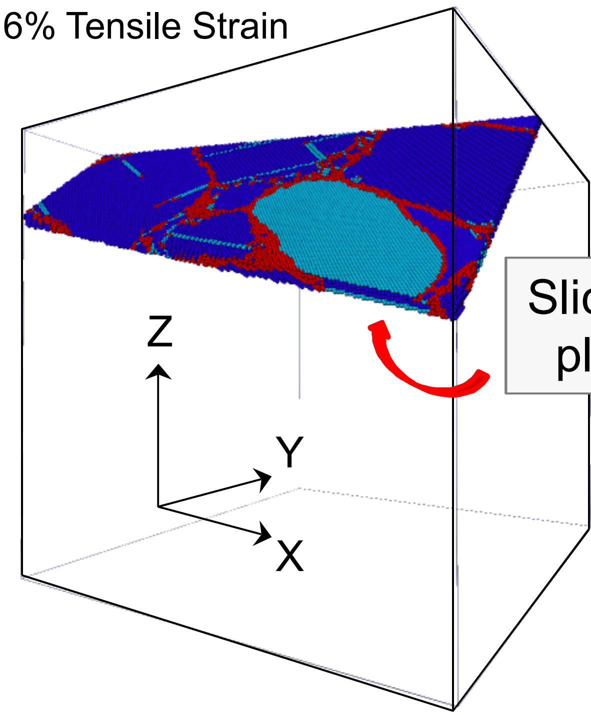


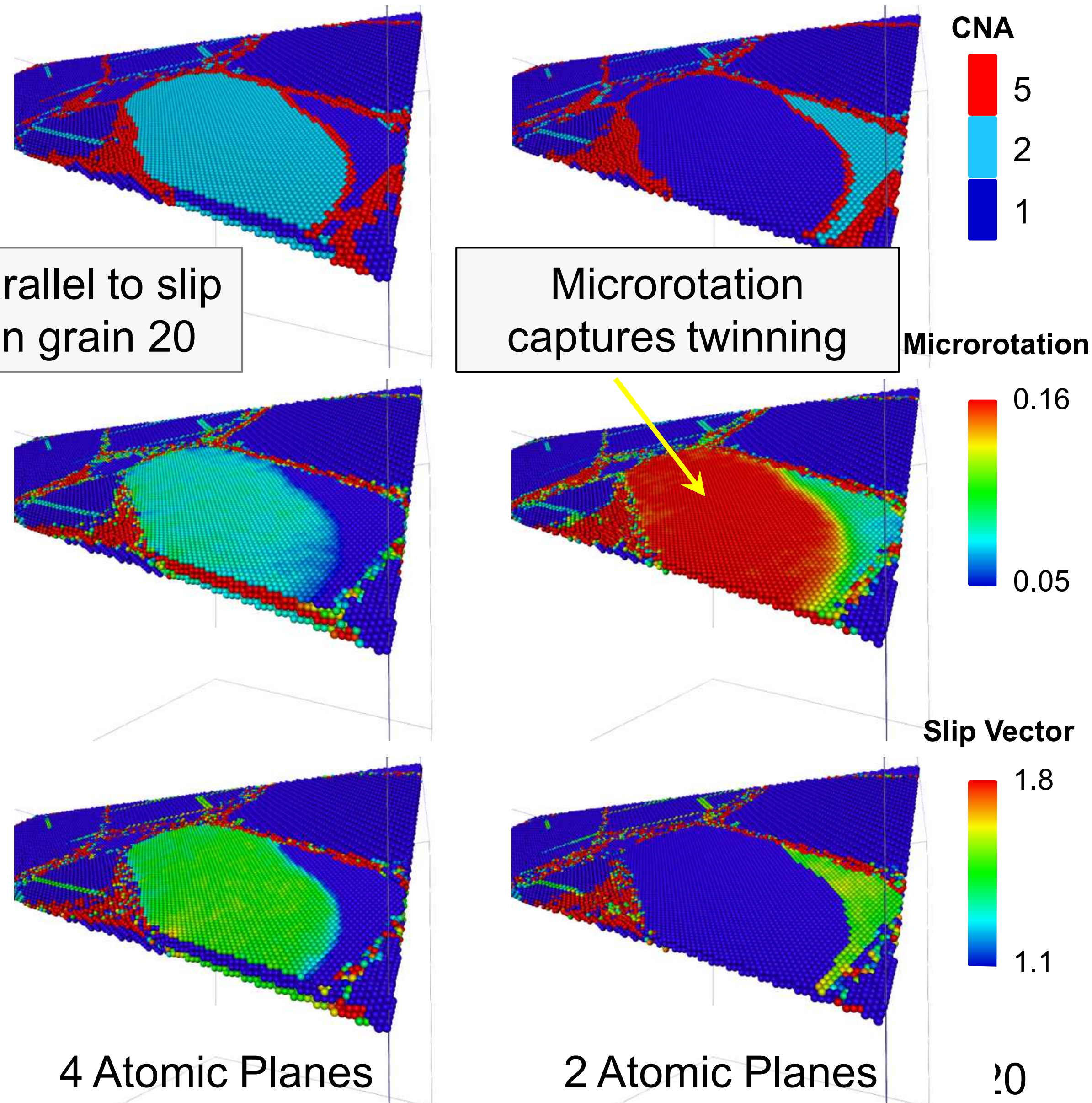






Advantage of Microrotation





- *Microrotation* is able to capture important deformation behavior (e.g. **dislocation slip**) and