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Georgia Institute of Technology

Resolving Deformation Modes of Nanocrystalline Metals using Continuum Metrics Based on Atomistic Simulations

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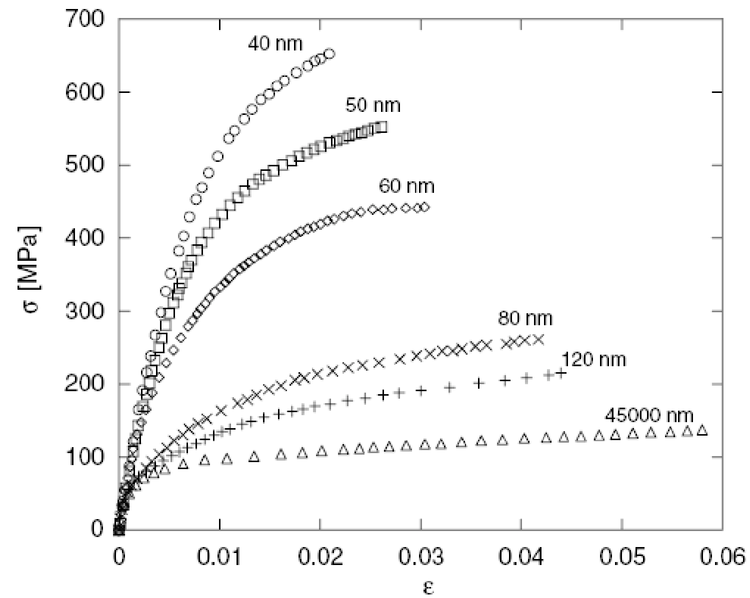
Introduction

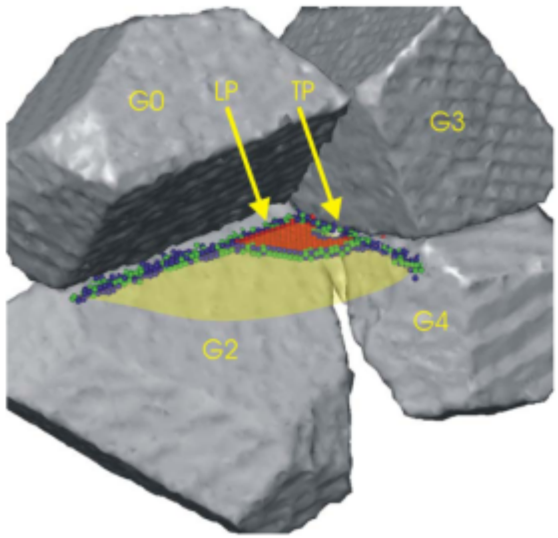
- Mechanical properties of <u>nanocrystalline</u> (NC) materials show potential improvement compared to larger grained polycrystalline materials (e.g. yield strength, fracture/fatigue resistance, and superplasticity).

- Higher number density of atoms are located in GB regions, need a deeper understanding of GB role in deformation processes, both elastic and inelastic.

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

Khan et al., IJP, 22 (2006).



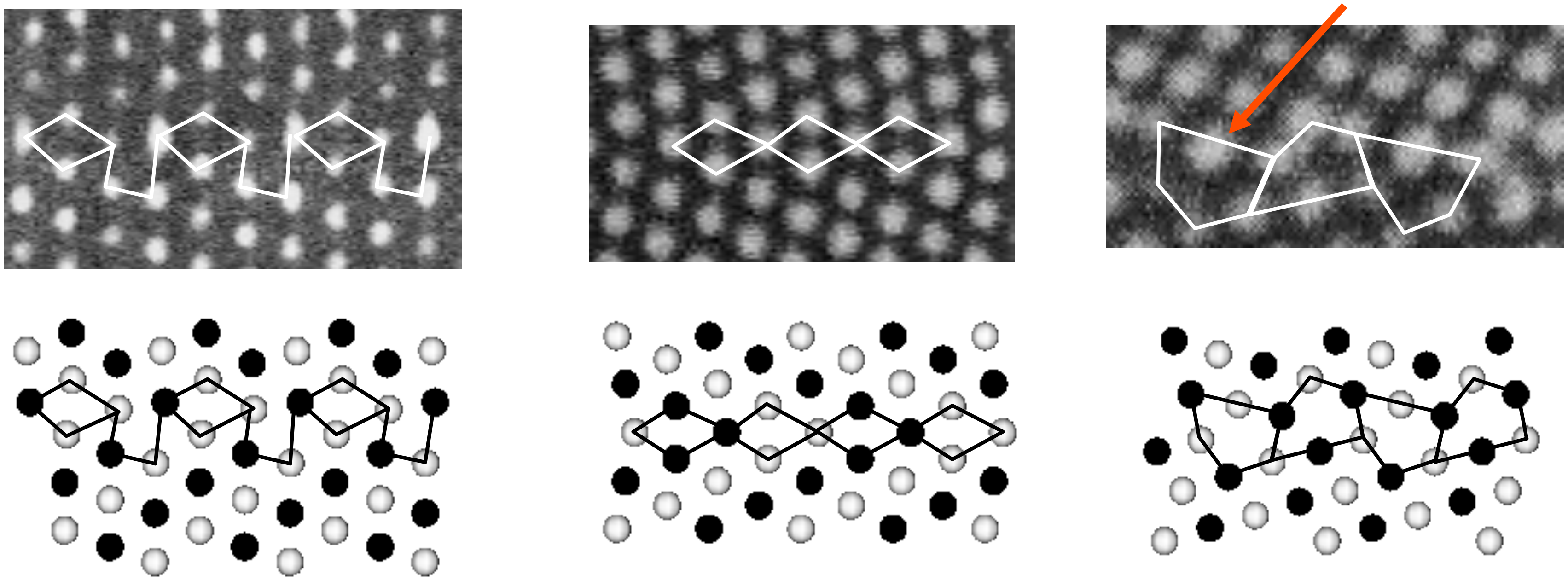


Van Swygenhoven et al., Acta Mat., (2006).

Atomistic 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))

E Structural Unit



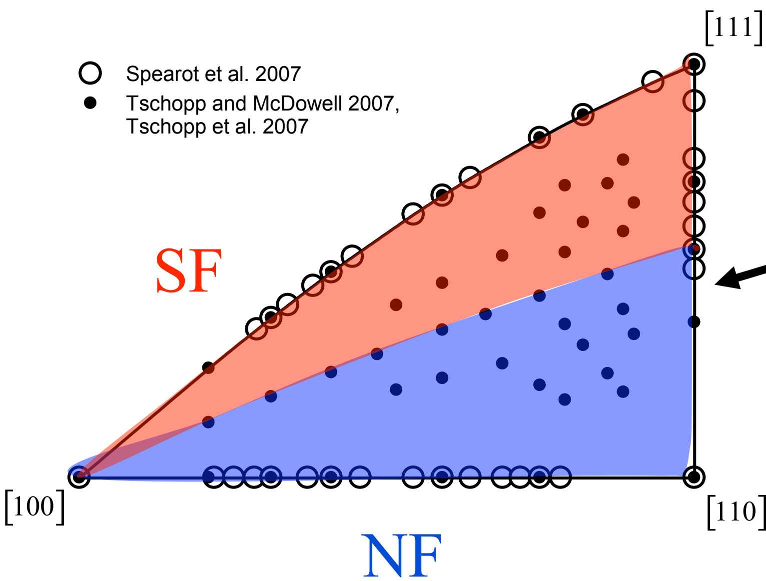
Σ3 (112) 70.5°   Σ11 (113) 50.5°   Σ9 (221) 141.1°

- 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

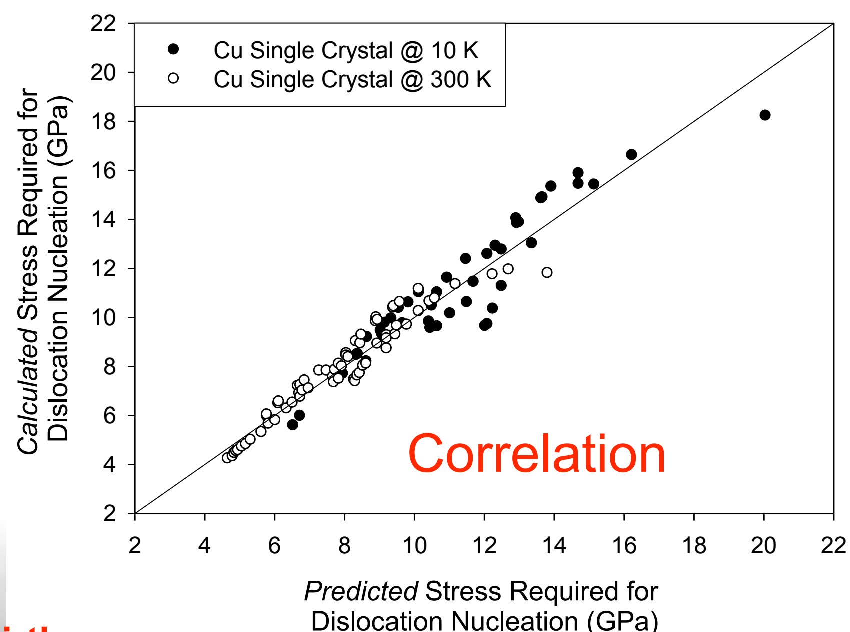
Homogeneous and heterogeneous nucleation

Spearot, Tschopp, Jacob, McDowell, Acta Materialia, 55 (2007) 705.

$$\sigma^{sc}_{max} = \begin{cases} \frac{\tau_{ideal}}{\mu_{s,1}SF+\mu_{n,1}NF}, & \text{if } \mu_{s,1}SF + \mu_{n,1}NF \geq \mu_{s,2}SF + \mu_{n,2}NF \\ \frac{\tau_{ideal}}{\mu_{s,2}SF+\mu_{n,2}NF}, & \text{if } \mu_{s,1}SF + \mu_{n,1}NF < \mu_{s,2}SF + \mu_{n,2}NF \end{cases}$$



Dislocation nucleation stresses are best correlated with the Schmid factor or normal factor in different regions of the stereographic triangle.



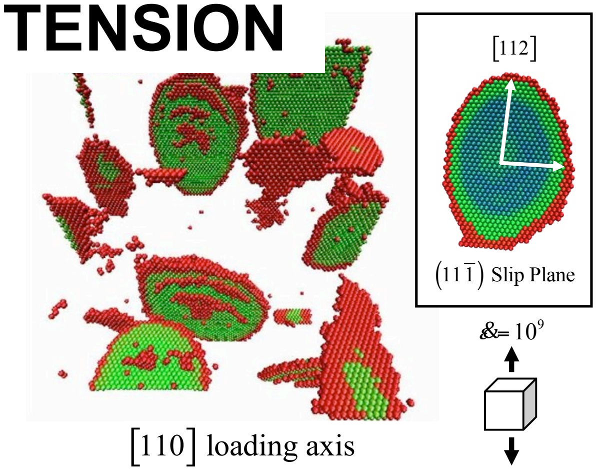
Boundary heterogeneous nucleation

$$\left(\sigma_{\max}\right)^{BC} = \left(1 - \xi D_c\right)\left(\sigma_{\max}\right)^{SC}$$

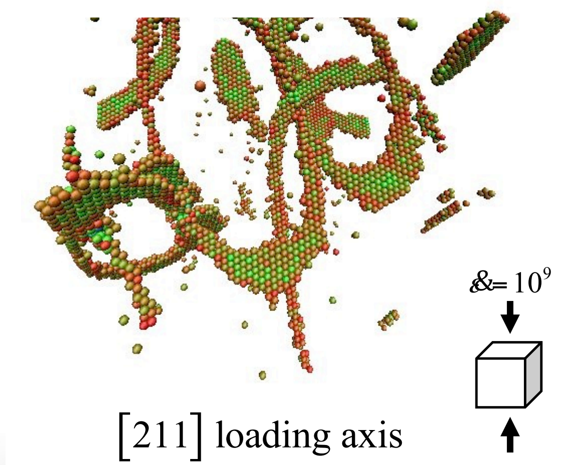
Tschopp, Spearot, McDowell, MSMSE, 15 (2007) 693.
Tschopp, Spearot, McDowell, Nabarro Tribute, Ed. J.P. Hirth, Elsevier, 2008, 43.

Dislocation Nucleation in Cu: Tension-Compression Asymmetry

TENSION

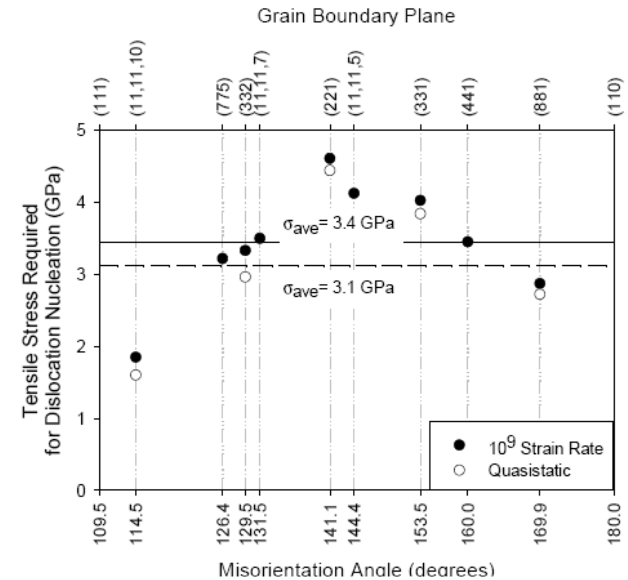


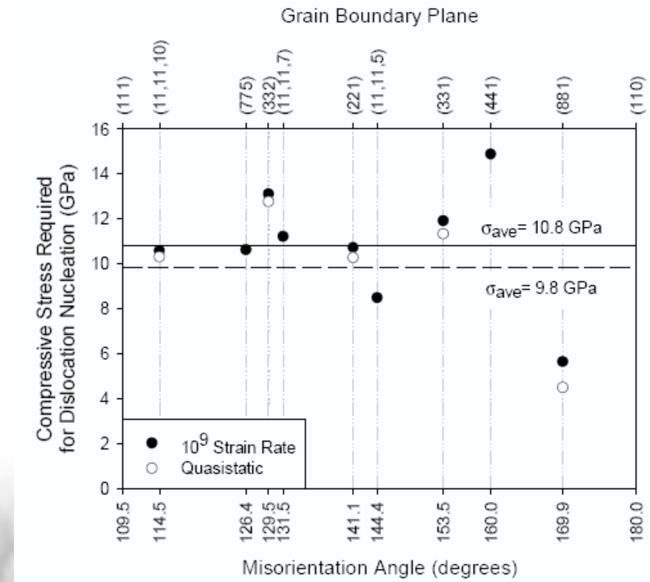
COMPRESSION



<110> grain boundary structures

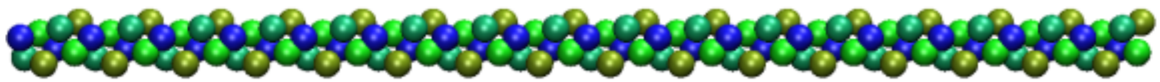
(Tschopp, Tucker, McDowell, Acta Mater. 2008)





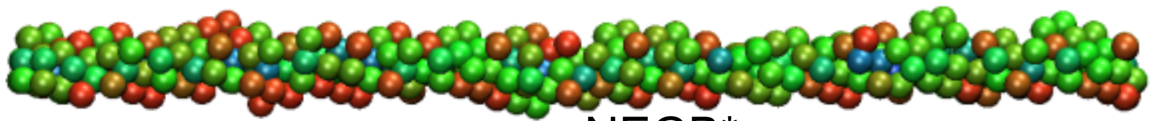
Tschopp, McDowell, JMPS, 56 (2008) 1806.

