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# Molecular Dynamics Simulations of Uniaxial Compression of Silicon Nanoparticles

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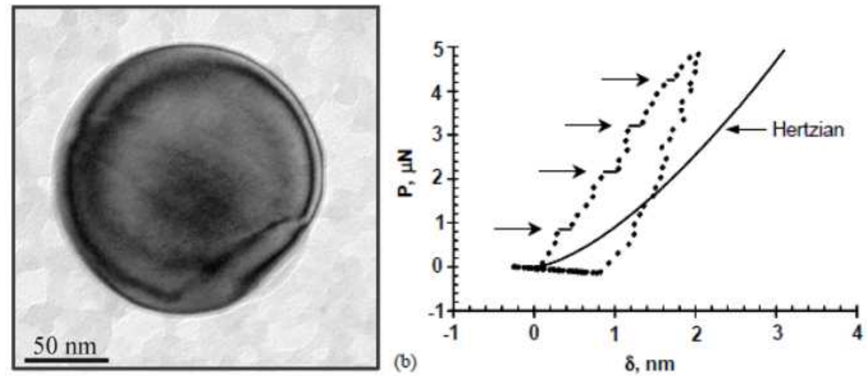
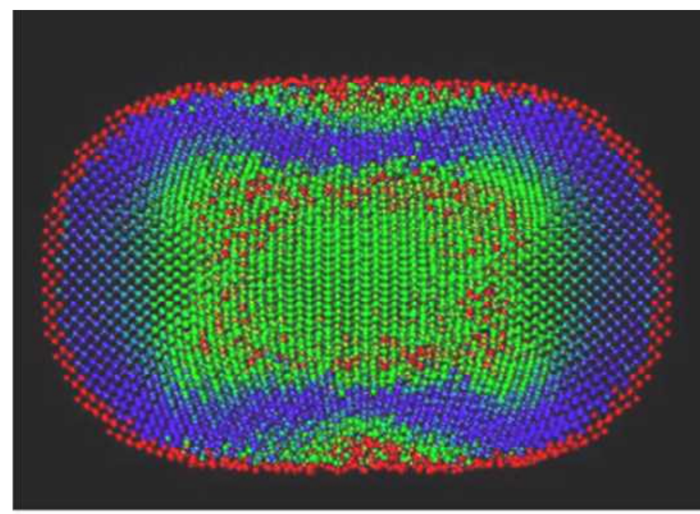
# Superhard Si Nanospheres

- History
  - Experimental
    - High contact stress values
    - Load discursions indicated dislocation activity
  - MD Simulation
    - [100] compression
    - Tersoff at 0 K
    - Phase transformation seen
    - High stress values
    - Concluded that hardening is due to phase transformation
- Purpose
  - Additional MD simulations to obtain a better understanding of hardening behavior
    - Phase transformations
    - Dislocations




Gerberich, et al. *J Mech. Phys. Solids* **51** (2003) 959



Valentini, et al. *Phys. Rev. Lett.* **99** (2007) 175701

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# Simulation Procedure

- LAMMPS MD code
- Planar indenter force potentials
- Displacement rate of 0.00625 A/ps = 6.25 m/s

| Atomic potentials | Sphere diameters | Compression |
|---|---|---|
| – Tersoff | – 10 nm | – [100] |
| – Stillinger-Weber | – 20 nm | – [110] |
| | | – [111] |


LAMMPS Molecular Dynamics Simulator. http://lammps.sandia.gov/.
J. Tersoff, Phys. Rev. B **38**, 9902 (1988).
F. H. Stillinger, and T. A. Weber Phys. Rev. B **31**, 5262 (1985).


