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Exploring the Evolution and Deformation of Twinned Nanocrystalline Metals with Microscale Kinematic Metrics and Molecular Dynamics Simulations

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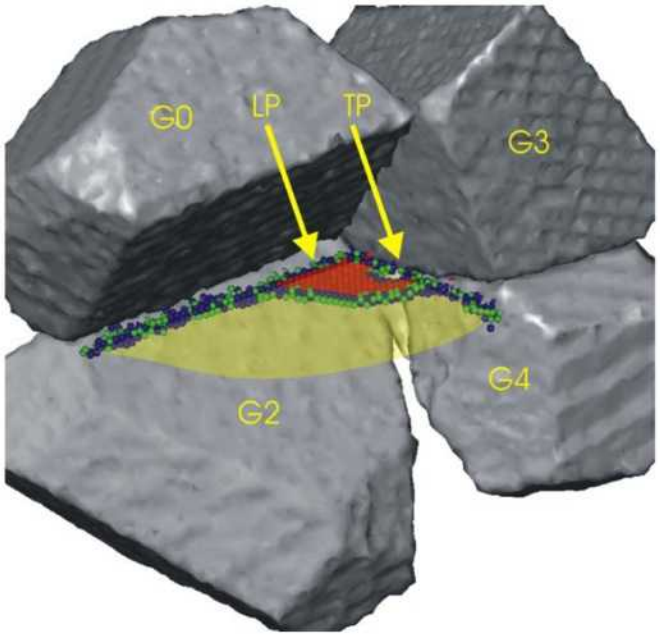
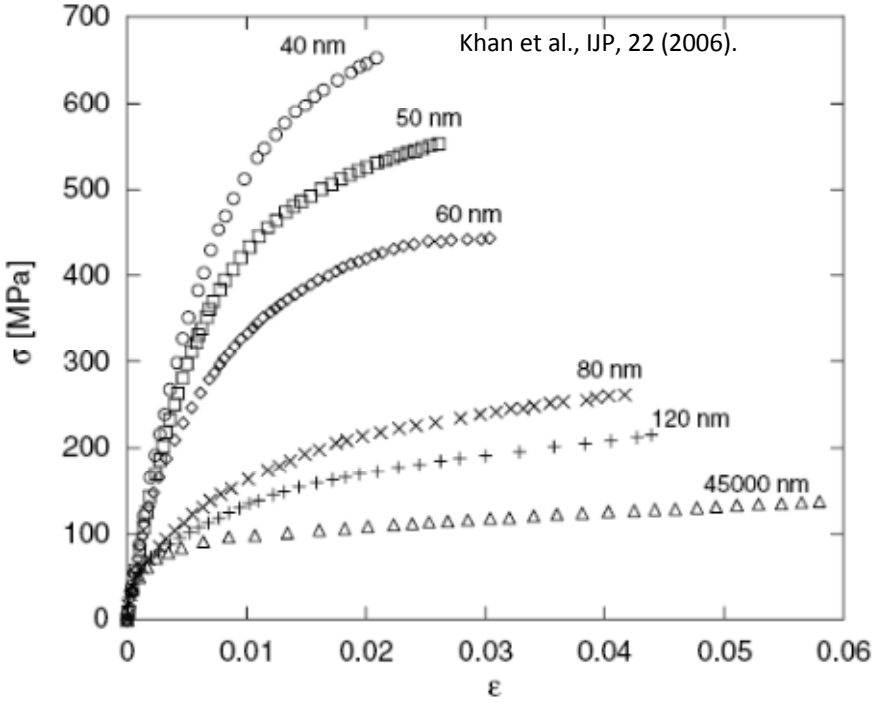
Why study Nanocrystalline Materials ?

- Mechanical properties of nanocrystalline (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 nanoscale deformation processes, both elastic and inelastic.



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

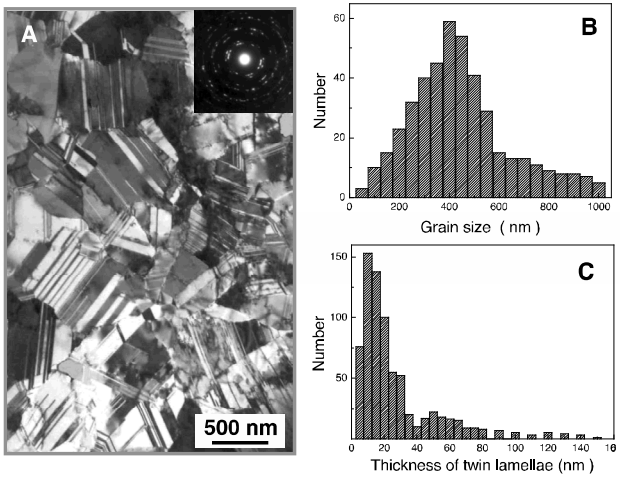


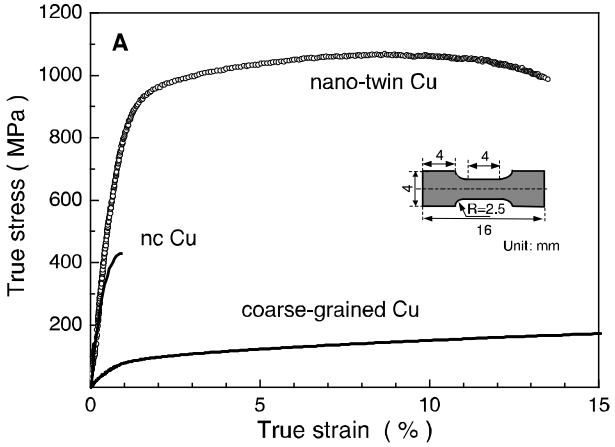
- Various deformation mechanisms have been observed to cooperate/compete to accommodation strain within NC metals.
- A direct relationship between nanoscale structure and properties for interfaces in NC materials.

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

Why Twinned Nanocrystalline Metals ?

- Nanocrystalline (NC) Cu samples with nanoscale growth twins from pulsed electrodeposition have displayed higher mechanical strength while preserving the electrical conductivity.
- Coherent twin boundaries (TBs) serve to block the migration of lattice dislocations* leading to the observed work hardening.



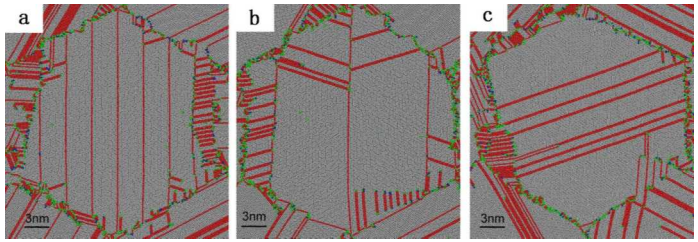


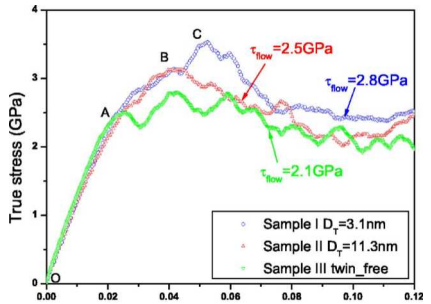
L. Lu et al., Science (2004)

* J.W. Christian and S. Mahajan, Prog. Mater. Sci (1995)

Molecular Dynamics Simulations

- MD simulations of <110> columnar NC Cu show that TBs can serve as dislocation nucleation sites as the TBs lose coherency.
- The presence of twin lamellar can influence the mechanical properties of strength and ductility.
- TBs serve as obstacles to migrating lattice dislocations and therefore can lead to high strain hardening rate in nanotwinned (NT) Cu.
- Thickness of twin lamellar also influences mechanics and tendency of TBs to act as sources.



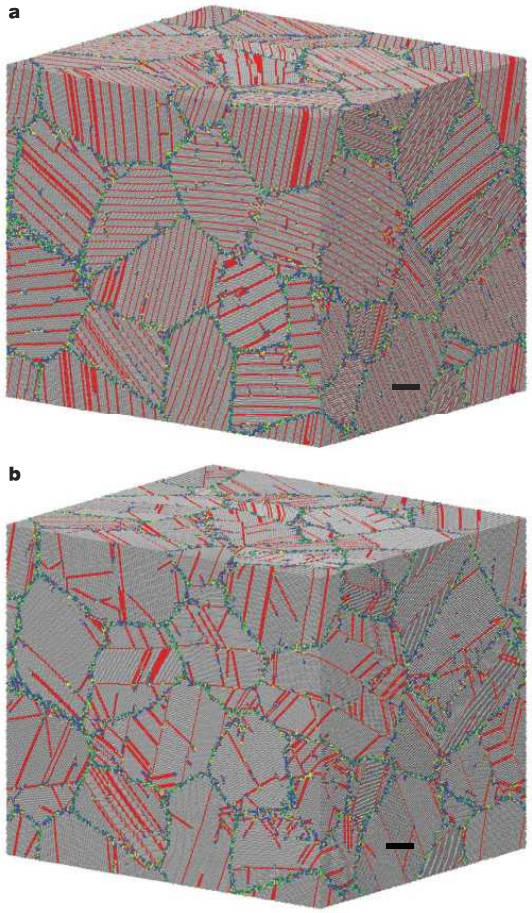


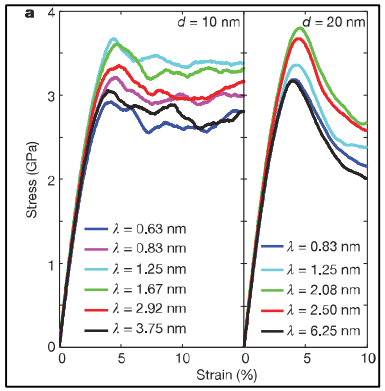
A.J. Cao and Y.G. Wei, J. of Applied Physics (2007)

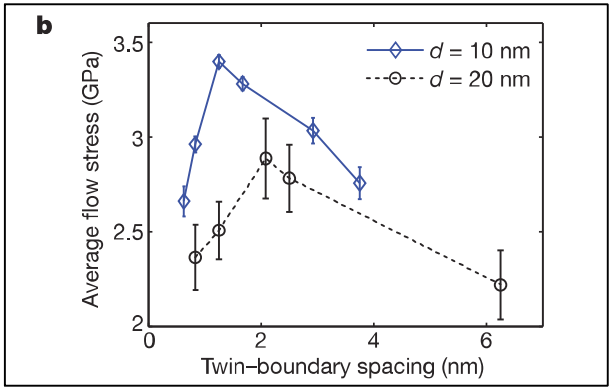
Why Twinned Nanocrystalline Metals ?