Non-eqilibrium GB structures



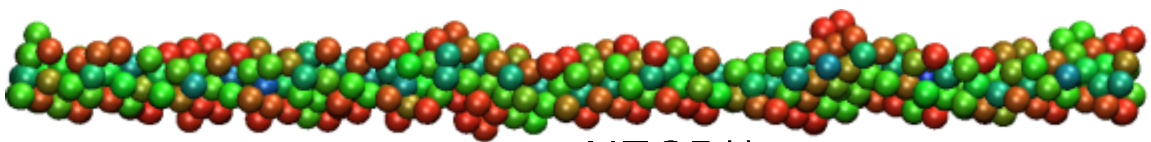
EGB

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



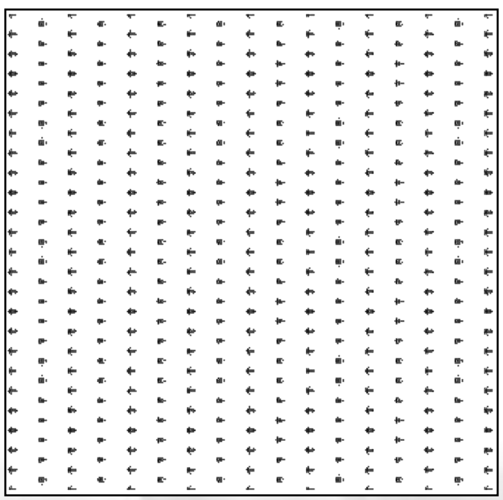
NEGB*

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

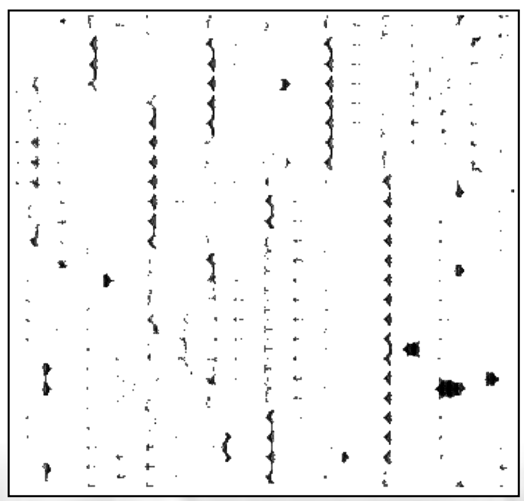


NEGB**

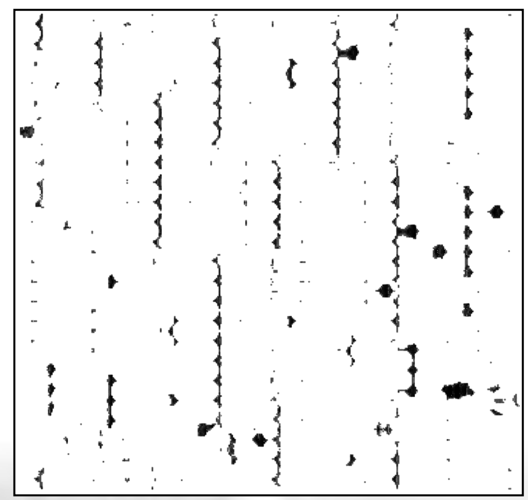
γ_{GB} = 919 mJ/m^2
FV_{GB} = 7.94e-04



EGB



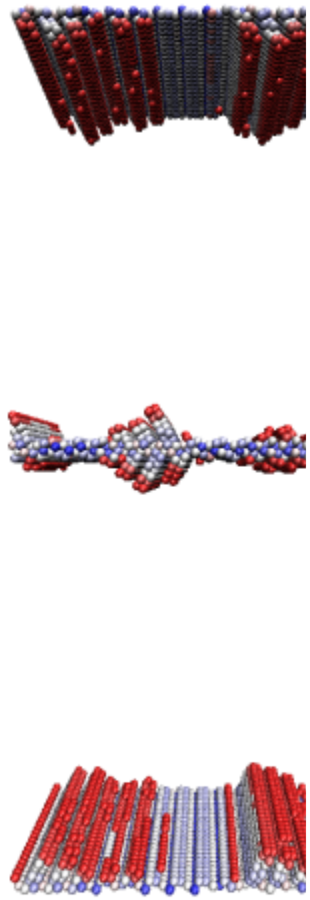
NEGB*



NEGB**

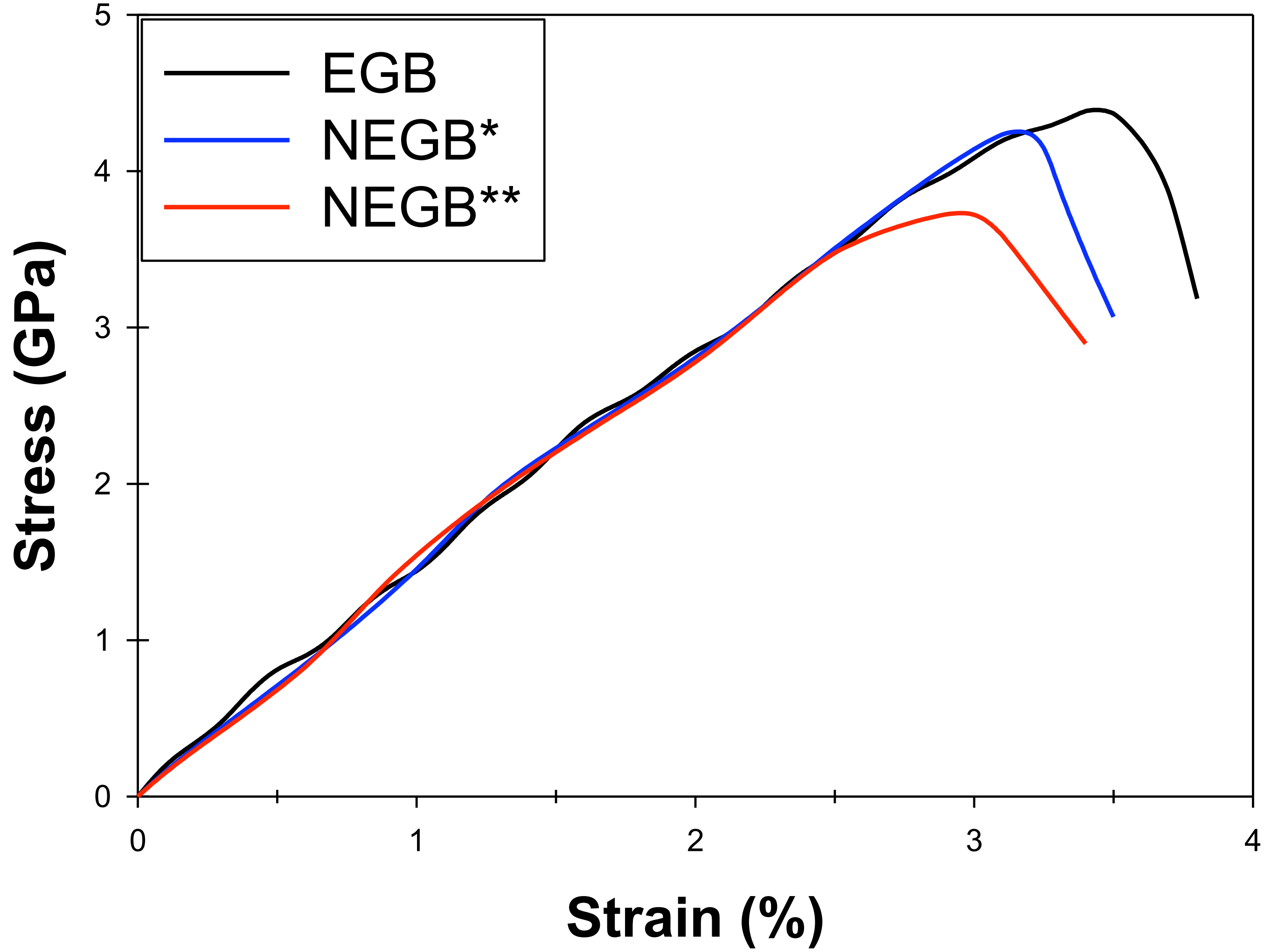
GB Deformation-Tension

GB Dislocation Nucle

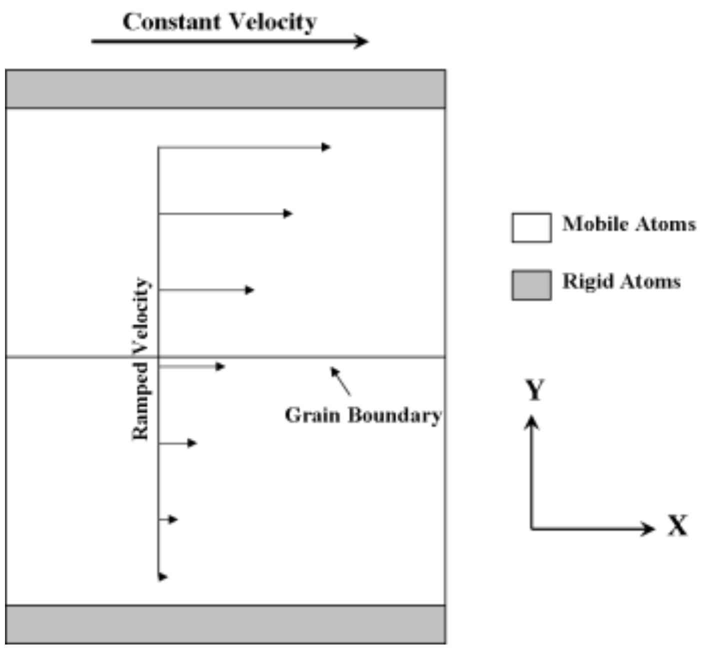


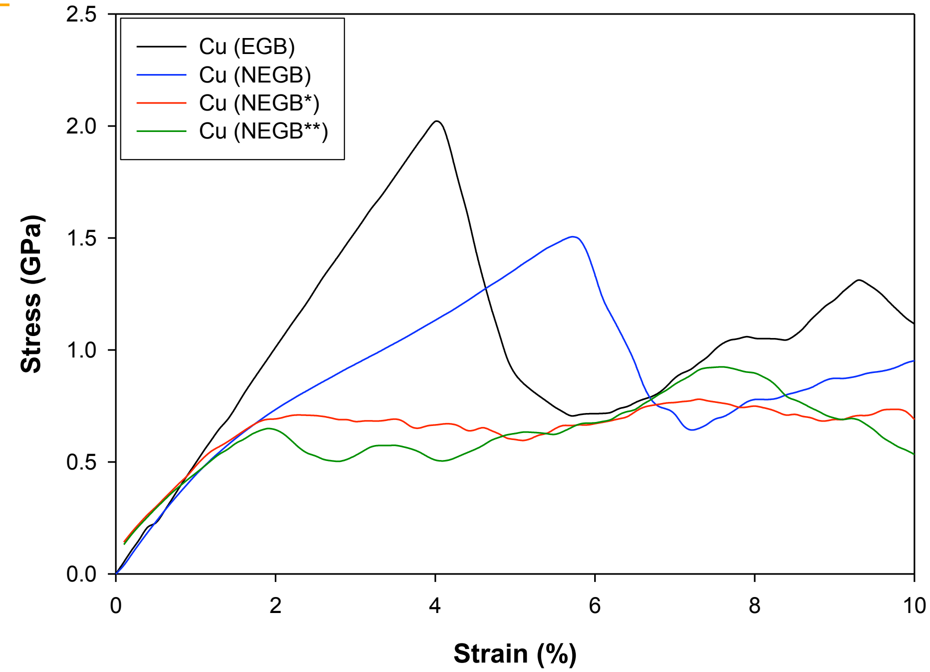
EGB

σ_{max} = 4.38



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

Some Implications for NC Metal Plasticity

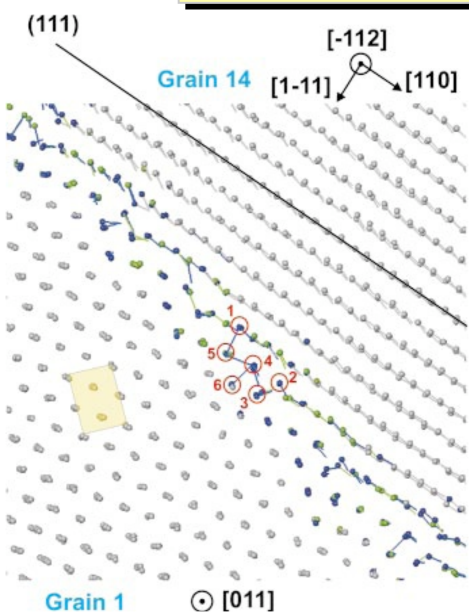
- ✓ Non-Schmid effects
- ✓ Tension-compression asymmetry
- ✓ Competing/combined effects of
  - GB reordering,shuffling/sliding, and/or migration
  - dislocation nucleation/absorption