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# Visualizing Defects

- Slip Vector
  - Marks region where dislocation has passed resulting in slip
  - Magnitude scaled to match Burgers vector

$$\vec{S}_i = -\frac{1}{N_s}\sum_{j\neq i}^{N}\left(\vec{R}_{i,j} - \vec{R}^{0}_{i,j}\right)$$

J. A. Zimmerman, *et al.*, *Phys. Rev. Lett.* **87** (2001) 165507

- Angular parameter
  - Compares bond angles to diamond cubic bond angle
  - Value can distinguish between different types of defects
  - Three body term of the Stillinger-Weber potential

$$Ang = \frac{1}{N_b}\sum_{j=1}^{N}\sum_{k=j+1}^{N}(\cos\theta_{ijk} - \cos\theta_{DC})^2$$

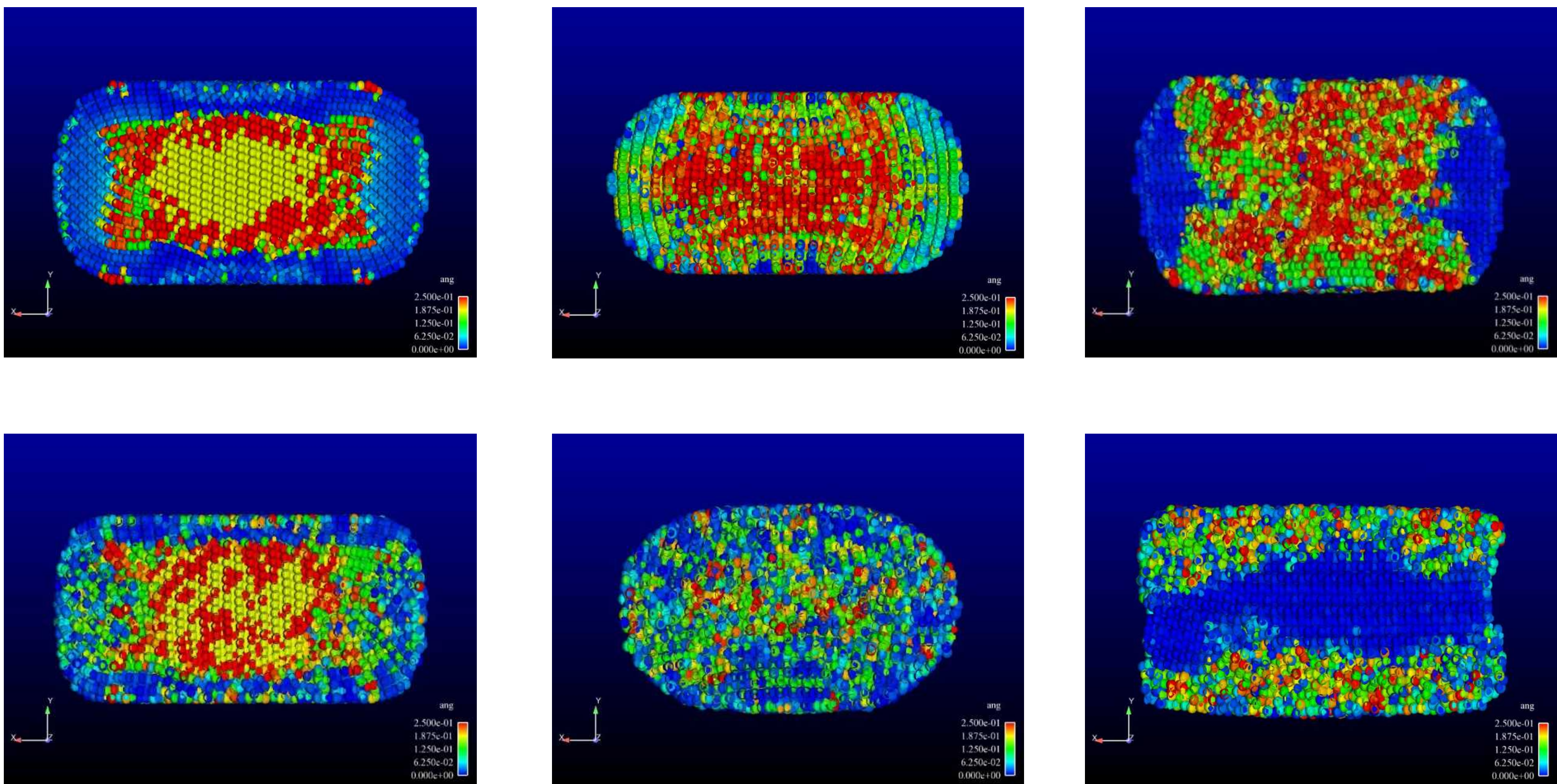
# Tersoff Yielding

- Only [100] compression results in $\beta$-Sn (yellow)
- 0 K runs show extensive elasticity before yield