structural features (e.g**. stacking fault**) usually visualized using *CNA* and atomic *slip vector* together.

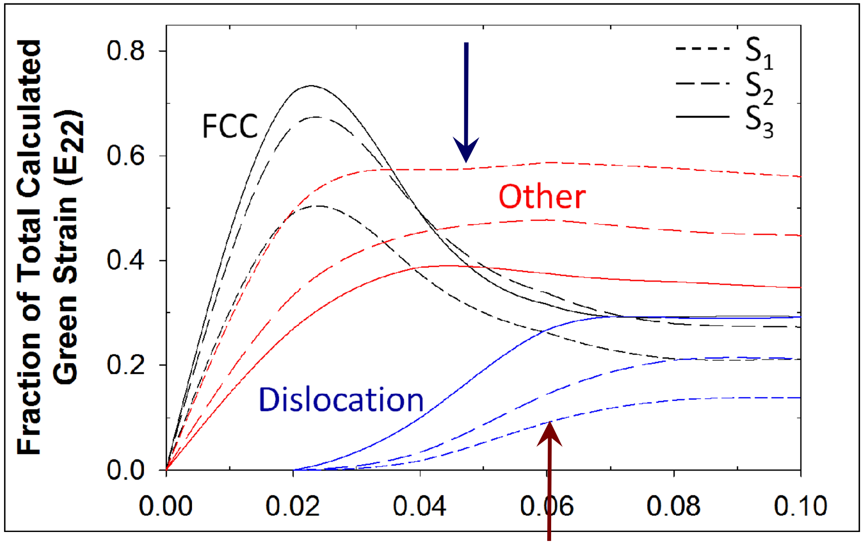
- Potential to be passed into continuum level models as kinematic variable.