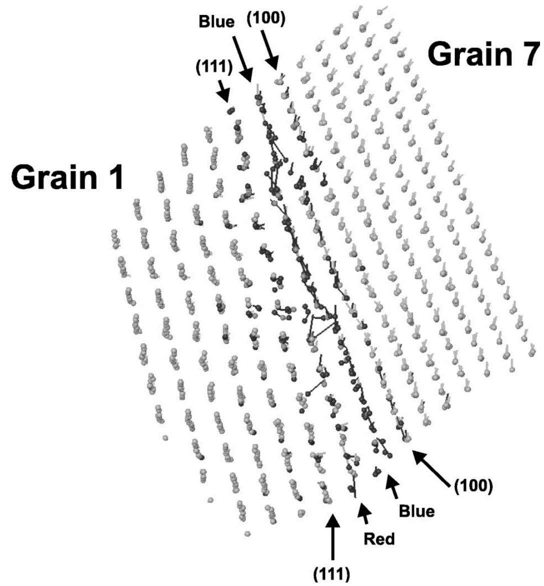
- ➢ Sensitive to GB network
- ➢ Affected by excess free volume – NEGB structures

****Deformation mechanisms are also thermally activated, which poses challenges for direct MD simulation of multiple mechanisms with different activation enthalpies.**

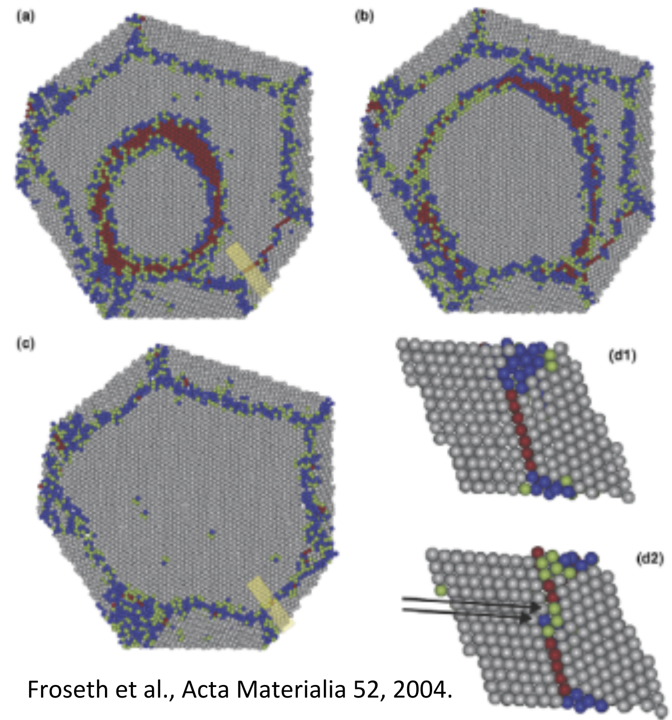
NC Inelastic Deformation Mechanisms

GB Sliding/Atomic Shuffling



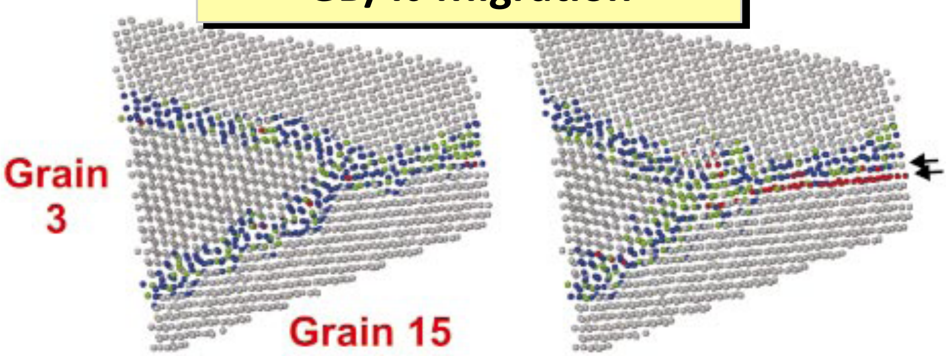


Dislocation Nucleation

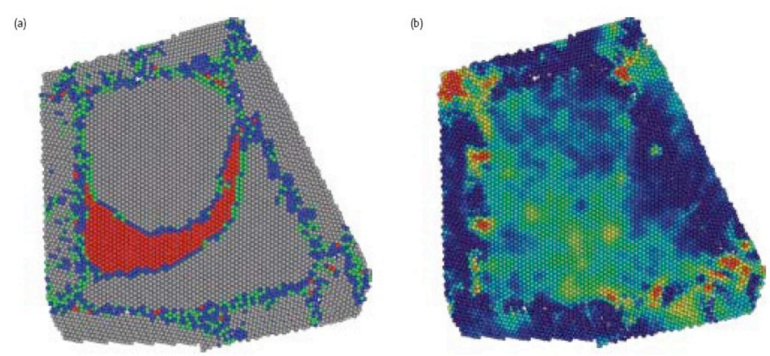


Froseth et al., Acta Materialia 52, 2004.

GB/TJ Migration

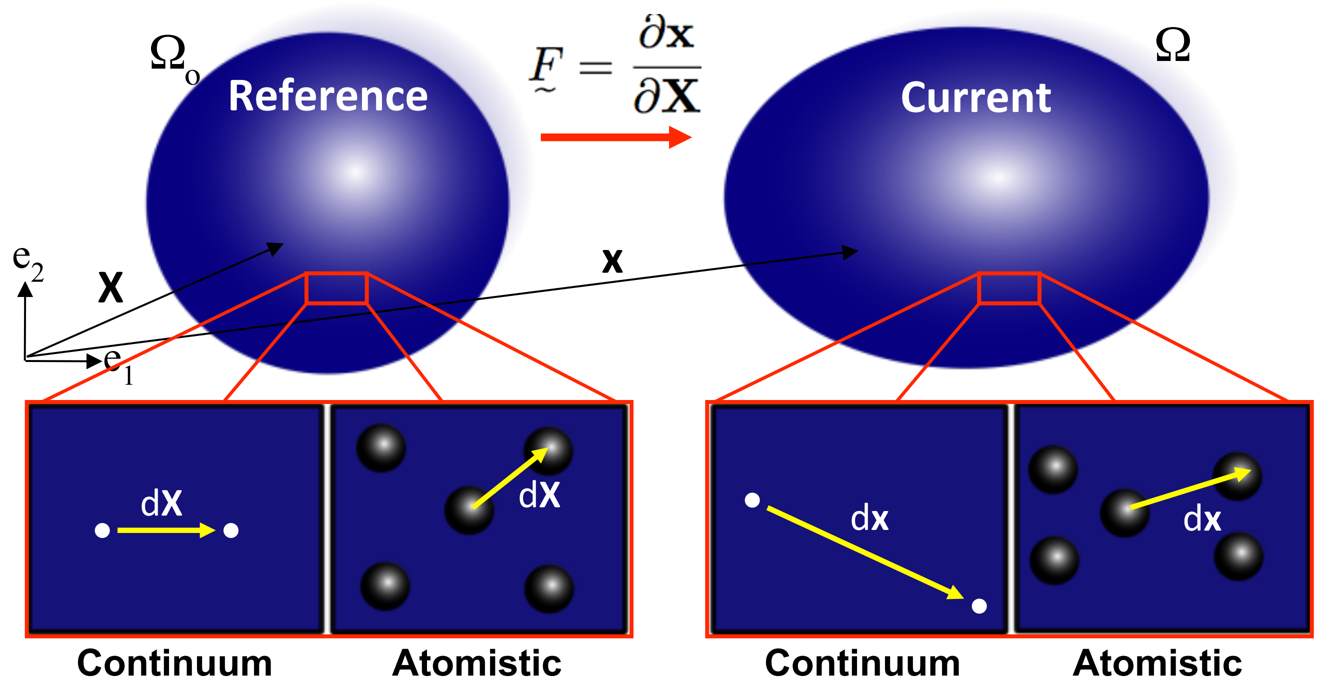


Van Swygenhoven and Derlet., PRB 64, 2001.



Van Swygenhoven, Materials Today 9, 2006.

Kinematics



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

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

* 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., submitted to Int. J. Engineering Science in memoriam to C. Eringen, July 2010.

Why Continuum Metrics?

Metal plasticity at the nanoscale is complex

- Various deformation mechanisms
- Use of centrosymmetry, slip vector, etc. is complicated in terms of characterization and visualization of high density of evolving line defects

Informing continuum models

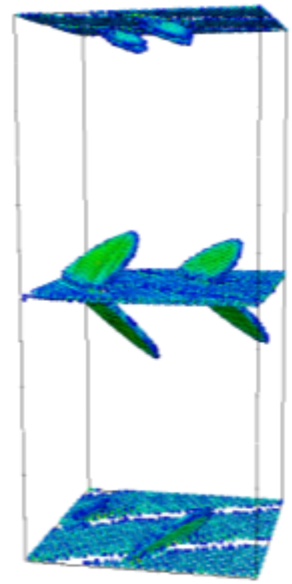
- Kinematics of continuum description can perhaps be bridged in terms of understanding based on statistical fields from atomistic simulations
- Check assumptions, trends from proposed continuum constitutive models (e.g., Khan et al. (2006), Capolungo et al. (2007), Wei and Anand (2004) and Wei et al.(2006))

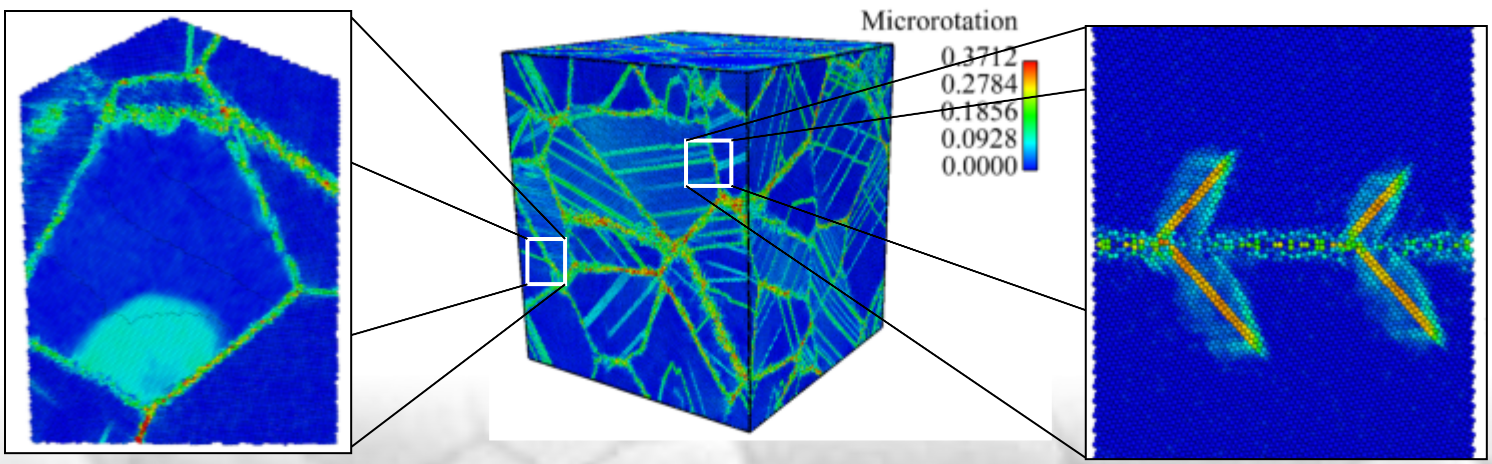
Some connections

- microrotation (**ϕ**) and its gradient [Atomistics]
- micro- strain and torsion-flexure tensors [Continuum]

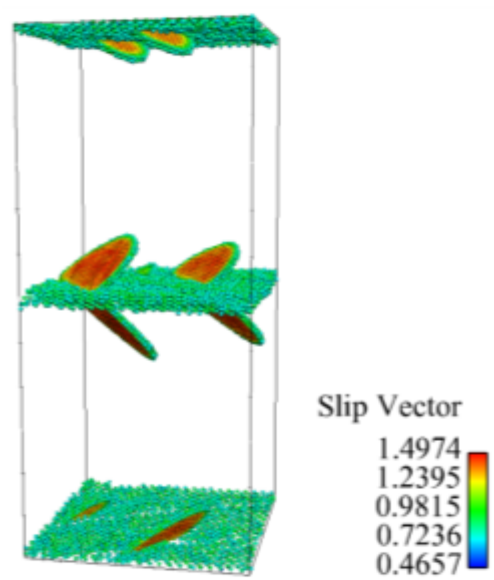
Objectives

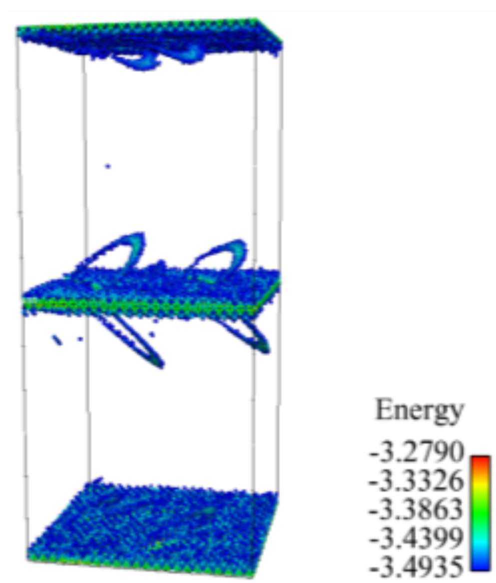
- Formulate continuum metrics for use in atomistic simulation analysis
- Investigate the evolution of metrics for various deformation mechanisms
- Resolve nanocrystalline copper deformation using continuum metrics
  - Dislocation Nucleation
  - GB Sliding/Atomic Shuffling