[100] [110] [111]

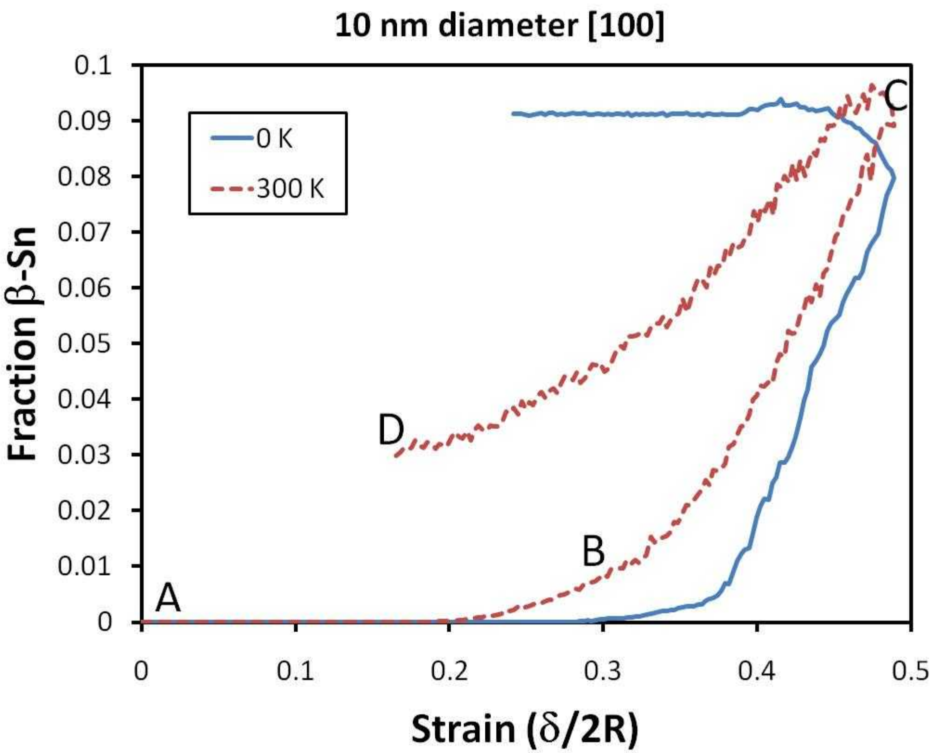
0K

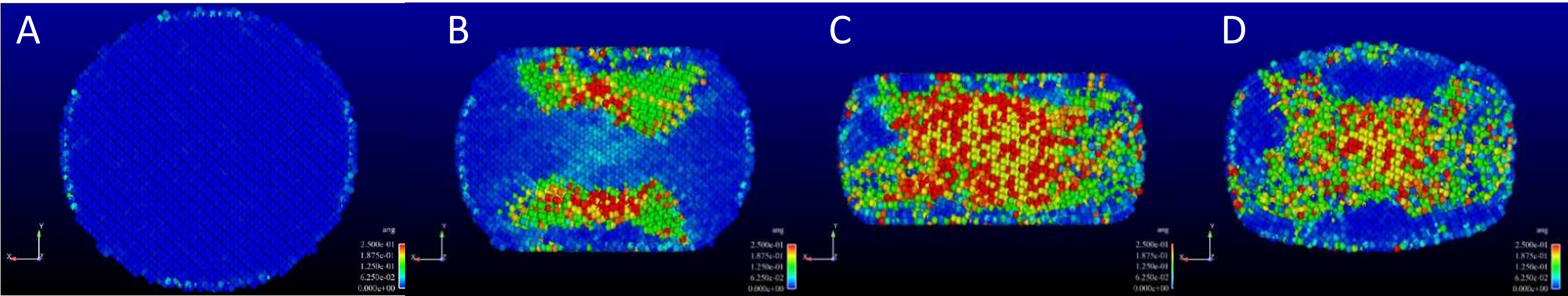
300K



# Tersoff: β-Sn Transformation

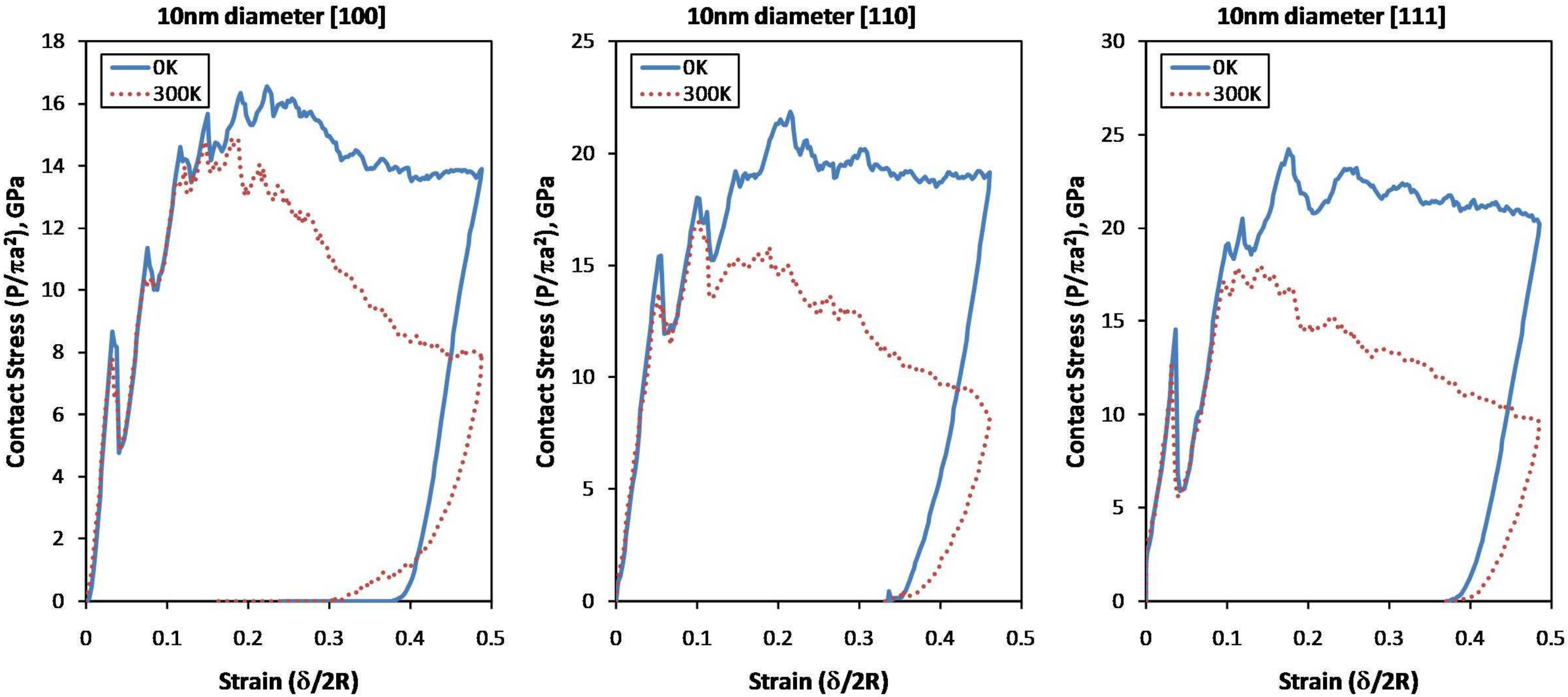
- Angular parameter used to estimate the atomic fraction of β-Sn
- Only 1-2% characterized as β-Sn for other orientations
- Reverse transition seen at 300 K on unloading