Molecular Dynamics Simulations

- Changes in the spacing of the initial TBs for a given average grain size results in different flow stresses and peak stress values.
- For small initial TB spacing samples, partial dislocation migration parallel to the TB plane is much more common, and therefore induces TB migration normal to the TB plane.
- As the spacing of initial TBs increases, more partial dislocations are observed to cut across the TB plane and TB migration is less common.
- The maximum observed flow stress is a function of both the TB spacing and the initial average grain size.
- As the initial grain size is increased from 10 to 20nm, the TB spacing at maximum flow stress also increases.



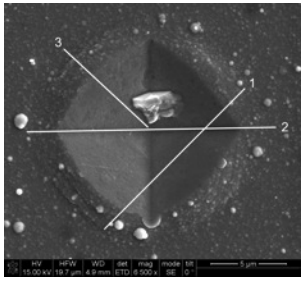


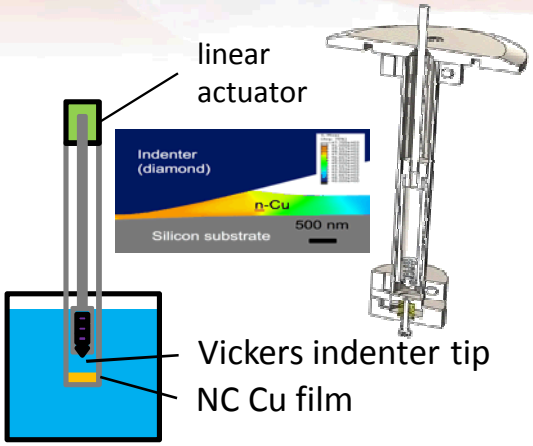


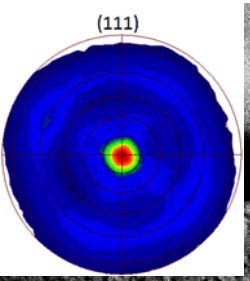
X. Li, Y. Wei, L. Lu, K. Lu, and H. Gao, Nature Letters (2010)

Why Twinned Nanocrystalline Metals ?

- Vicker's indentation can apply high stresses at cryogenic temperatures (4K, 77K).
  - 20 g load results in Maximum Von Mises stress of 800 MPa.
  - Samples are removed, sectioned via FIB, and examined by SEM and TEM.





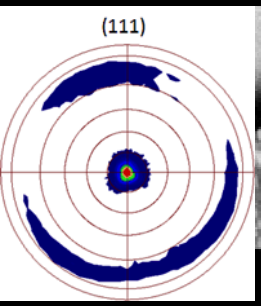


Rapid high energy pulse plated NC Cu
-Equiaxed grains

Deposited by Tim Renk, (indented at 4K, 55 g load)

Two different structures of NC Cu do not show noticeable grain growth during indentation

1 μm



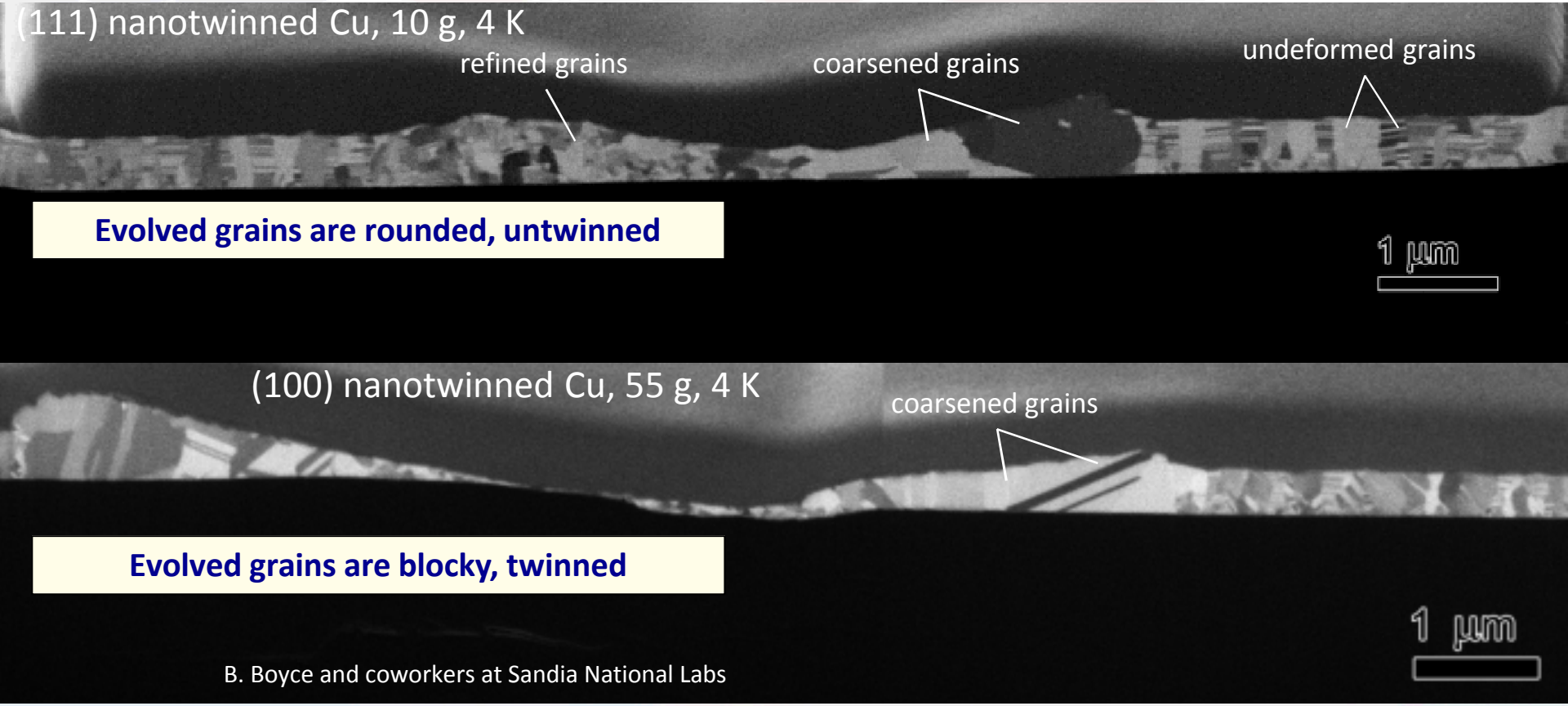
Pulsed laser deposited nanocrystalline Cu
-Columnar grains

Deposited by Jim Knapp, (indented at 4K 55 g load)

1 μm

B. Boyce and coworkers at Sandia National Labs

Why Twinned Nanocrystalline Metals ?

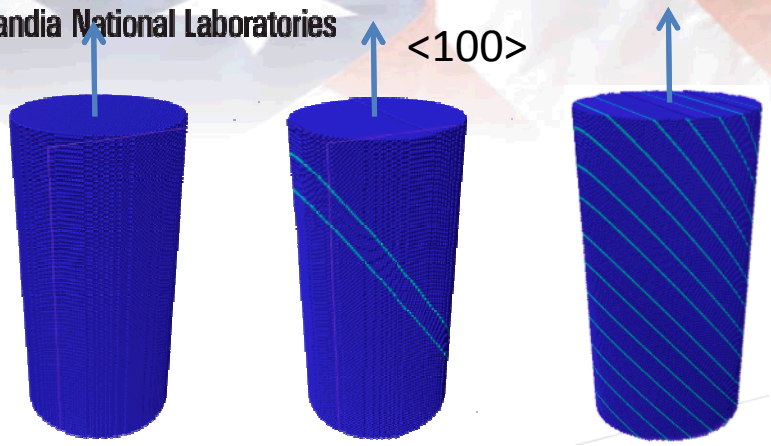


B. Boyce and coworkers at Sandia National Labs

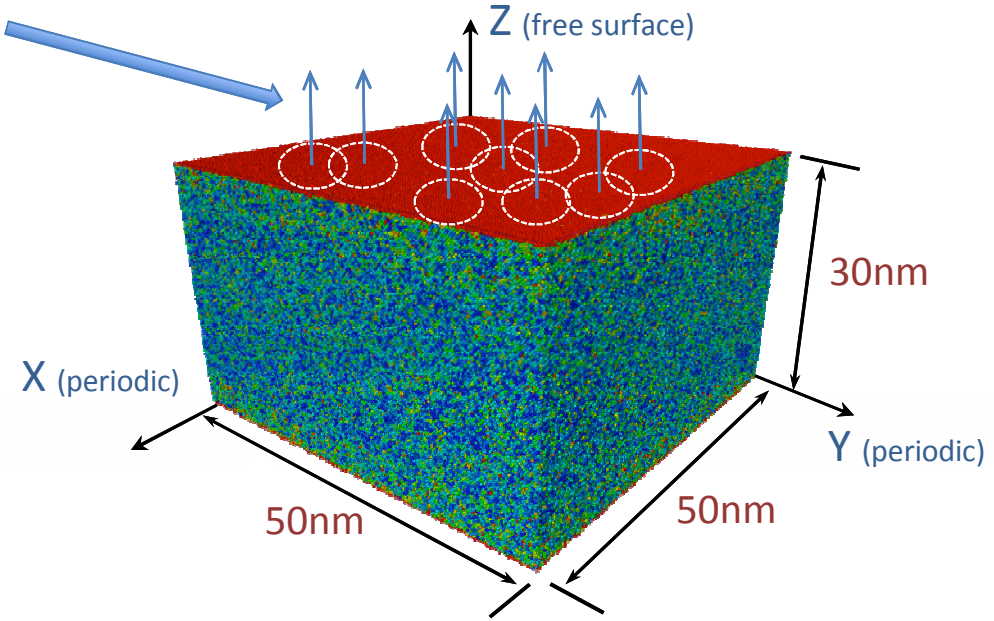
- TBs lead to significantly different microstructural evolution in columnar NC Cu under indentation cryogenic temperatures.
- Grain growth is enhanced with grown in TBs.
- Texture dependence on the role of TBs?
- How do grown in TBs influence underlying mechanisms and microstructure evolution?