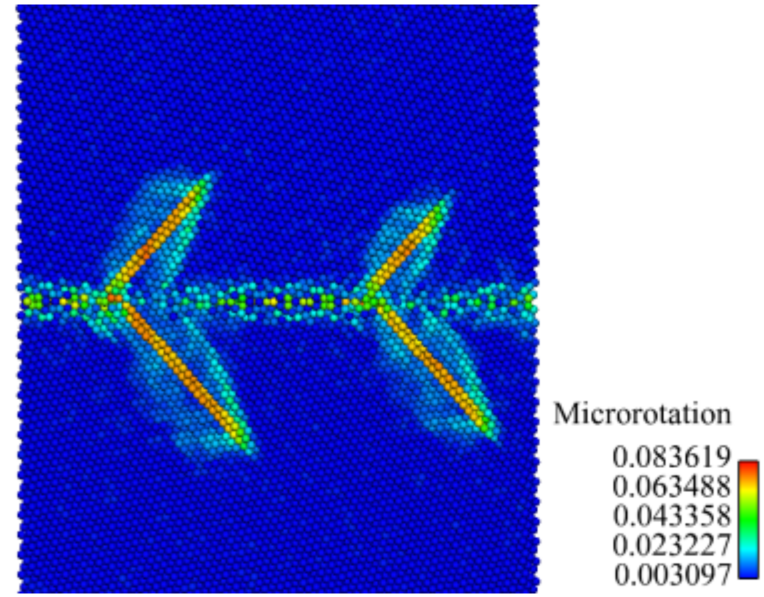


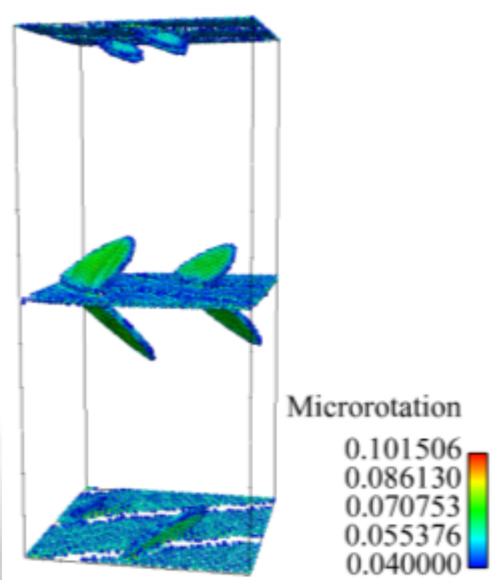


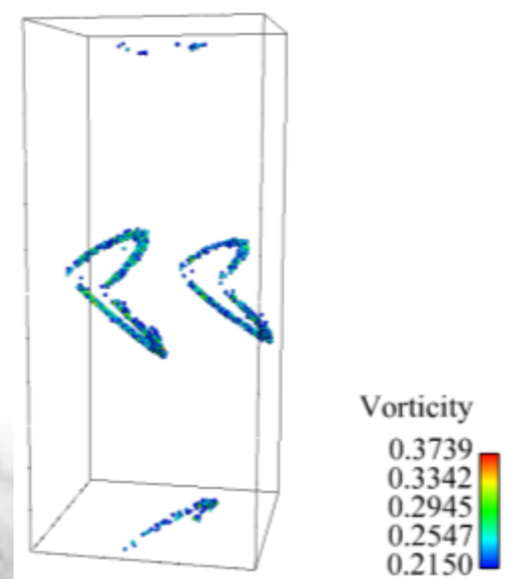
3D Dislocation Nucleation

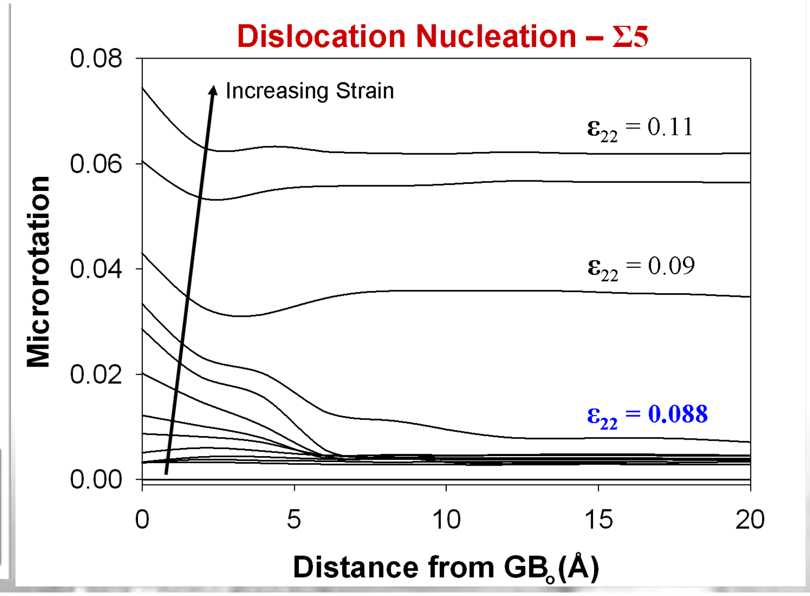






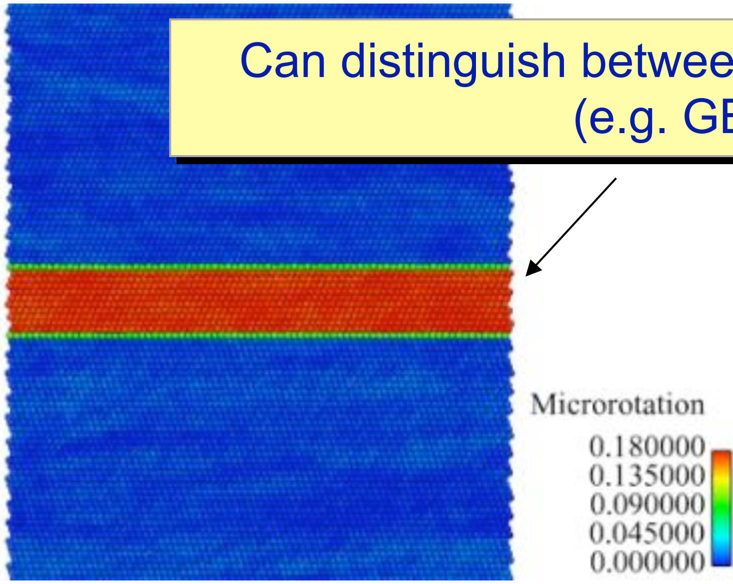


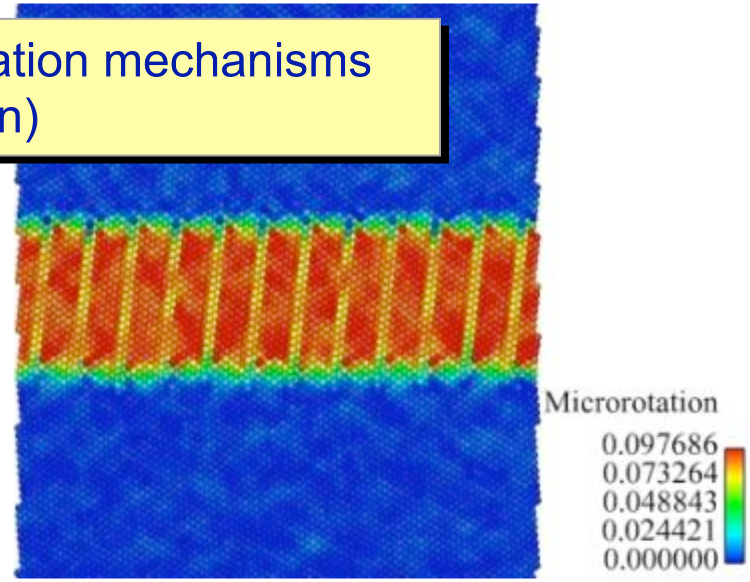


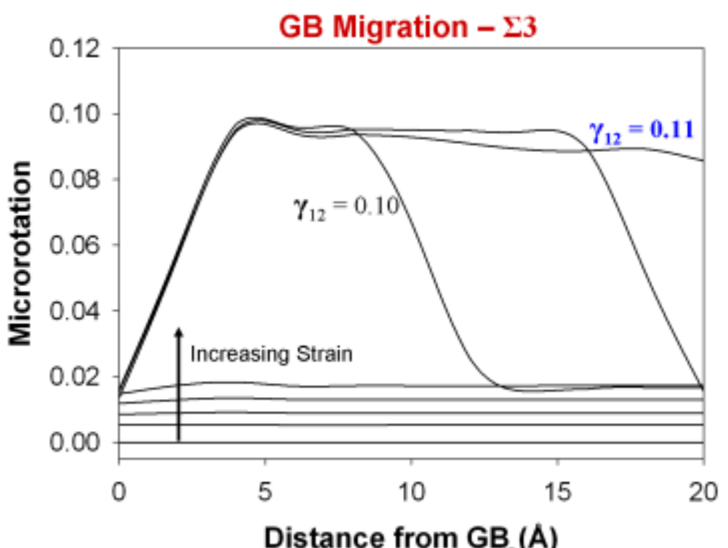


3D GB Migration

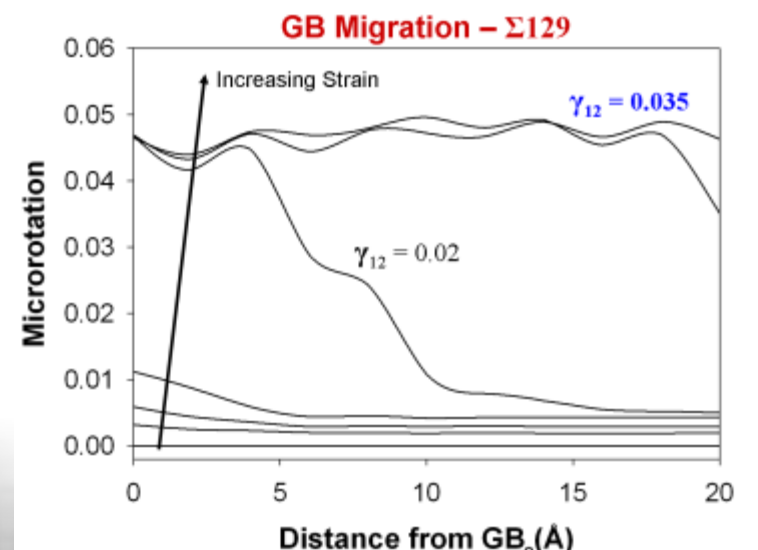
Can distinguish between deformation mechanisms (e.g. GB migration)







Average microrotation over slices || to boundary

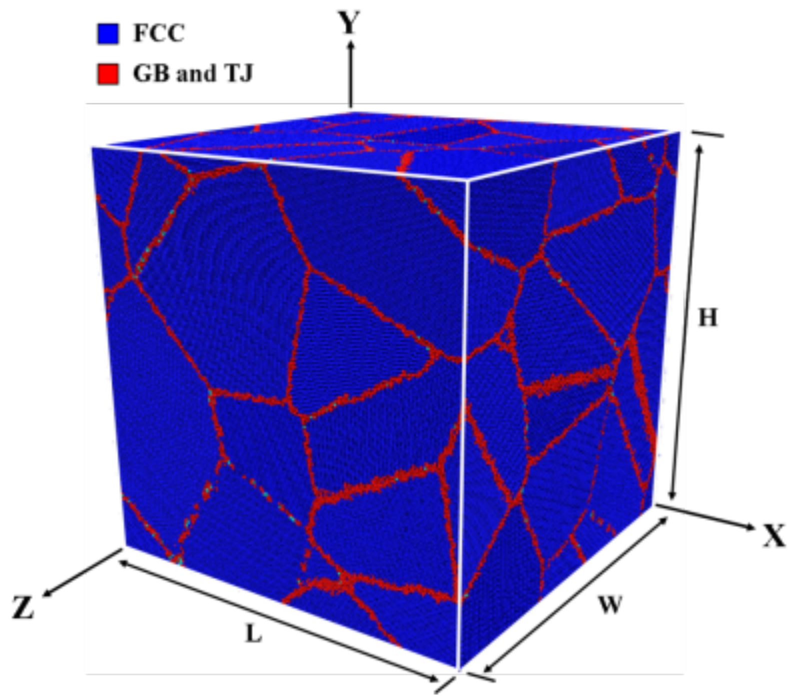


Tucker, G.J., Zimmerman, J.A., and McDowell, D.L., MSMSE 18(1) 2010, 015002.