# Tersoff: Temperature Dependence

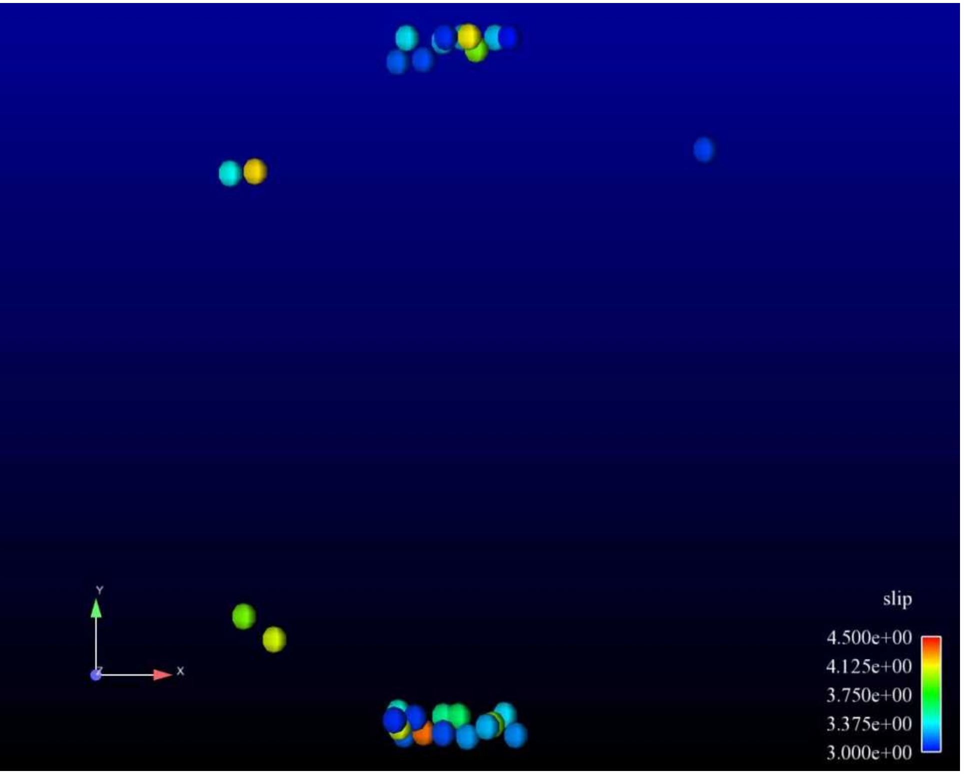
- For 0 K runs, contact stress plateaus near maximum
- For 300 K runs, contact stress decreases after maximum
- Unloading stiffness 50-100% greater at 0 K
- Hardness previously seen not due to β-Sn