Questions to Address:

- How do TBs influence the mechanical behavior of <100> columnar NC Cu?
- How does the evolution of different deformation mechanisms rely on TB density and loading?
- Do TBs influence the onset of plastic deformation?
- How do TBs effect strain accommodation in columnar NC Cu?



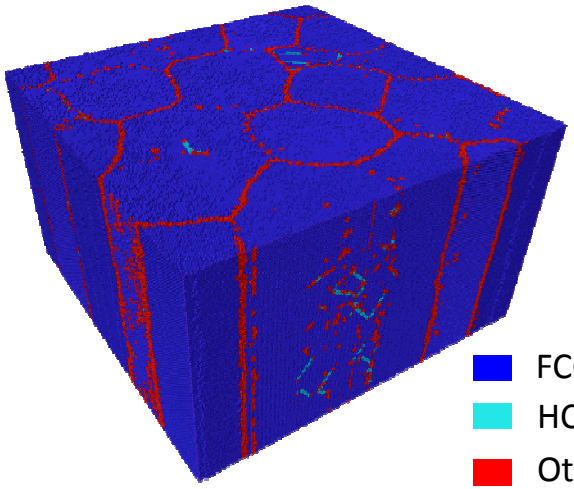
- Constant twin thickness (2nm)
- Varying concentration of TBs
- Common <100> vertical axis



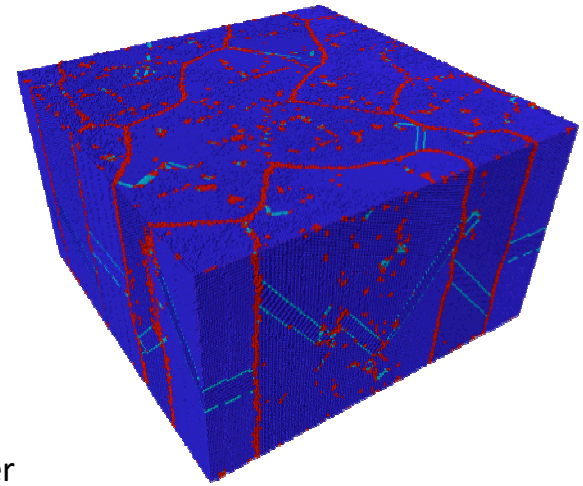
3 NC copper columnar structures

- 6,000,000 atoms
- Varying TB density
- Randomly oriented grain seeds
- Insert grain seeds into amorphous slab
- Delete overlapping atoms and minimize energy
- 10 nanosecond equilibration at 300K
- 14 grains, d ~ 13-14 nm