3D NC simulations

- 3D periodic simulation domain
  - Orthogonal Box with edges oriented along X,Y,Z axis
  - Voronoi [1] tessellation to partition domain into grains
  - 25 grains

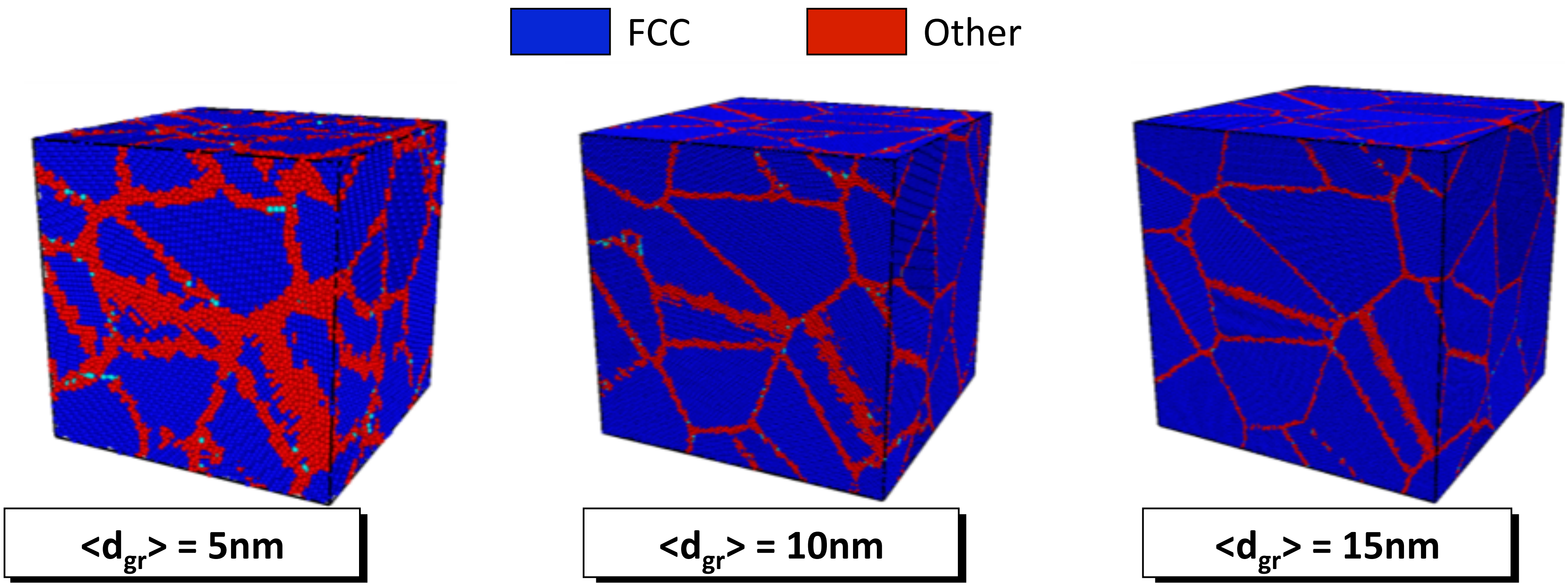
- Average Grain size= 5 - 15 nm
  - Lattice orientations chosen randomly for each grain



$$\langle g \rangle = \sqrt[3]{\frac{LHW}{n}}$$

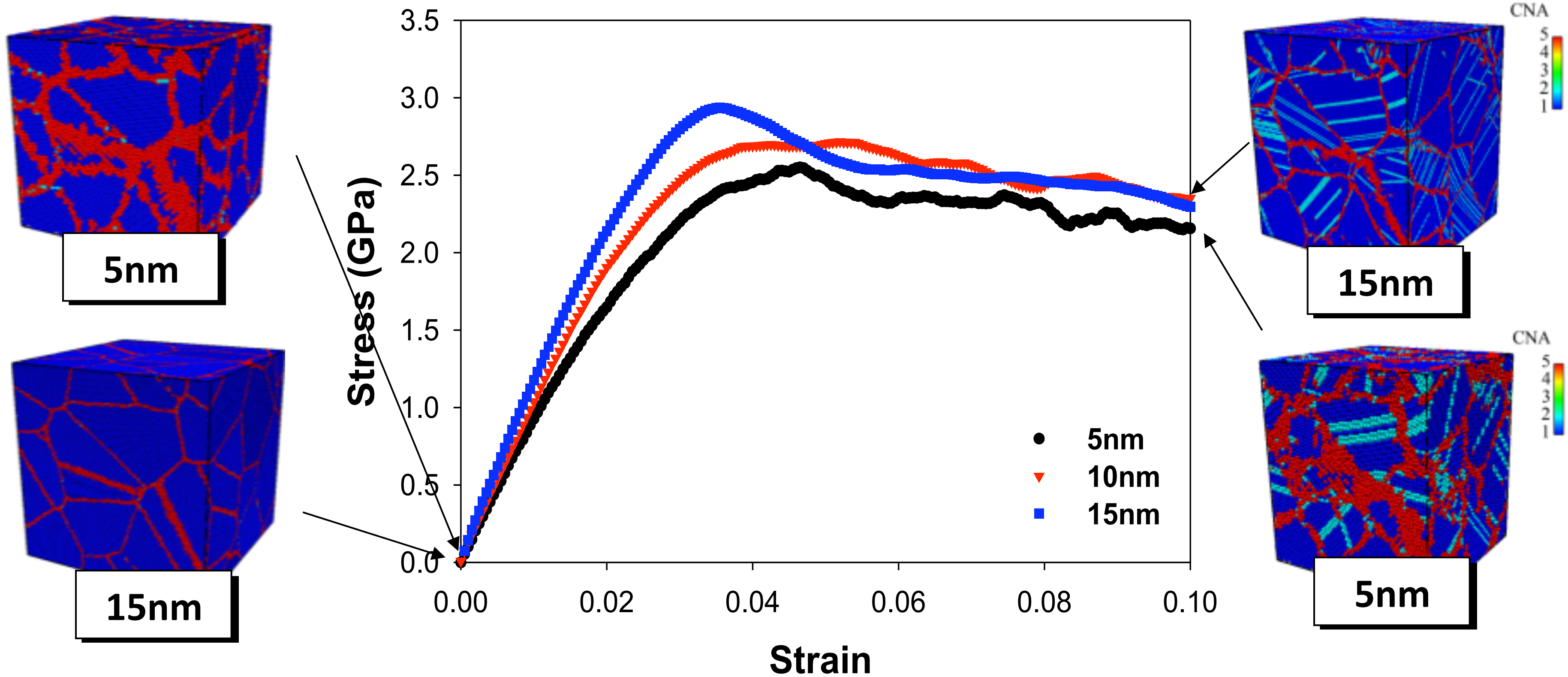
[1] Voro++., http://math.lbl.gov/voro++/

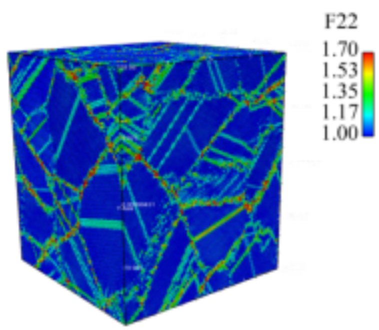
Nanocrystalline Copper



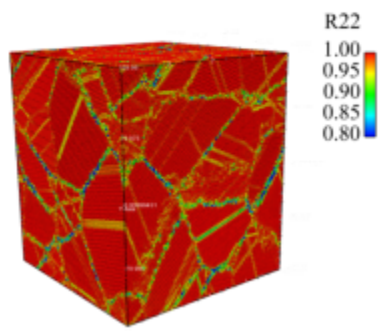
- Full 3D nanocrystalline structure (Voronoi Tessellation, random lattice orientations)
- 3D periodic BCs
- Atom overlap deletion and equilibration for 50 ps
- Uniaxial tension at 10K under NPT, const strain rate 10^9 s^{-1}
- Analysis of deformation mechanisms using microscale continuum metrics