# Stillinger-Weber: Dislocations

**10 nm diameter sphere**

**20 nm diameter sphere**



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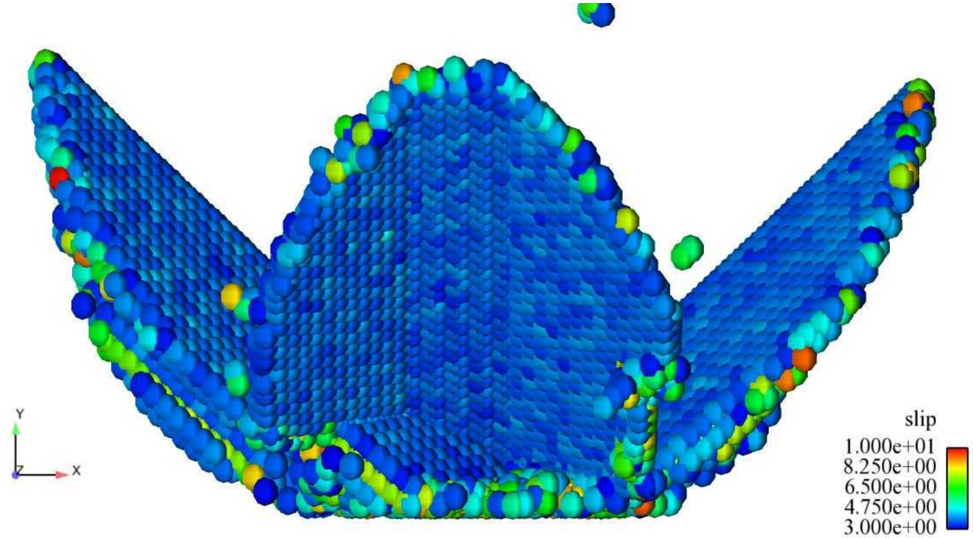
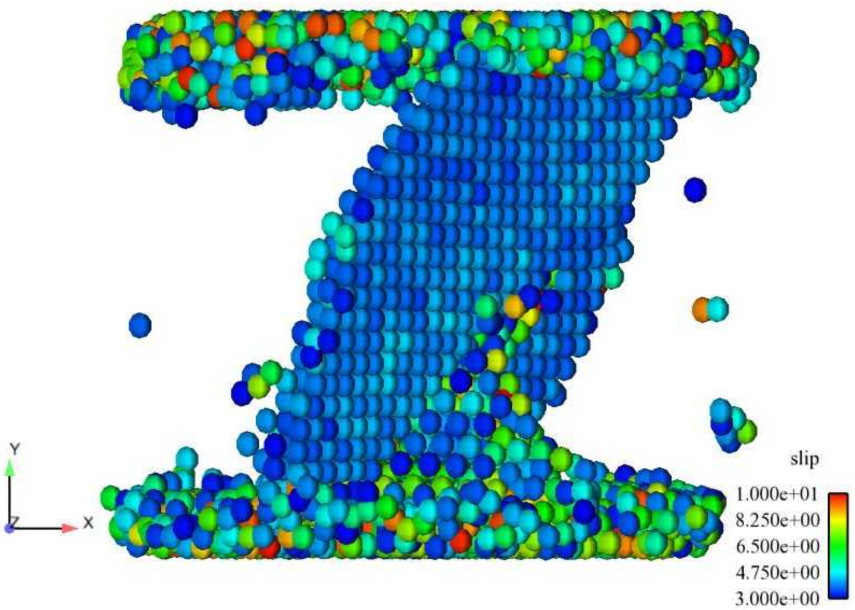
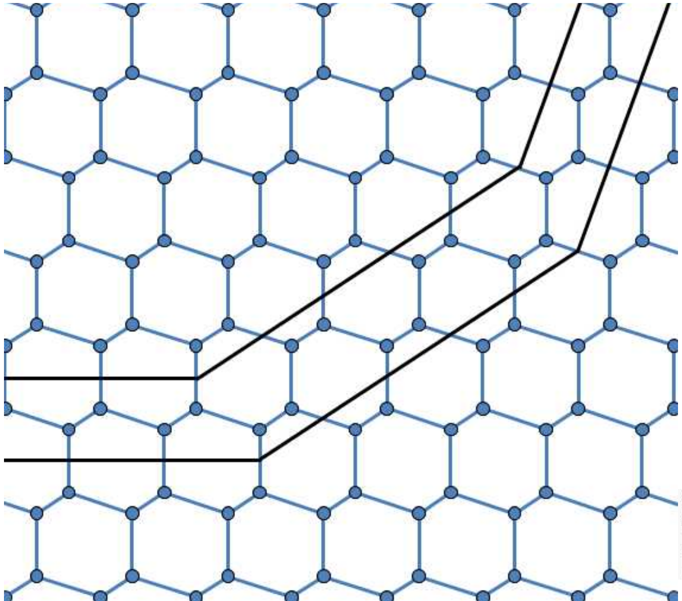
# Stillinger-Weber: Dislocation Morphology