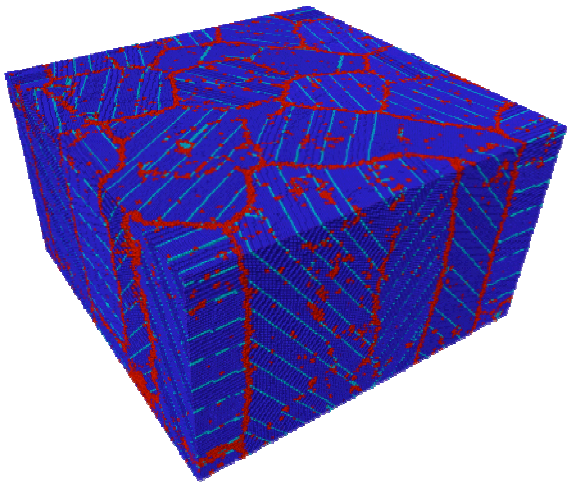
No twins inserted



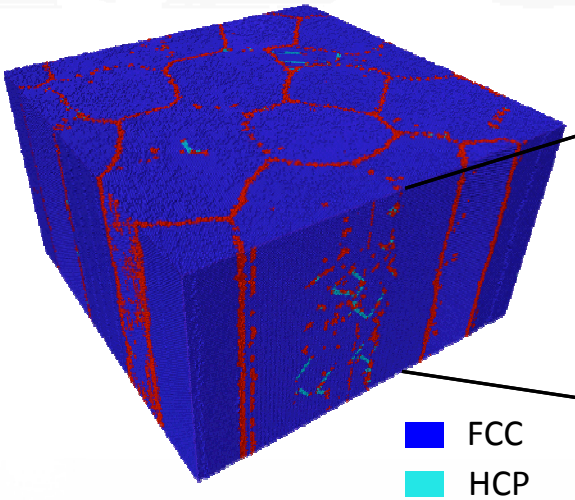
Two TBs per grain

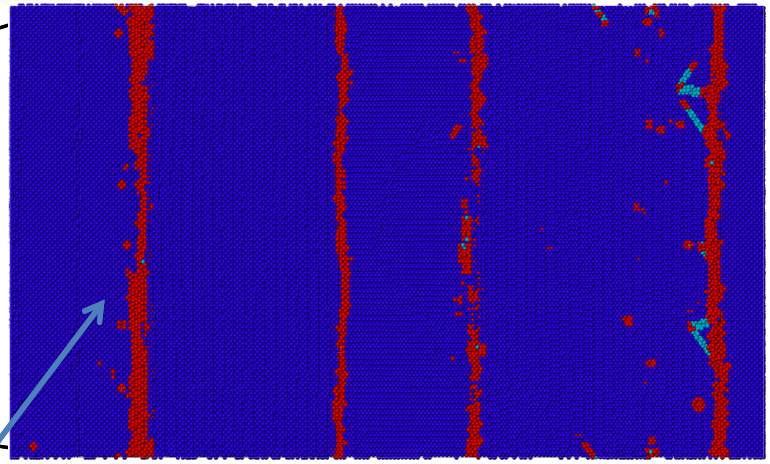


Multiple TBs per grain



No twins inserted



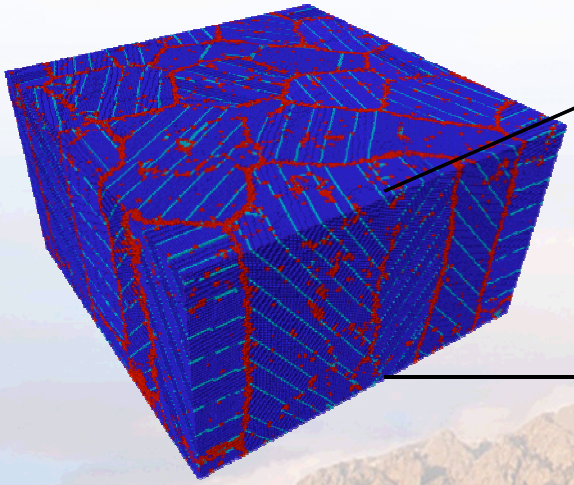


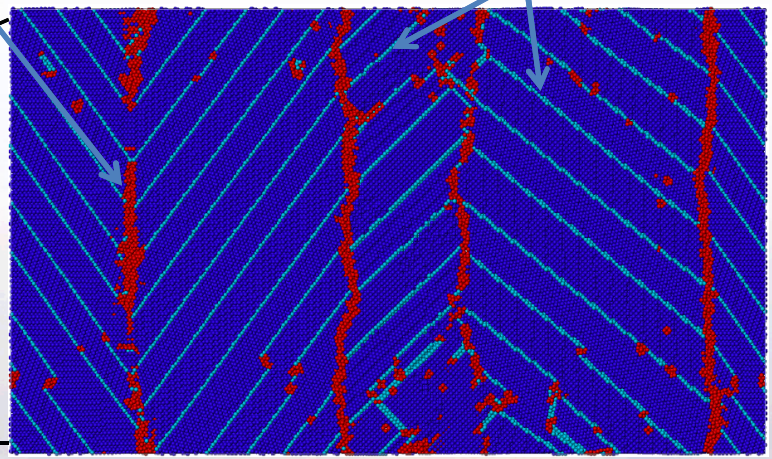
FCC
HCP
Other

Grain Boundaries

Twin Boundaries

Multiple TBs per grain

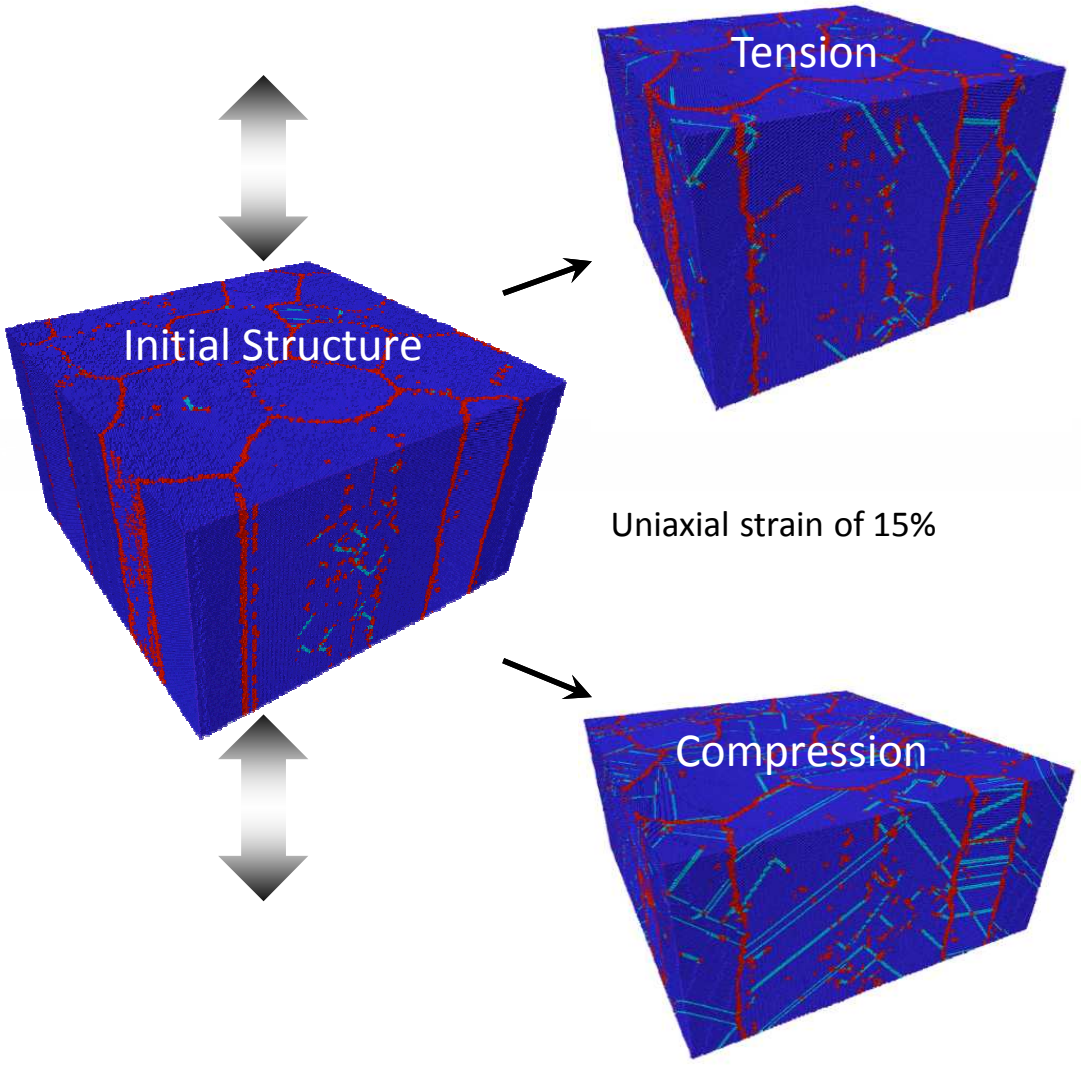




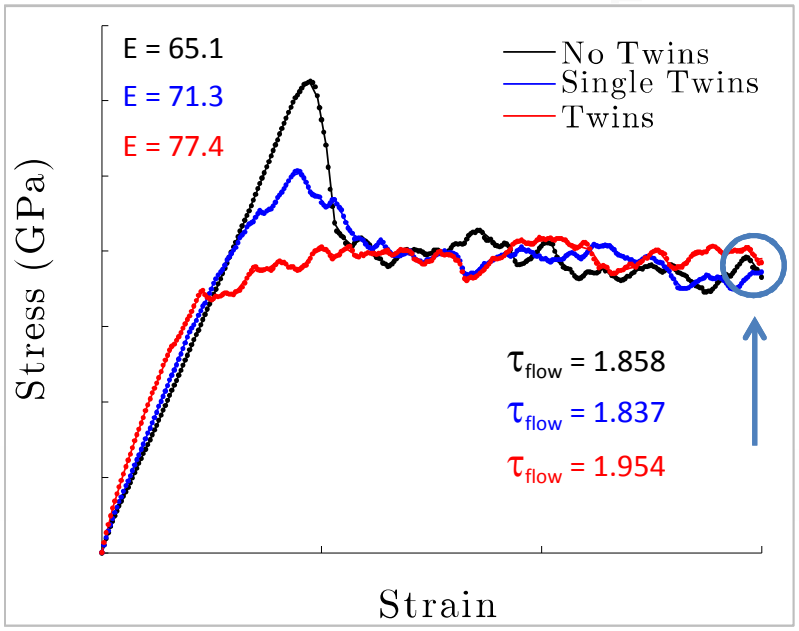
TB spacing is initially about 2nm

Uniaxial Deformation Methodology

- Embedded atom method (EAM) interatomic potential (Mishin et al., 2001) for Cu.
- Uniaxial Tension and Compression
- Constant strain rate (10^8 s^{-1}) applied parallel to grain axis.
- NPT at 300K
- Zero normal stress (transverse dimensions)
  - $\sigma_{xx} = \sigma_{yy} = 0$
  - σ_{zz} not prescribed
- Deformation continues until approximately 15% strain (1.5 nanoseconds).
- Simulation snapshots every 1,000 timesteps or 1 ps.
- Virial stress computed per atom and globally
- Common neighbor analysis (CNA) provides atomic structure



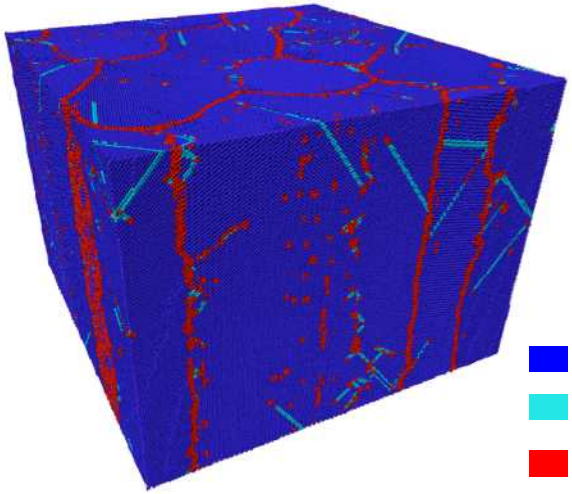
Uniaxial Tension at 300K



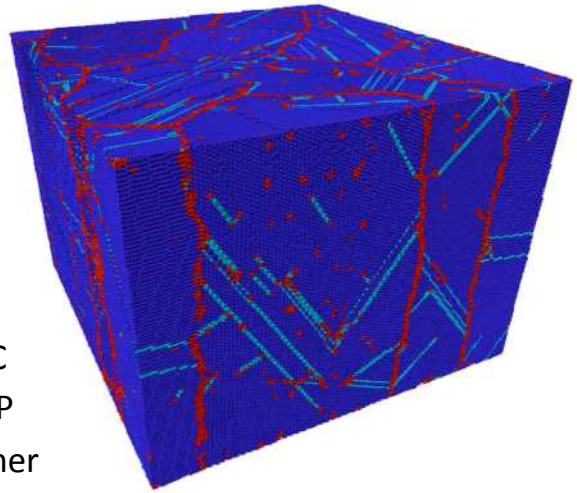
Initial Observations:

- No significant deformation TBs in 'No Twins', but there are stacking faults.
- Presence of both TBs and stacking faults in 'Single Twins', but slightly more TBs than at 0% strain.
- Higher concentration of TBs in the 'Twins' structure, and stacking faults are also evident.
- Deformation twinning and detwinning appear to have occurred in 'Twins'.
- No significant grain growth has occurred, and initial grain geometry has been mostly preserved.

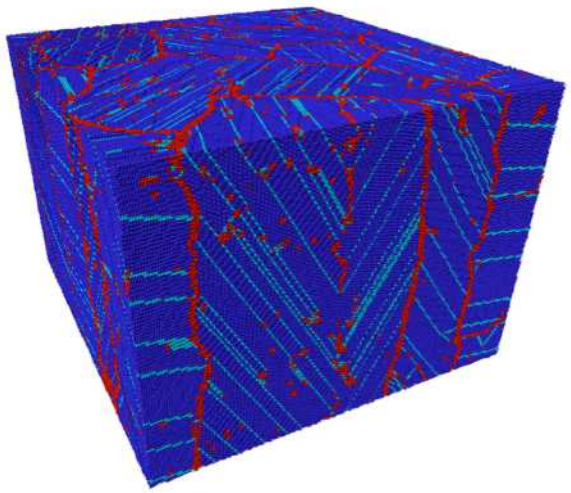
No Twins



Single Twins



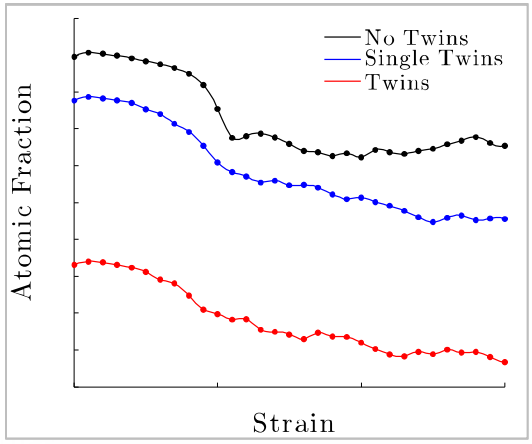
Twins



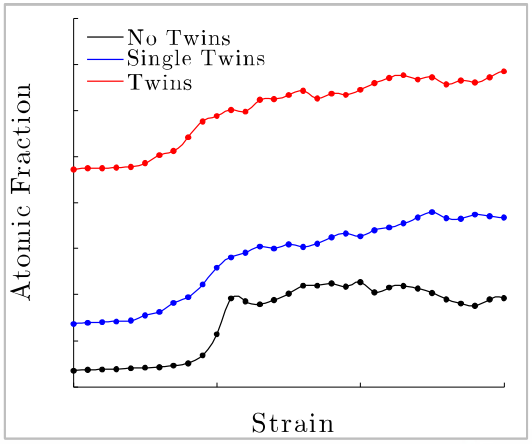
FCC
HCP
Other

Uniaxial Tension at 300K

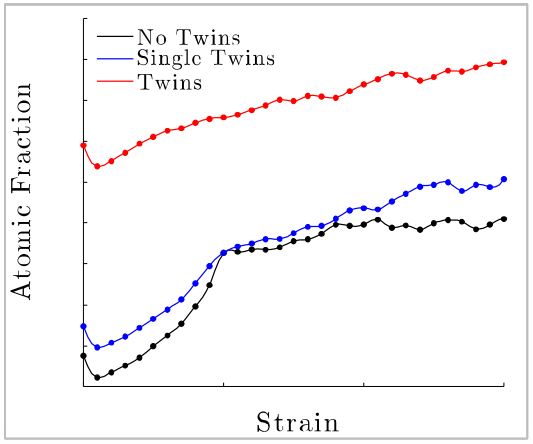
FCC



HCP

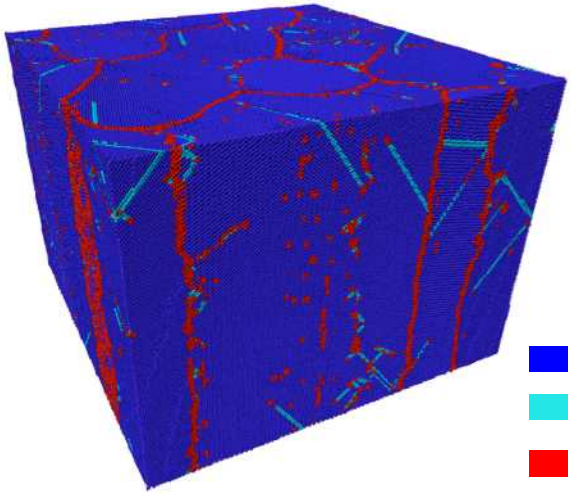


Other

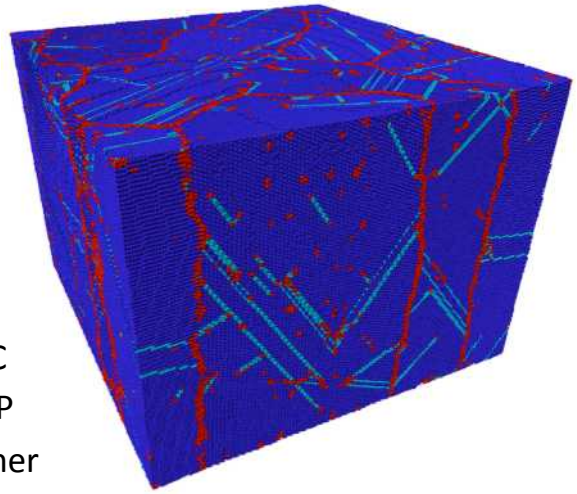


- During straining, the atomic fraction of FCC or lattice atoms decreases, while the fraction of both HCP and Other (GB and defect) atoms increases.