Nanocrystalline Copper

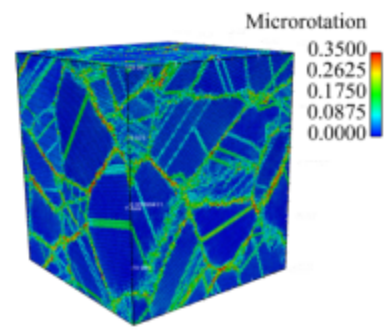




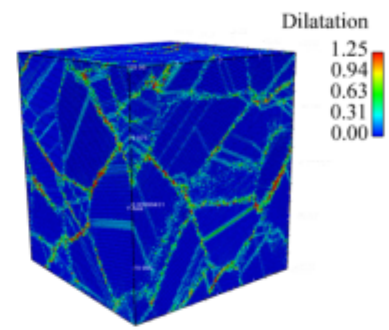
Deformation Gradient



Rotation Metric



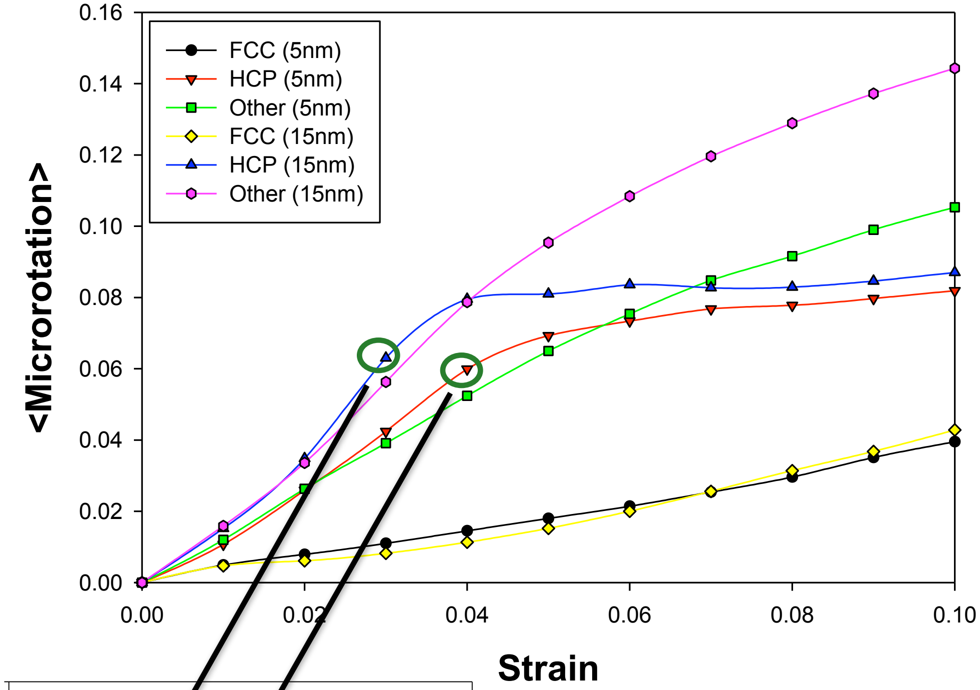
Microrotation

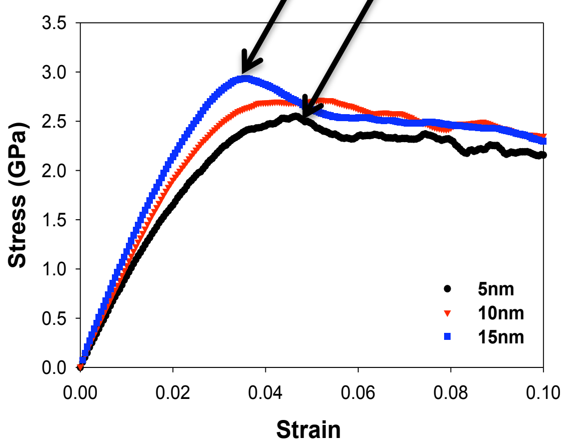


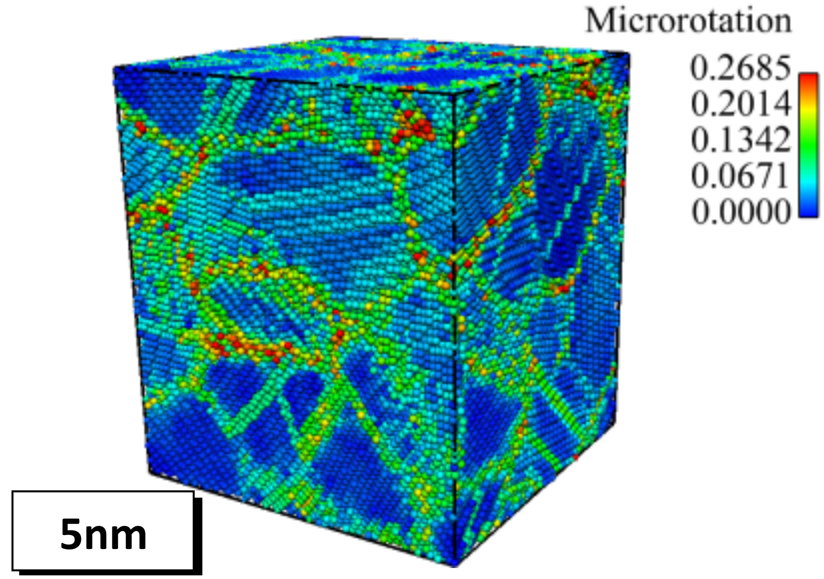
Dilatation

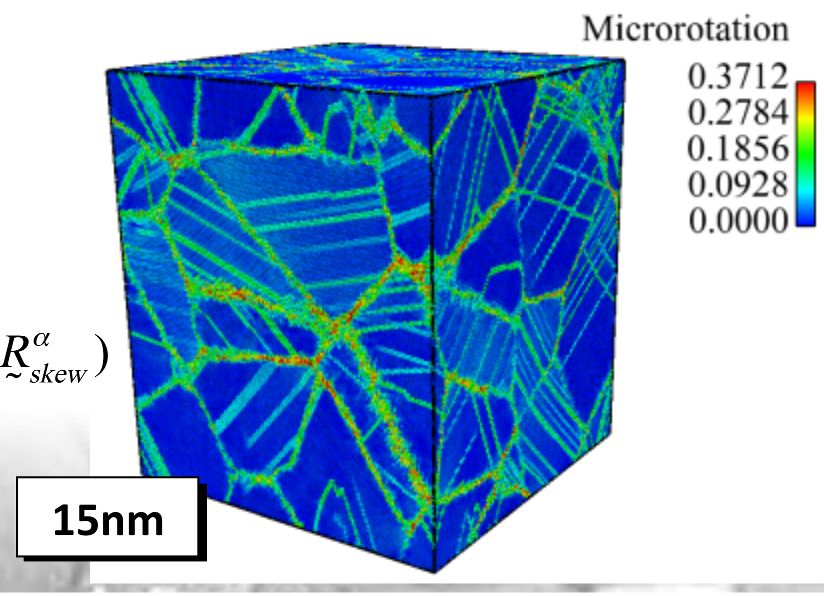
Nanocrystalline Copper

Phase averaged microrotation





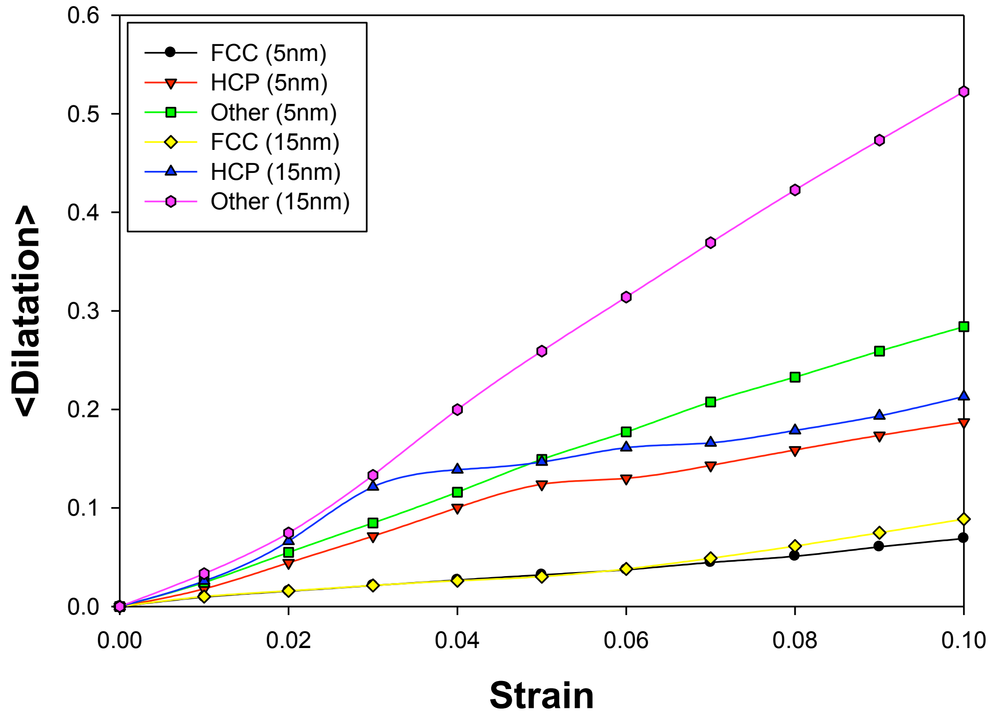


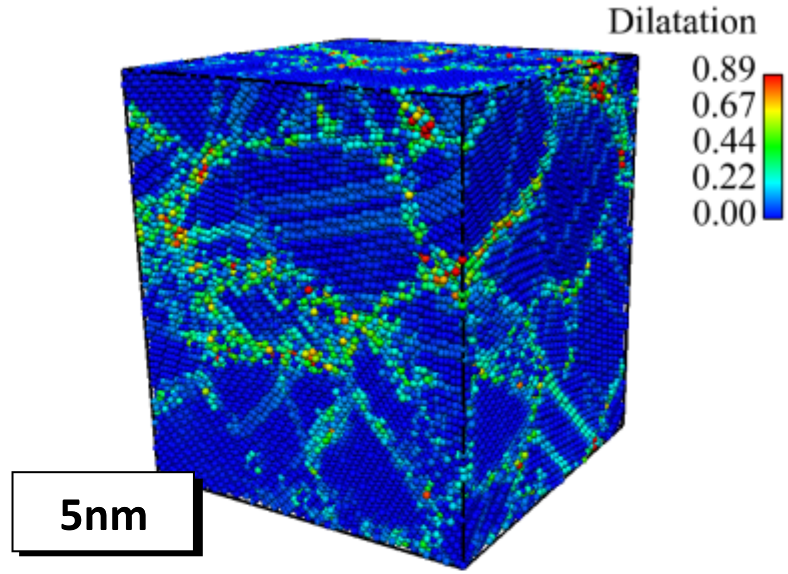


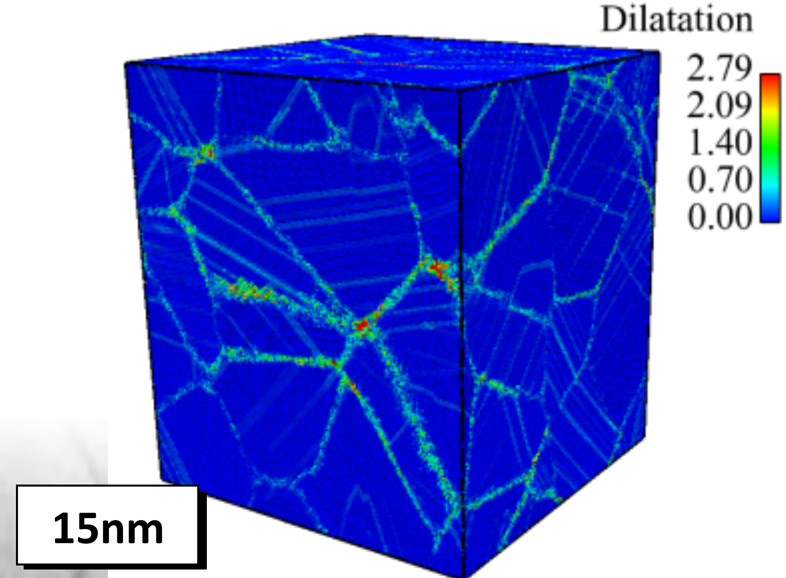
$$microrotation \equiv \vec{\phi}^{\alpha} = -\frac{1}{2}\underset{\sim}{\varepsilon}(\underset{\sim}{R}^{\alpha}_{skew})$$

Nanocrystalline Copper

Phase averaged dilatation



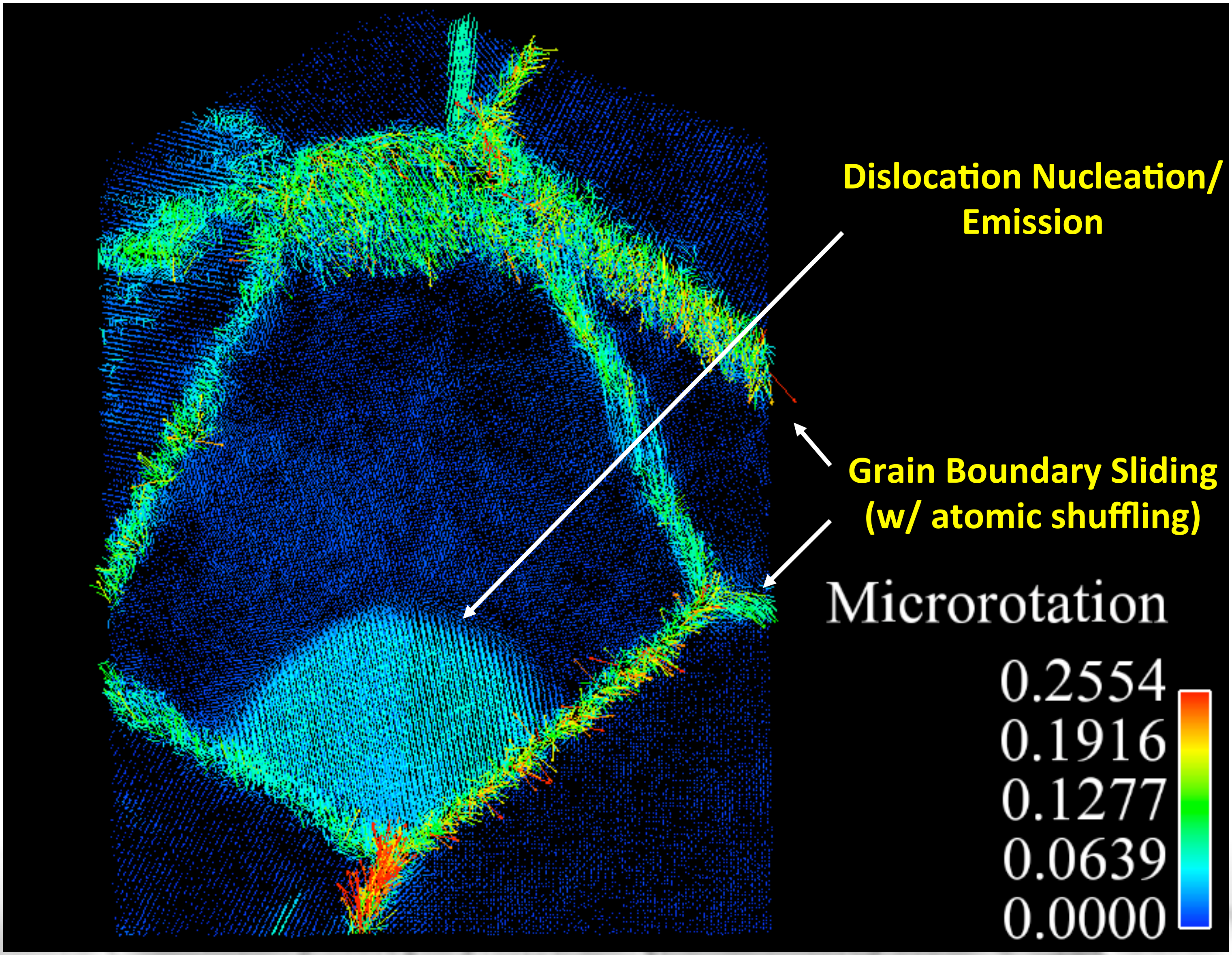




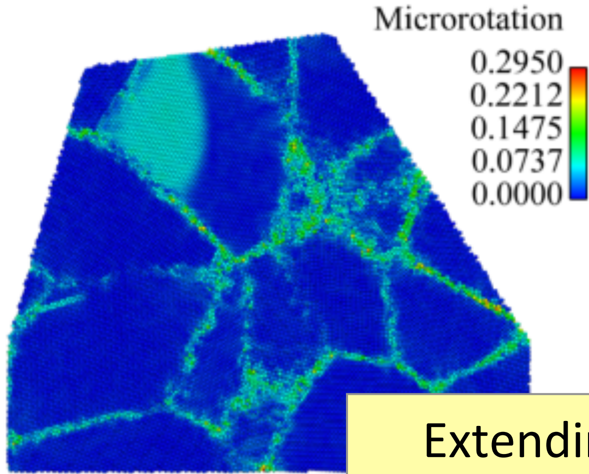
$$\underset{\sim}{E} = \frac{1}{2}\left[\underset{\sim}{F}^T \underset{\sim}{F} - \underset{\sim}{I}\right]$$

$$\longrightarrow \quad dilatation \equiv e^{\alpha} = tr(\underset{\sim}{E}^{\alpha})$$