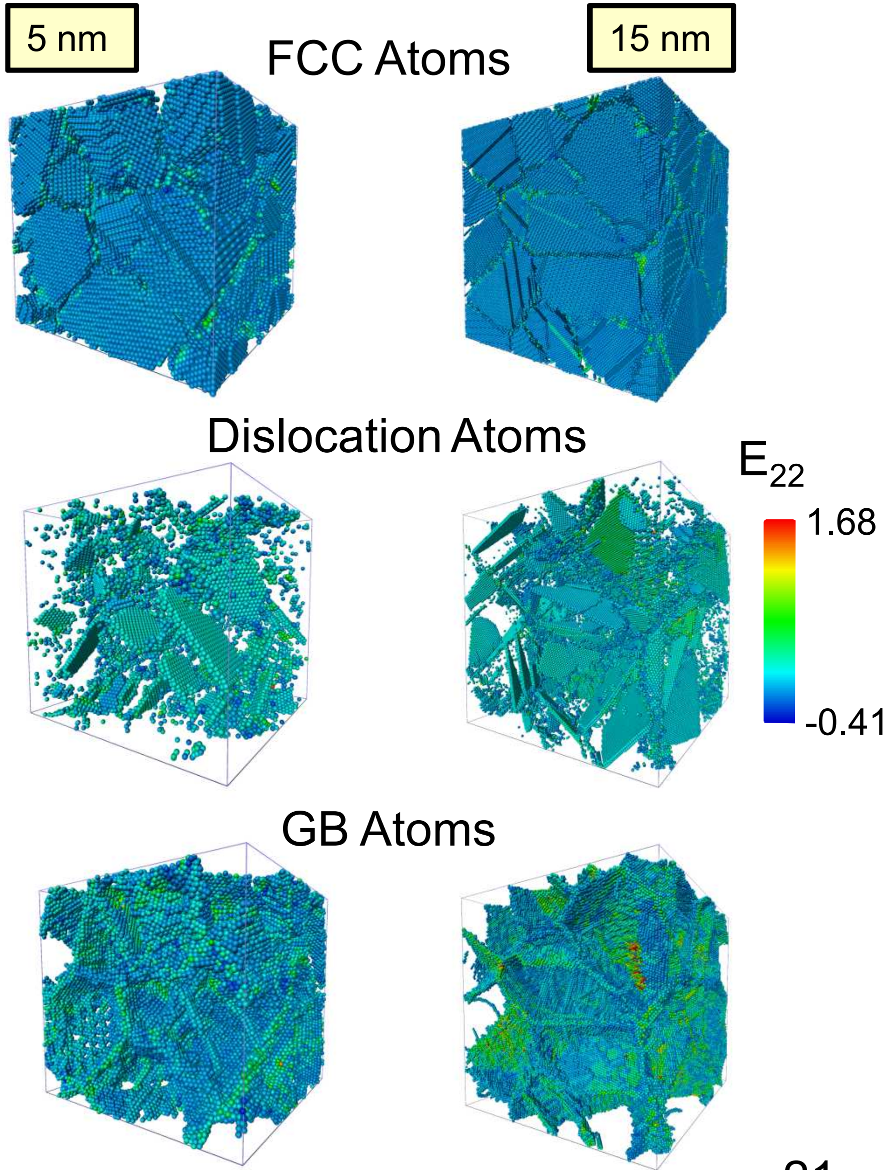
Green Strain

Green Strain Tensor

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^{\mathrm{T}} \cdot \mathbf{F} - \mathbf{I})$$

- E_{22} from all atoms in a group (e.g. FCC, GB, Dislocation).
- Overall, GBs account for a higher fraction of tensile strain in smaller grain structures. In contrast, *dislocation activity accounts for a higher fraction in larger grain structures*.





Conclusions/Future Work

- Different mechanisms provide distinct kinematic signatures and a sense of deformation history is captured by certain metrics.
- The non-locality of various mechanisms can be probed by employing the volume-averaging scheme using atomic neighbor lists (*1st, 2nd, 3rd, and reference/current*).
- Insight into complex deformation landscape in NC materials is provided through the implementation of microscale continuum metrics, and we can begin to resolve mechanism contributions to overall deformation.
- Deformation avalanches are of interest (inversion points and plateaus), also from point of view of distribution of shedding of microkinetic energy.

❖ Investigate tension/compression asymmetry and stress-state dependent behaviors

❖ Quantify the distribution of dislocation slip vs. GB processes during deformation as a function of grain size.

Acknowledgements

- **NSF CMMI #0758265** - Multiresolution, Coarse-Grained Modeling of 3D Dislocation Nucleation and Migration (metrics)
- **NSF DMI #1030103** - Methods for Atomistic Input into Initial Yield and Plastic Flow Criteria for Nanocrystalline Materials (nanocrystals)
- **Dr. Jonathan Zimmerman** (*Sandia National Labs*)
- Sandia National Laboratories (*EPSRI Internship – Summer 2008*)
- Carter N. Paden Jr. Distinguished Chair in Metals Processing
- NSF **TeraGrid** Science Gateways program.

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