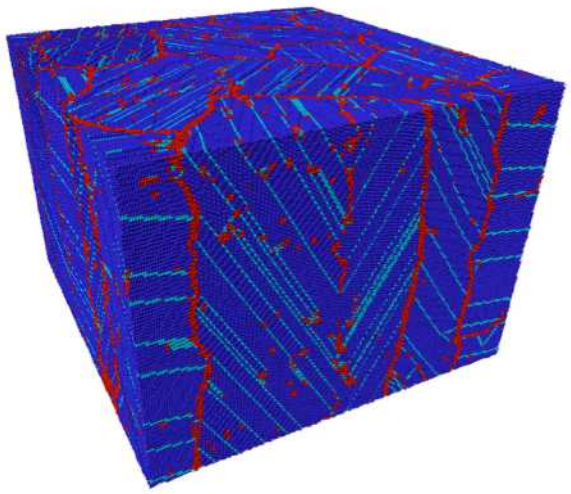
No Twins



Single Twins

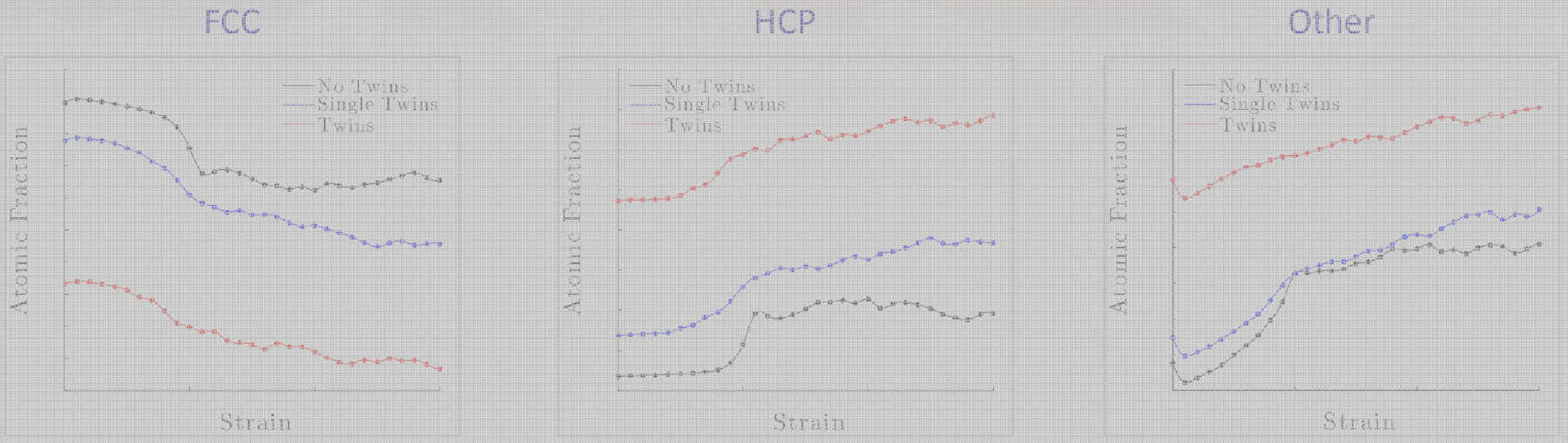


Twins

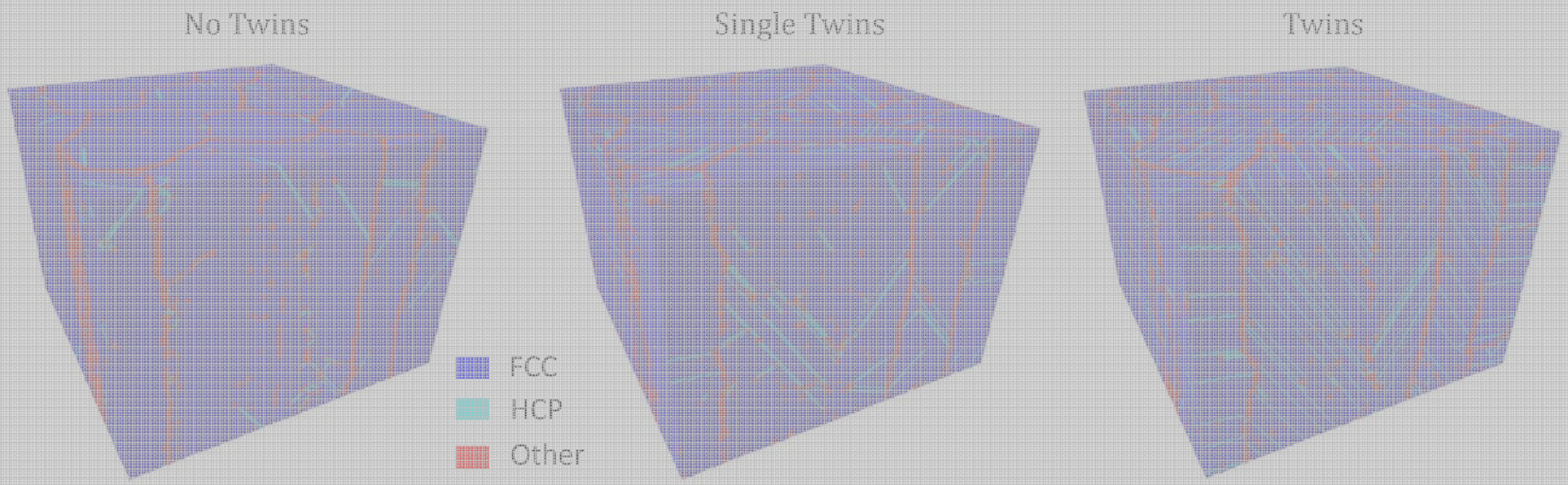


FCC
HCP
Other

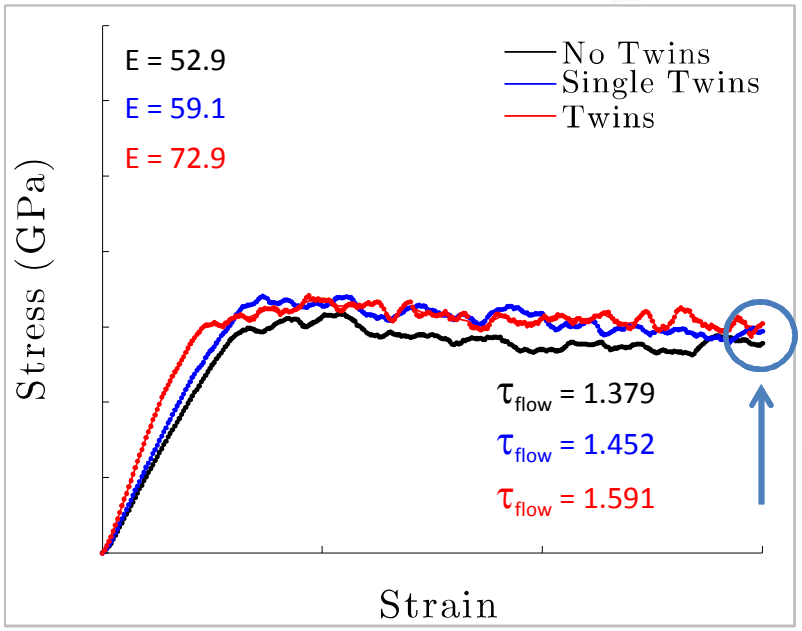
Uniaxial Tension at 300K



What mechanisms are fundamental to these microstructural changes and is there a difference in those mechanisms during uniaxial compression?



Uniaxial Compression at 300K

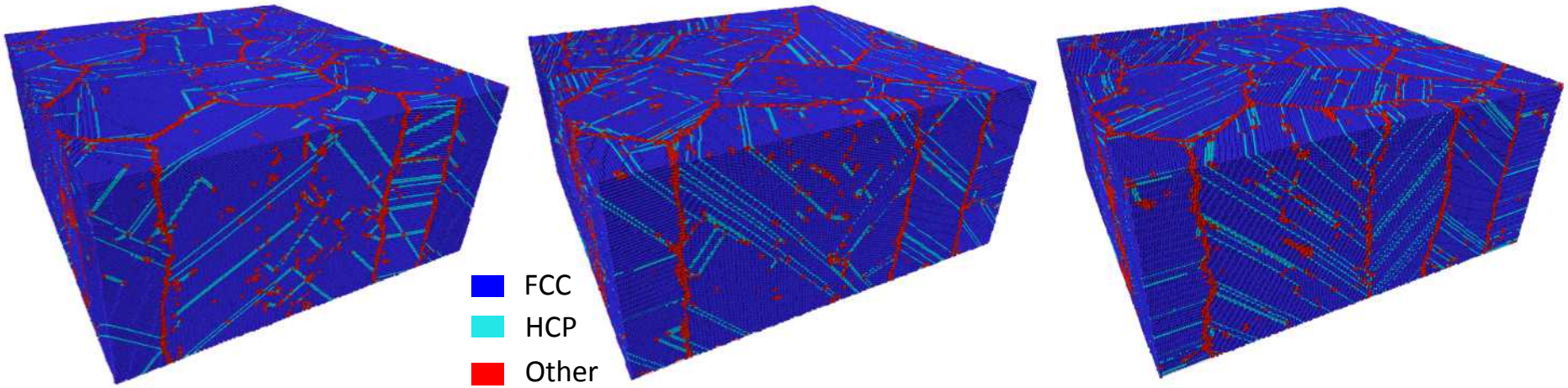


Initial Observations:

- A large number of TBs in both the 'No Twins' and 'Single Twins' structures at 15% compressive strain.
- Presence of stacking faults in all three structures.
- Full dislocations (i.e., entire stacking fault with both leading and trailing partial dislocations) are observed.
- Both deformation twinning and detwinning by the migration of twinning dislocations (or disconnections)* appear to be evident during high strain regime.