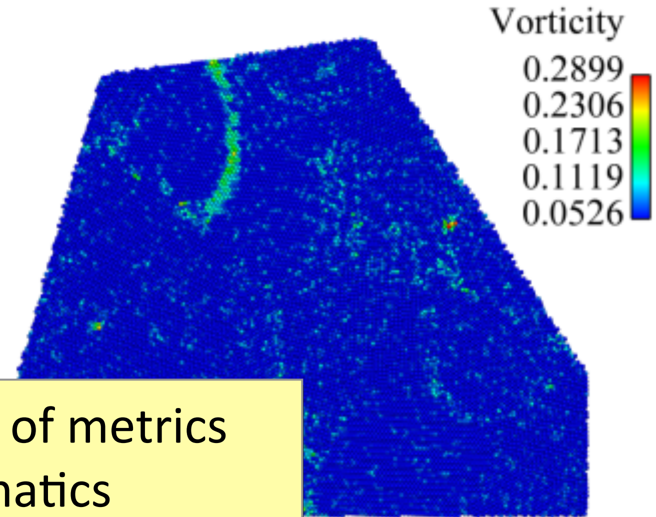
Microrotation – Vector Field



Effects of Averaging Nonlocality

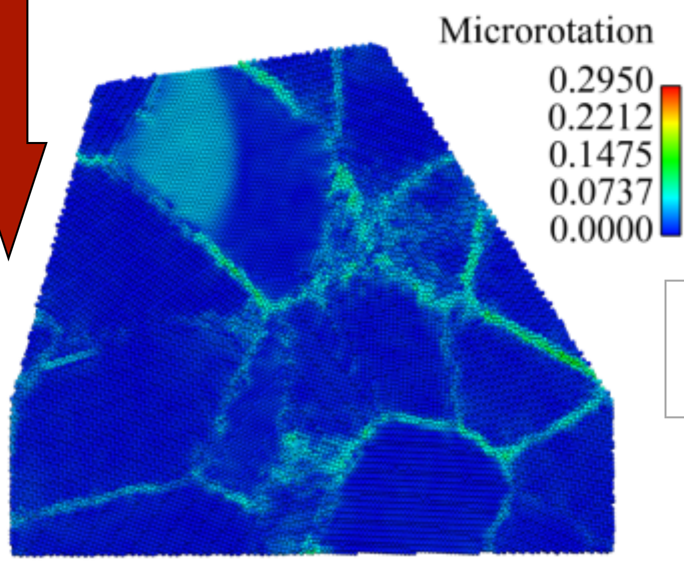


1st Nearest Neighbors only

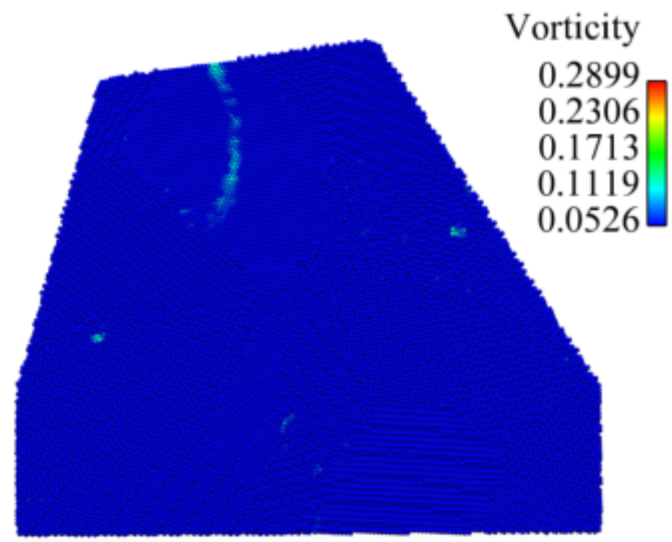


Increasing non-locality

Extending non-locality of metrics 'filters' the kinematics

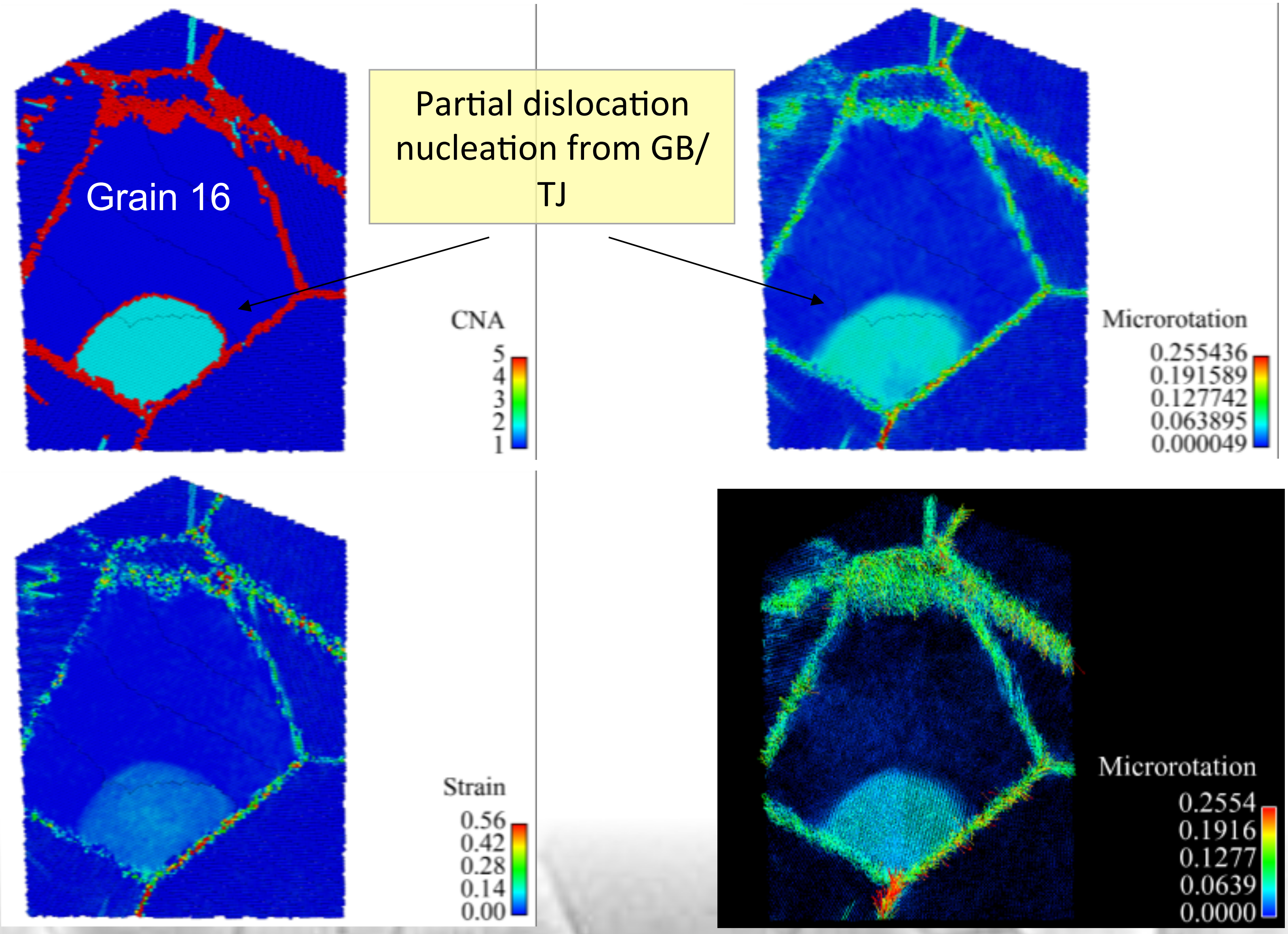


3rd Nearest Neighbors

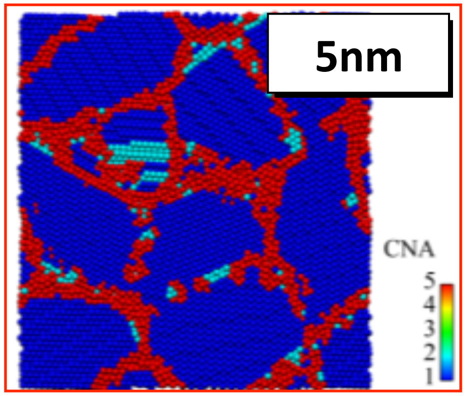


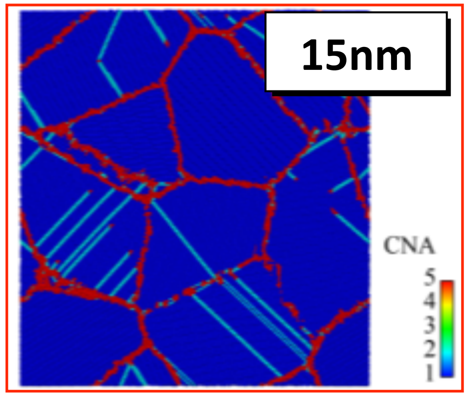
Nanocrystalline Copper

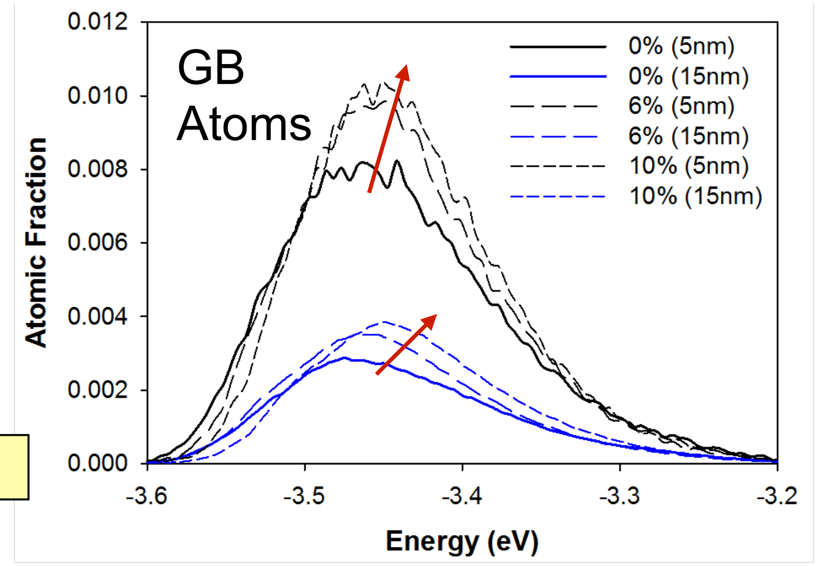
Partial dislocation nucleation from GB/TJ

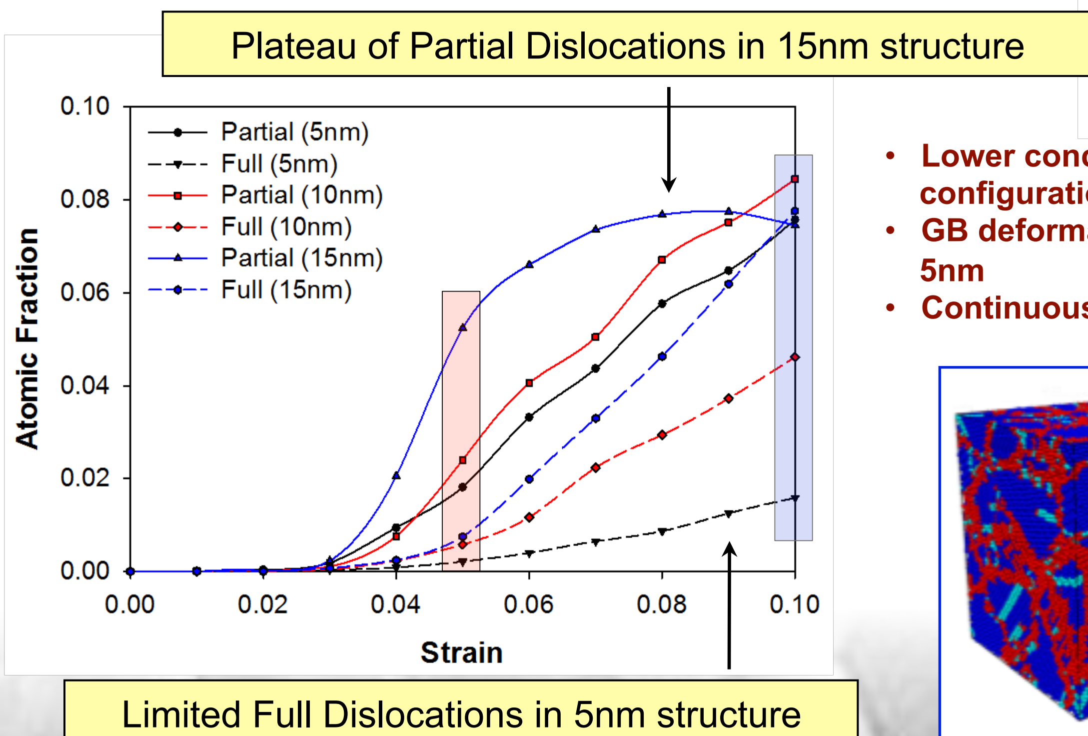


Dislocation/GB Deformation

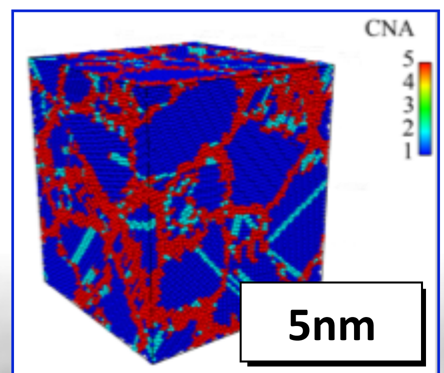


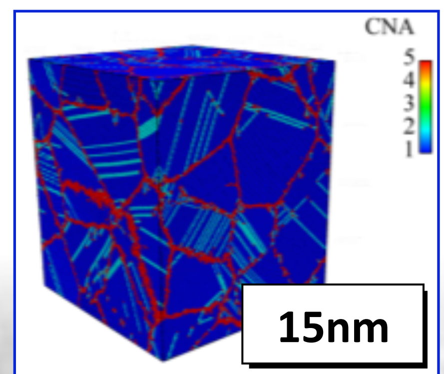




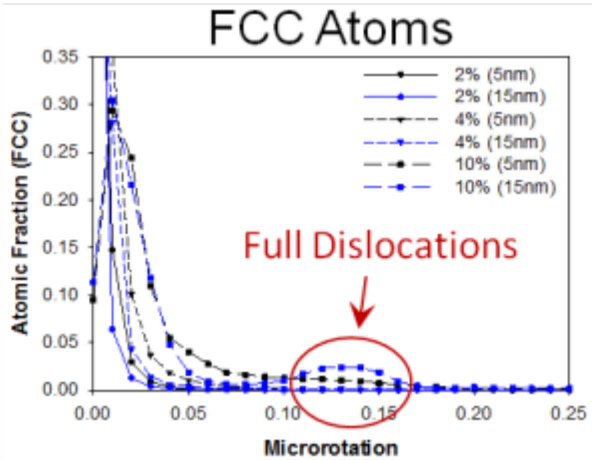


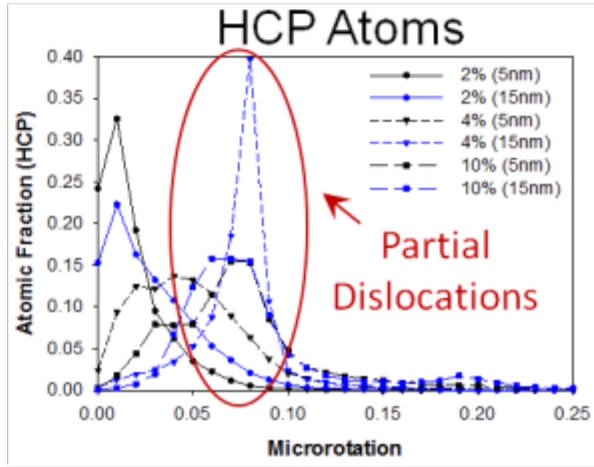
- Lower concentration and lower energy GBs in 15nm NC configuration than in the 5nm structure at 0% tensile strain
- GB deformation is dominant and begins at lower strains – 5nm
- Continuous GB accommodation with dislocation slip – 15nm