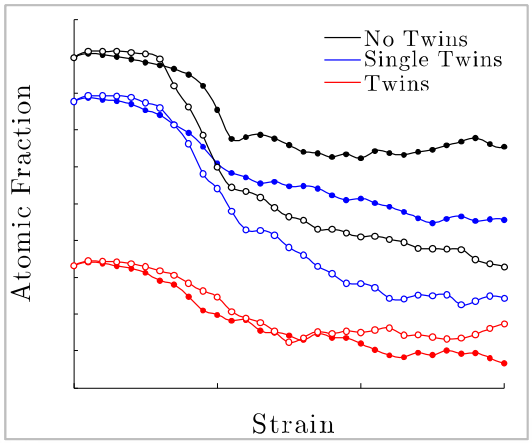
* J. Wang et al., Acta Mat. 2010.

No Twins | Single Twins | Twins

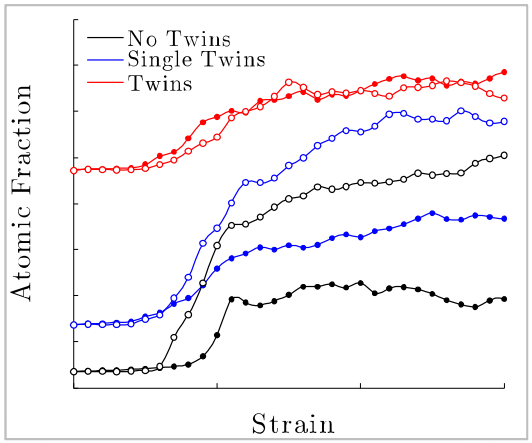


Tension/Compression Structural Evolution

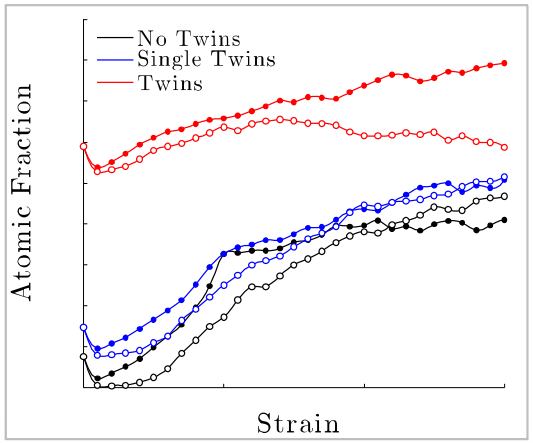
FCC



HCP



Other



- Tension
- Compression

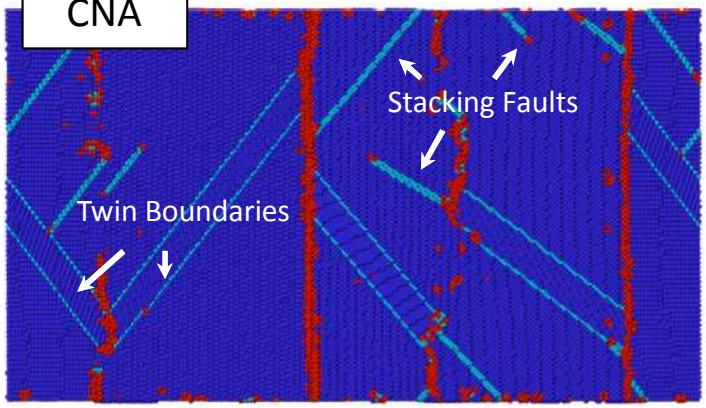
- Under both tension and compression, FCC decreases while both HCP and Other increase.
- A larger variance in the structural evolution is observed in tension, as compared to compression.
- Under compression, a higher atomic fraction of atoms are HCP at higher strains.
- Less tension/compression asymmetry is observed in the 'Twins' structural evolution behavior than in the other two structures.

Can we estimate the role of the deformation mechanisms and compute their evolution with imposed strain?

Dislocations and Twin Boundaries

How to determine both dislocation and TB atomic groups?

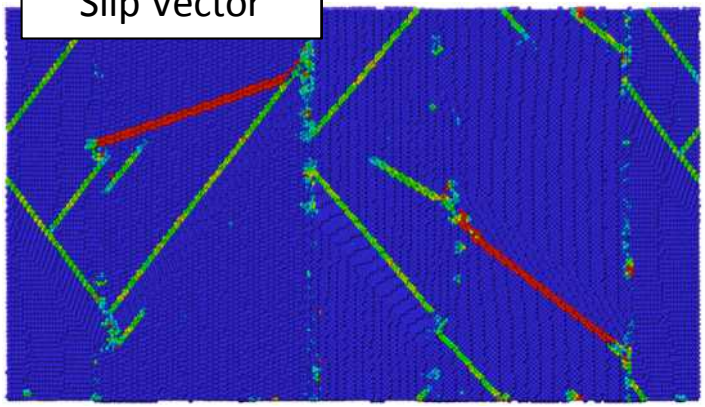
CNA



FCC
HCP
Other

- Atoms in both stacking faults and TBs are HCP, so we must distinguish.
- Both perfect lattice atoms and those that have been fully slipped are FCC, so we must distinguish.

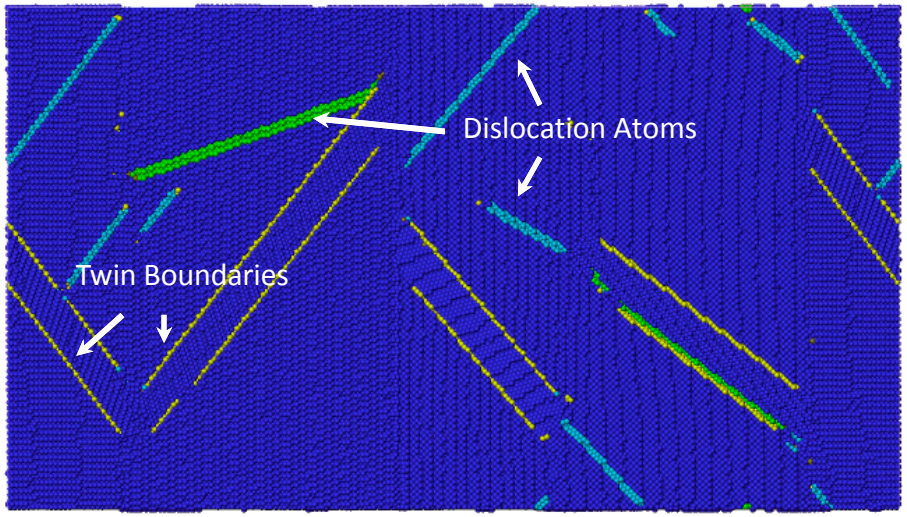
Slip Vector



Partial Slip
Full Slip

Slip vector for each atom α

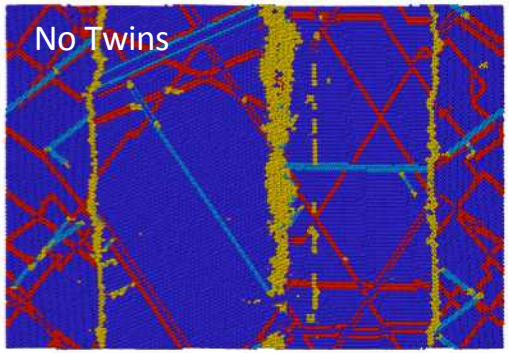
$$s^{\alpha} = -\frac{1}{n_s}\sum_{\beta \neq \alpha}^{n}(x^{\alpha\beta} - X^{\alpha\beta})$$

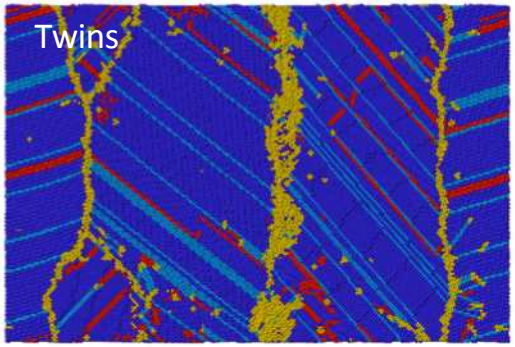


- Criteria is dependent upon both atom α and it's neighbors β.

Now, we can compute the evolution of both Dislocation and TB densities as a function of structure and imposed strain.

Dislocations and Twin Boundaries

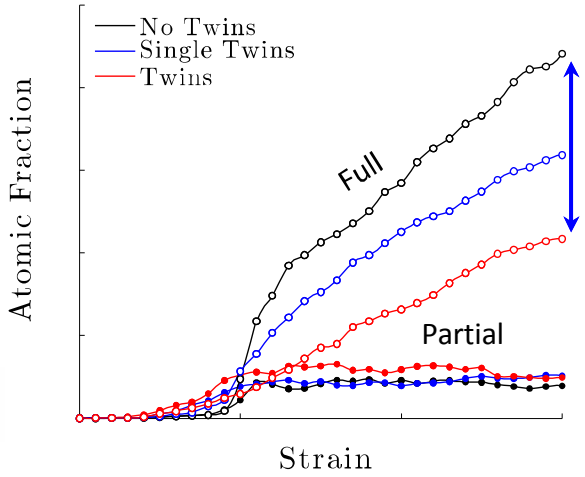




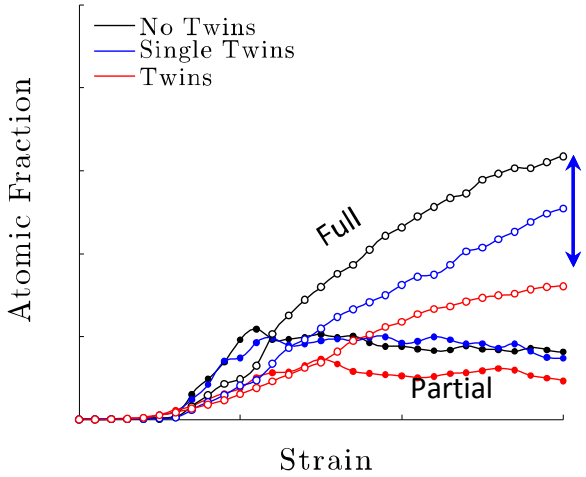
FCC
HCP
Other
Full Dislocations

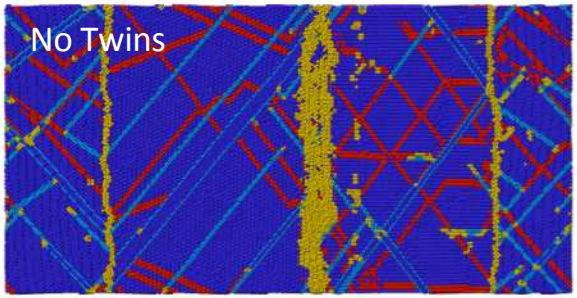
- TBs inhibit wide-spread dislocation activity.
- Localized slip planes parallel to TBs.

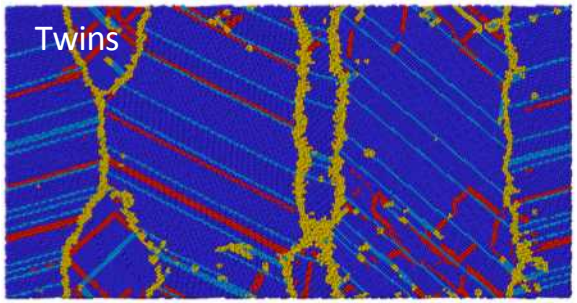
Tension



Compression



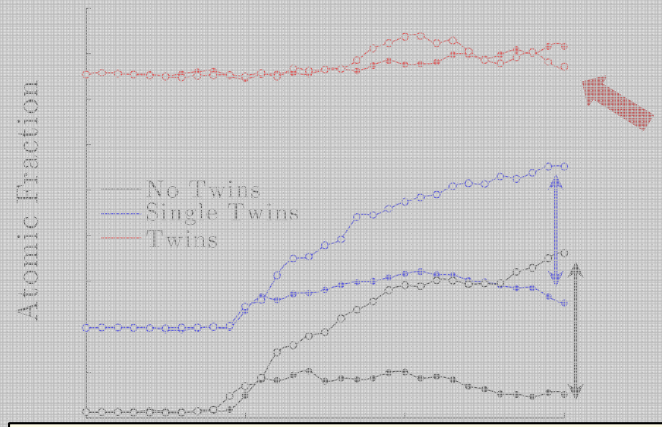




- TBs inhibit wide-spread dislocation activity.
- Localized slip planes parallel to TBs.
- Lower dislocation activity to accommodate strain, as compared to Tension → Why?

Dislocations and Twin Boundaries

TB Density Evolution



Maybe deformation twinning?

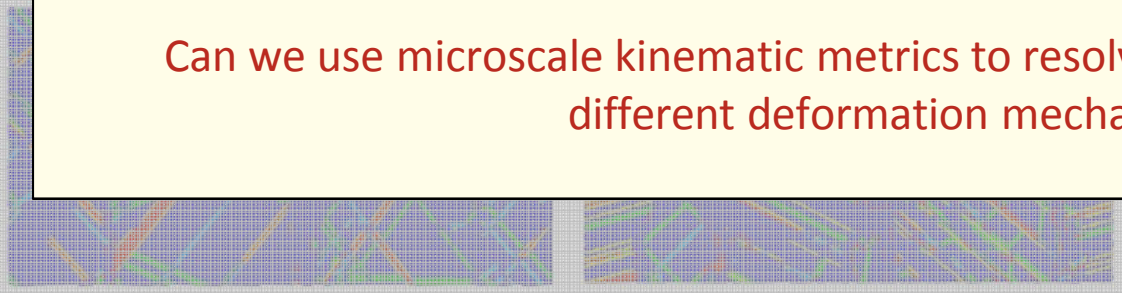
- Under compression, TB density is greater at higher imposed strains, as compared to under tension.
- This might explain low dislocation activity under compression.
- However, this is not the case for the 'Twins' structure.

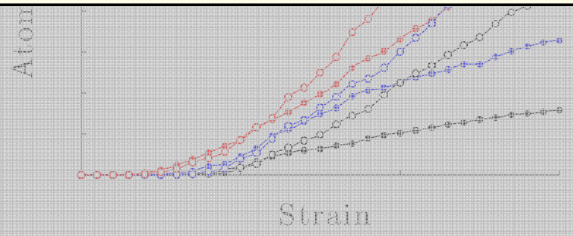
What other strain accommodation mechanism could

What does this mean?

- Coherent TBs alter the macroscopic response by altering the nanoscale mechanisms
- Higher density of TBs inhibits dislocation nucleation/migration
- Resolved stress state is fundamental for controlling mechanisms and strain accommodation

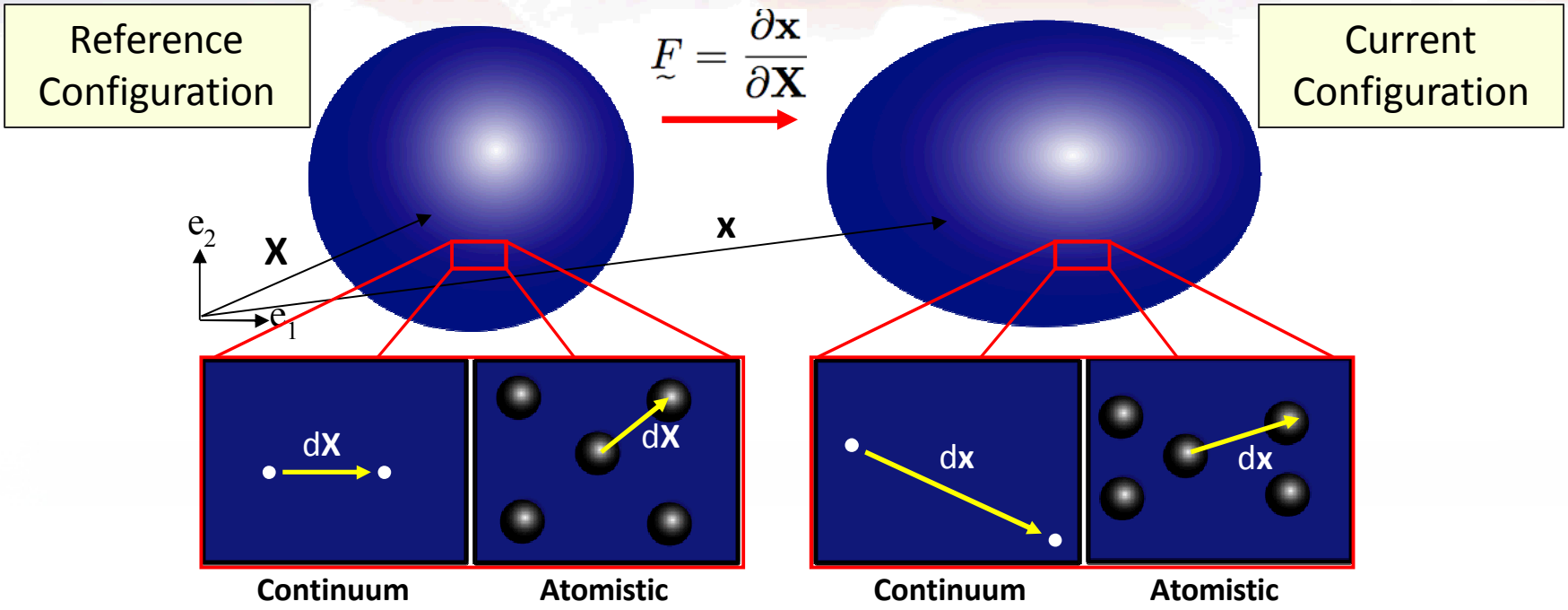
Can we use microscale kinematic metrics to resolve strain accommodation by different deformation mechanisms?





- TB migration is enhanced under compression.
- The atomic fraction of twinned regions, is greatest in the 'Twins' structure.

Microscale Kinematic Metrics



Deformation Gradient

$$F = \frac{\partial x}{\partial X} \rightarrow \sum_{\beta=1}^{n}(x_i^{\alpha\beta} X_M^{\alpha\beta} - F_{iI}^{\alpha} X_I^{\alpha\beta} X_M^{\alpha\beta}) = 0 \rightarrow \boxed{F_{iI}^{\alpha} = \omega_{iM}^{\alpha} \left(\eta^{\alpha}\right)_{MI}^{-1}}$$

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

where $\omega_{iM}^{\alpha} = \sum_{\beta=1}^{n} x_i^{\alpha\beta} X_M^{\alpha\beta}$

and $n_{iM}^{\alpha} = \sum_{\beta=1}^{n} X_I^{\alpha\beta} X_M^{\alpha\beta}$

Microrotation

$$\underset{\sim}{F} = \underset{\sim}{R}\underset{\sim}{U} \text{ where } \underset{\sim}{R} = \underset{\sim}{R}_{sym} + \underset{\sim}{R}_{skew} \rightarrow \underset{\sim}{R}_{skew} = \frac{1}{2}(\underset{\sim}{R} - \underset{\sim}{R}^{T}) \rightarrow \boxed{\phi_k = -\frac{1}{2}\varepsilon_{ijk}\left(R_{skew}\right)_{ij}}$$

* Tucker *et al.*, MSMSE (2010)