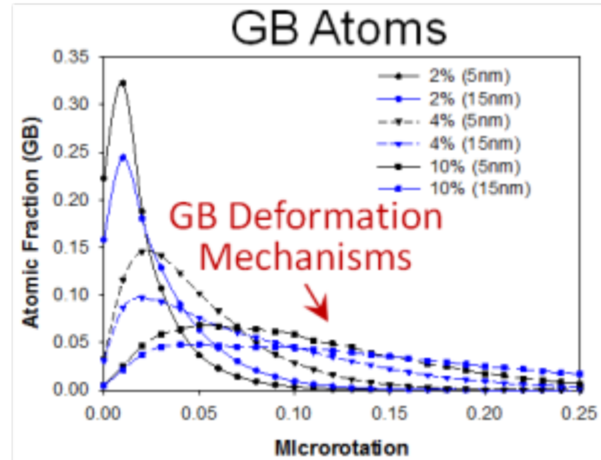


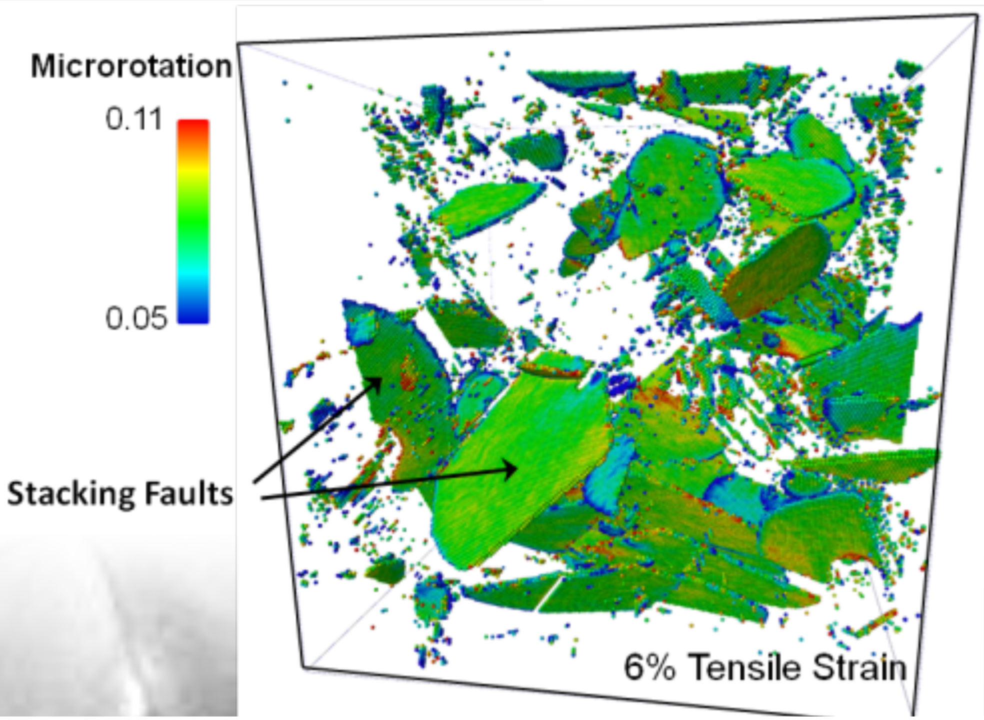


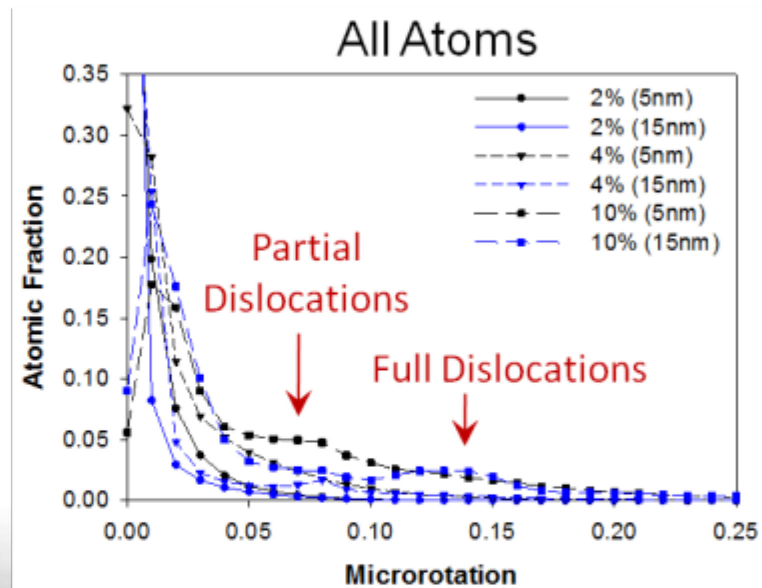
Microrotation Distribution



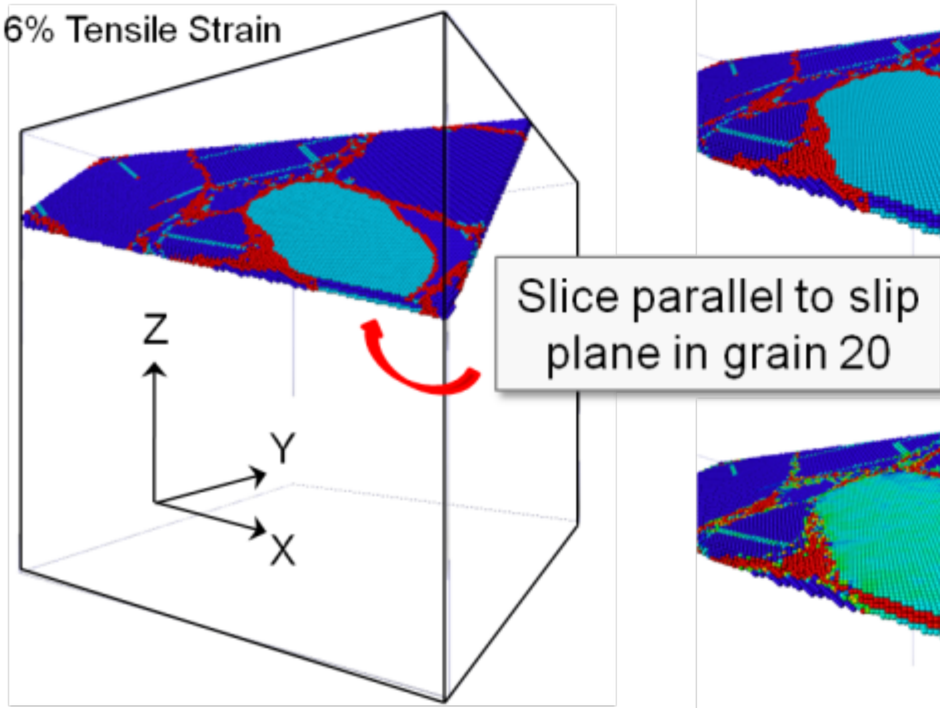




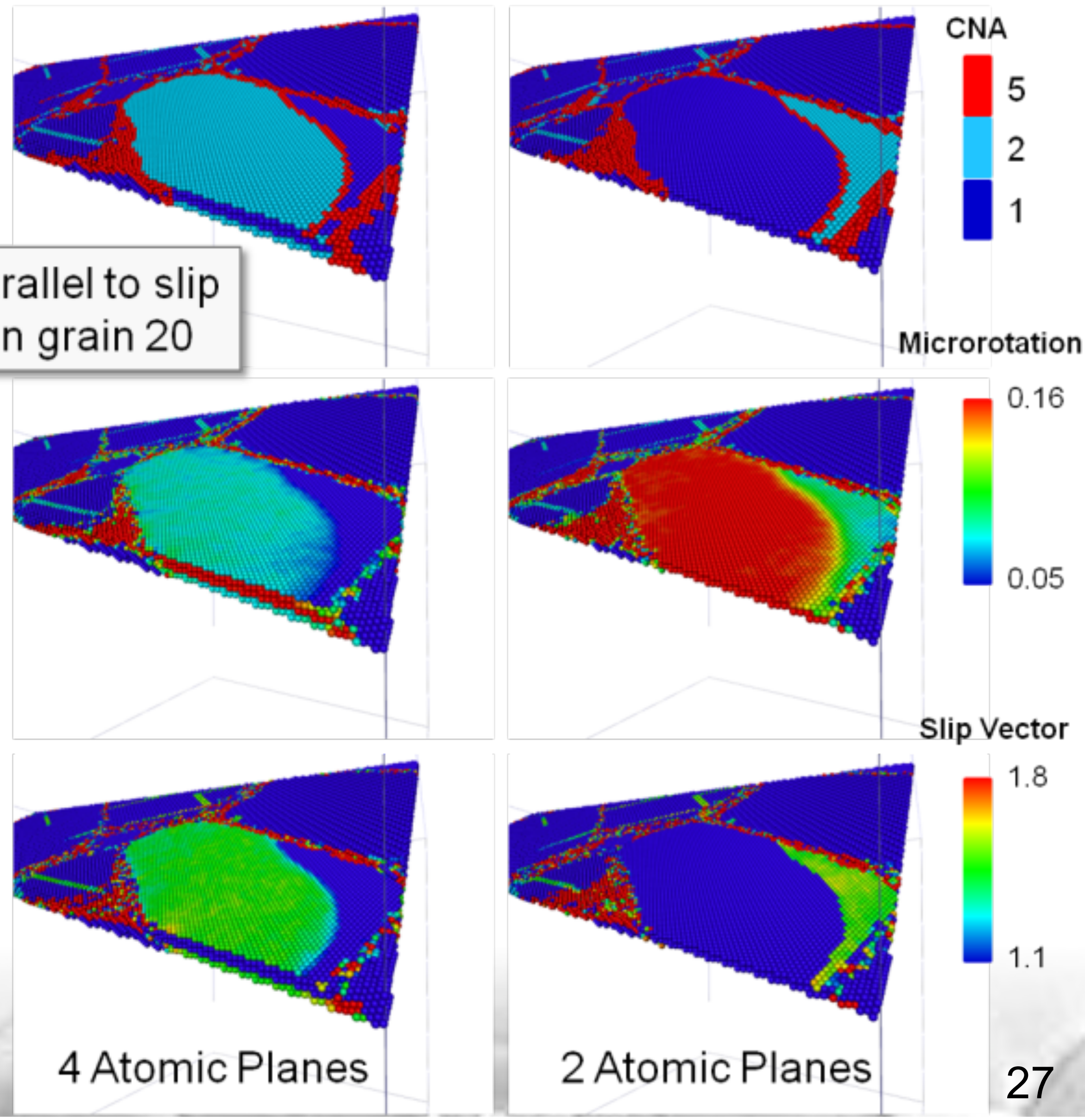




Advantage of Microrotation



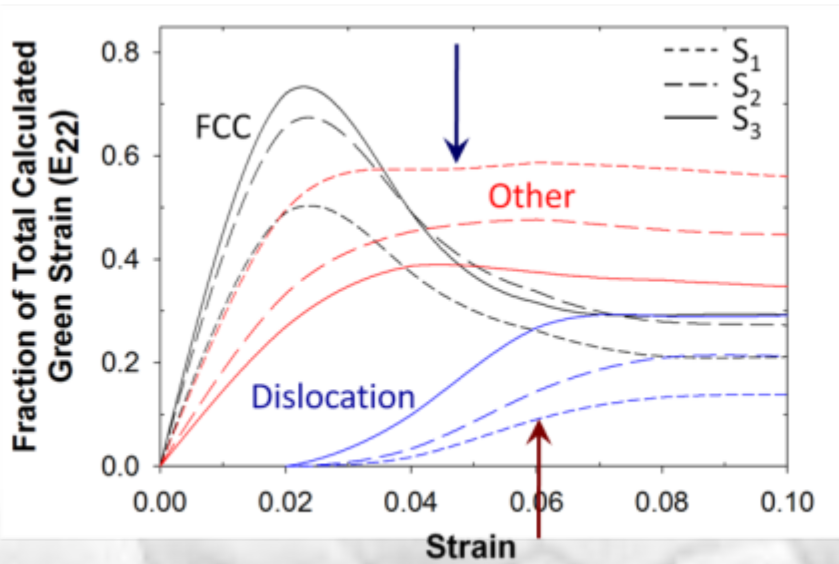
- *Microrotation* is able to capture important deformation behavior (e.g. **dislocation slip**) and structural features (e.g. **stacking fault**) usually visualized using *CNA* and atomic *slip vector* together.
- Potential to be passed into continuum level models as kinematic variable.

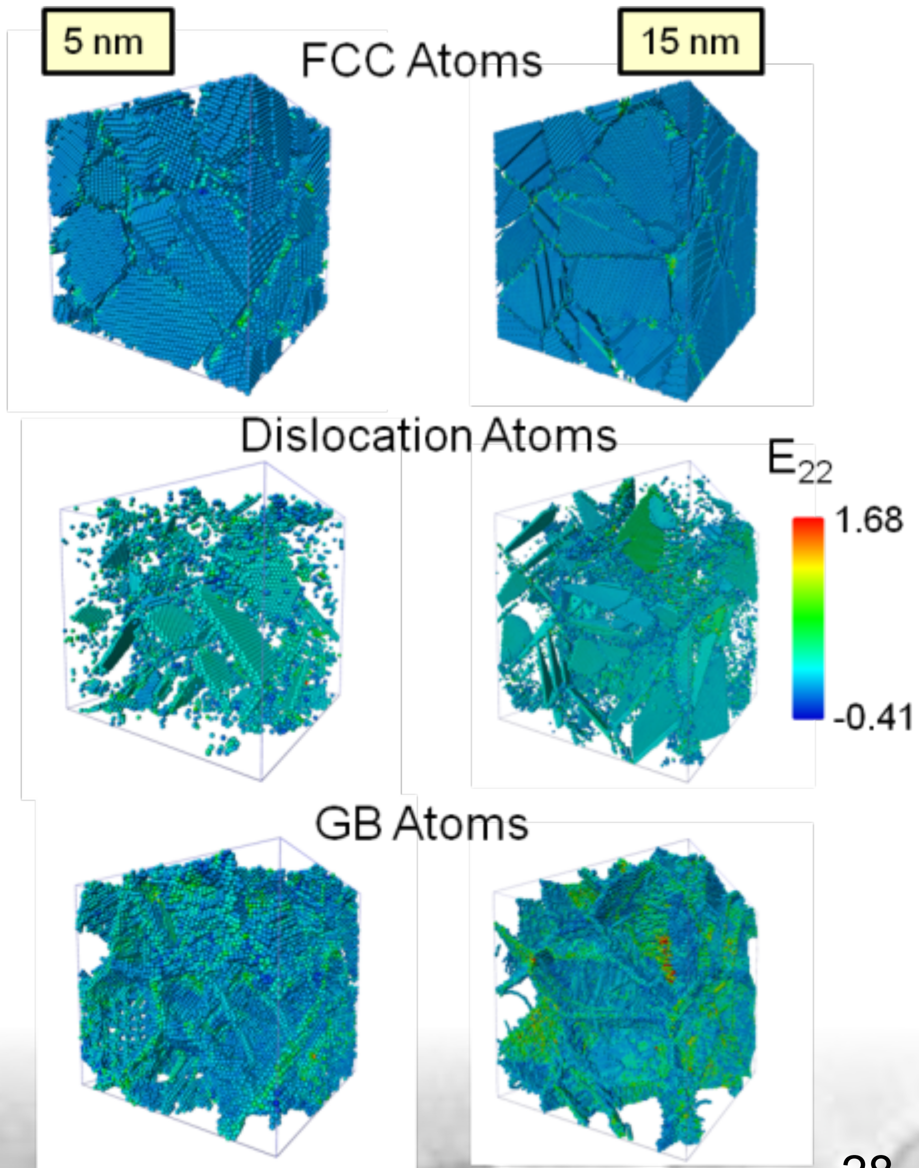


Green Strain

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

- E_{22} from all atom in a phase (e.g. FCC, GB, Dislocation) added together.
- 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.

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