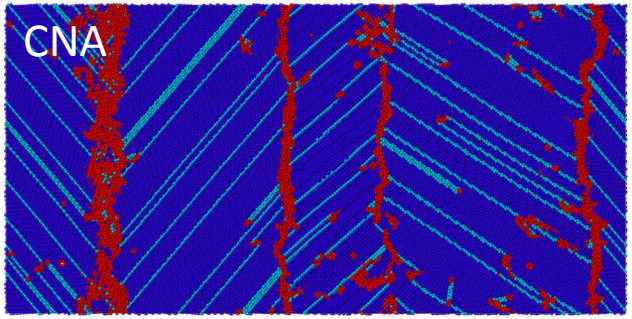
Green Strain

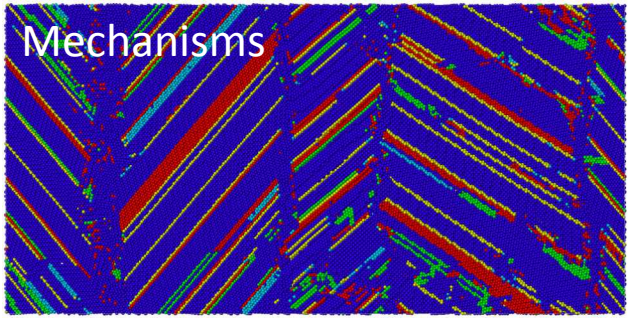
$$\boxed{\mathbf{E} = \frac{1}{2}(\mathbf{F}^{\mathrm{T}} \cdot \mathbf{F} - \mathbf{I})}$$

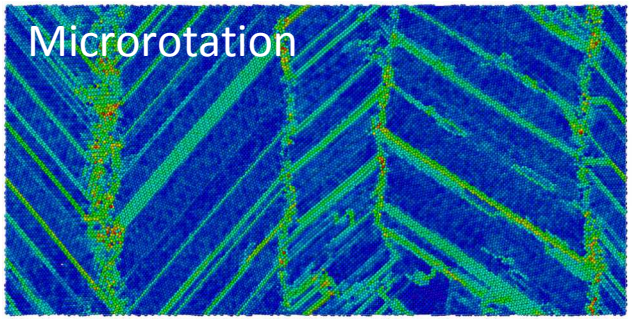
* Tucker *et al.*, JMPS (2012)

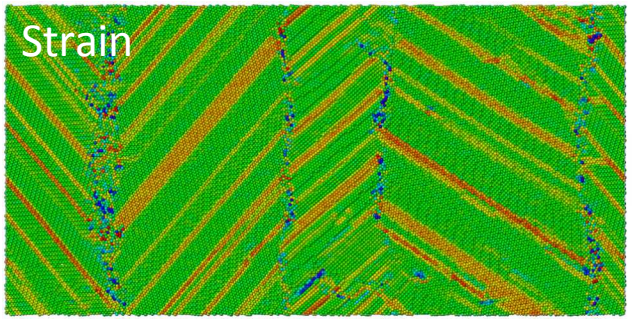
and $I_1(E) = tr(E)$

Microscale Kinematic Metrics









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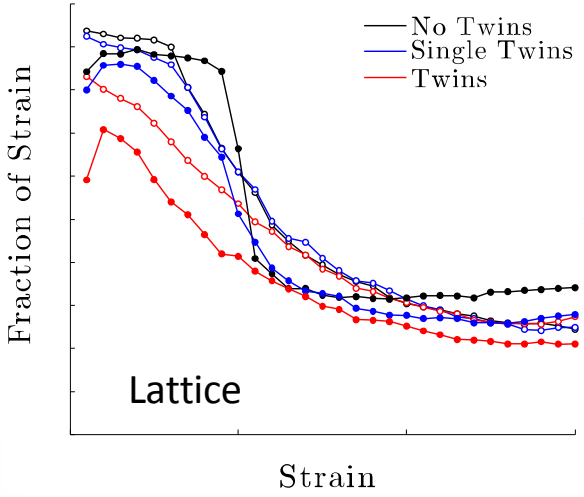
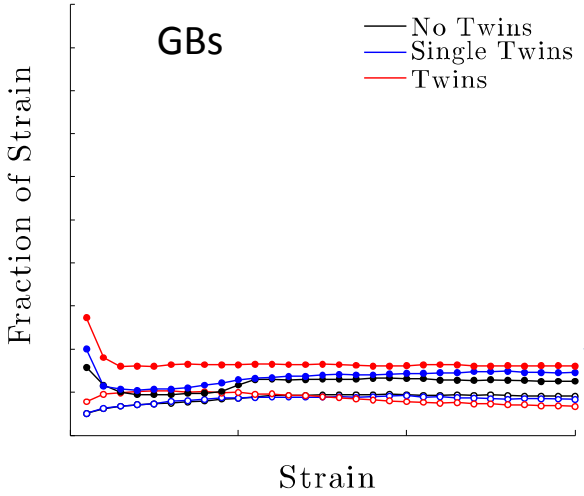
and $I_1(E) = tr(E)$

Resolving the Strain Contributions



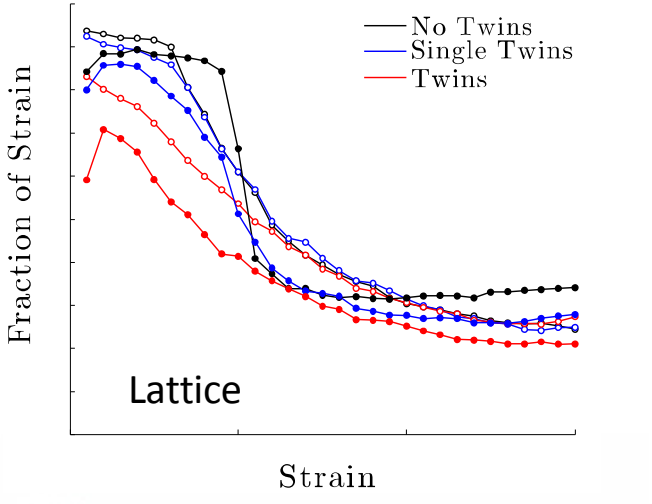
Lattice estimates do not consider atoms that have been fully slipped or traversed by migrating TBs

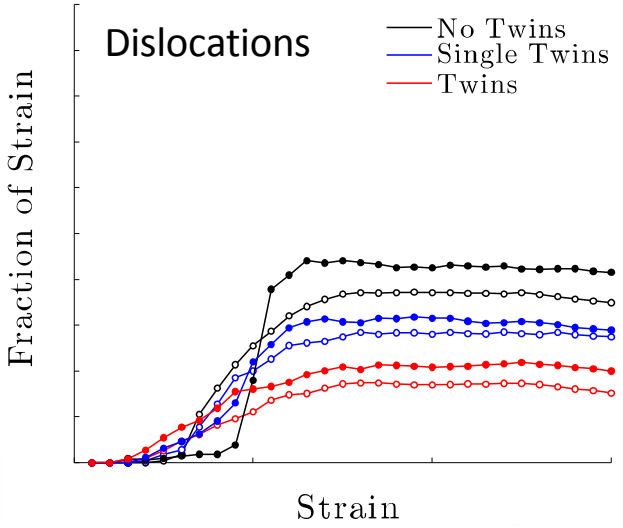
- Tension
- Compression



There is very little strain accommodation in GBs, and the role of GB strain accommodation is greater in tension than in compression.

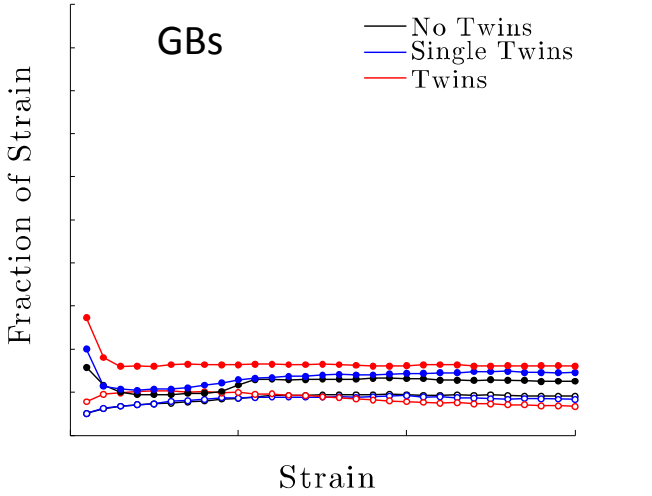
Resolving the Strain Contributions

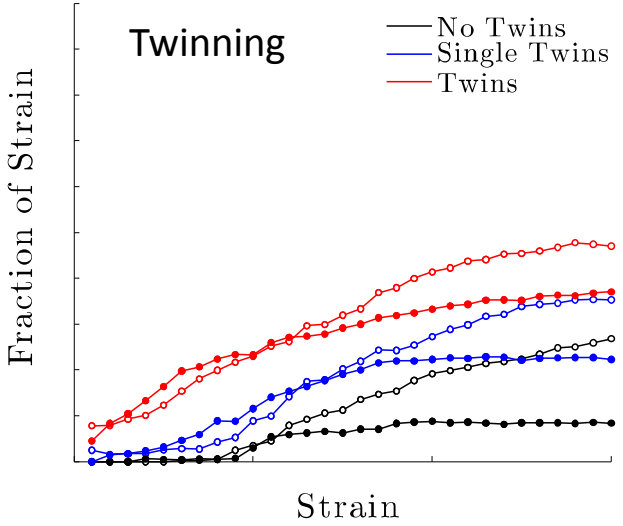




Dislocation strain is more significant during tension than under compression

- Tension
- Compression





Twinning (TB **nucleation** and **migration**) is more significant during compression than under tension

Conclusions

- Atomistic simulations have shown that TBs influence microstructural evolution and the mechanical behavior of <100> columnar NC Cu under uniaxial tension and compression at room temperature.
- The cooperation/competition of various deformation mechanisms to accommodate imposed strain during loading is influenced by TBs.
- The nucleation and migration of dislocations is suppressed in heavily twinned structures and during compression.
- **TBs alter the contribution of different mechanisms to the overall strain in NC metals, and play a more important role in deformation under compression and in twinned microstructures.**

Future Work:

- Explore the influence of TBs on the propensity of grain growth in the columnar structures under indentation.
- Investigate how TBs influence strain accommodation under shear loading and at lower temperatures.

Acknowledgements:

- Stephen Foiles, Henry Padilla, Brad Boyce, Corbett Battaille, and Liz Holm
- Sandia National Laboratories – LDRD and BES