- [100]
  - "V" shaped slip
- [111]
  - Single planes



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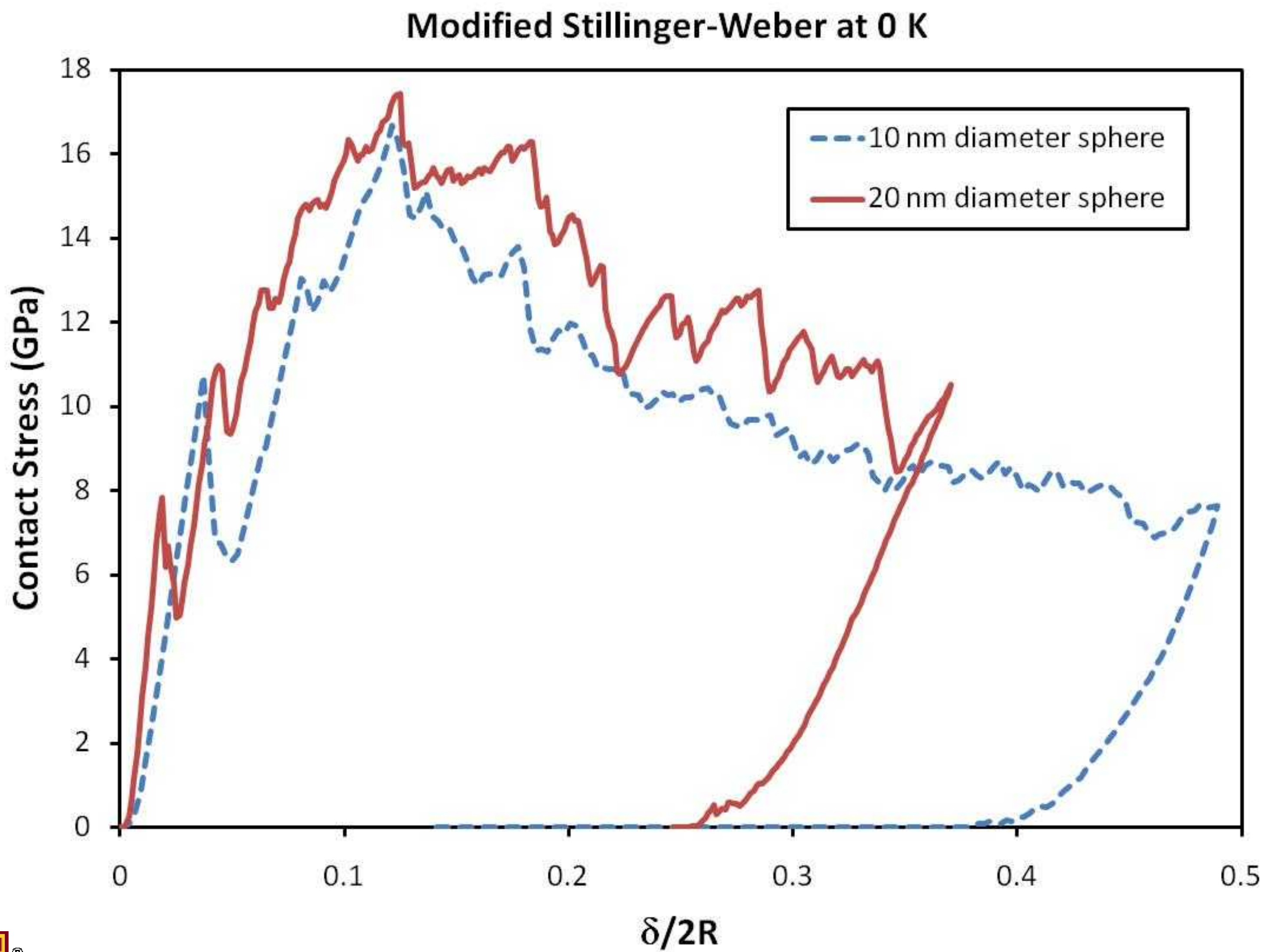
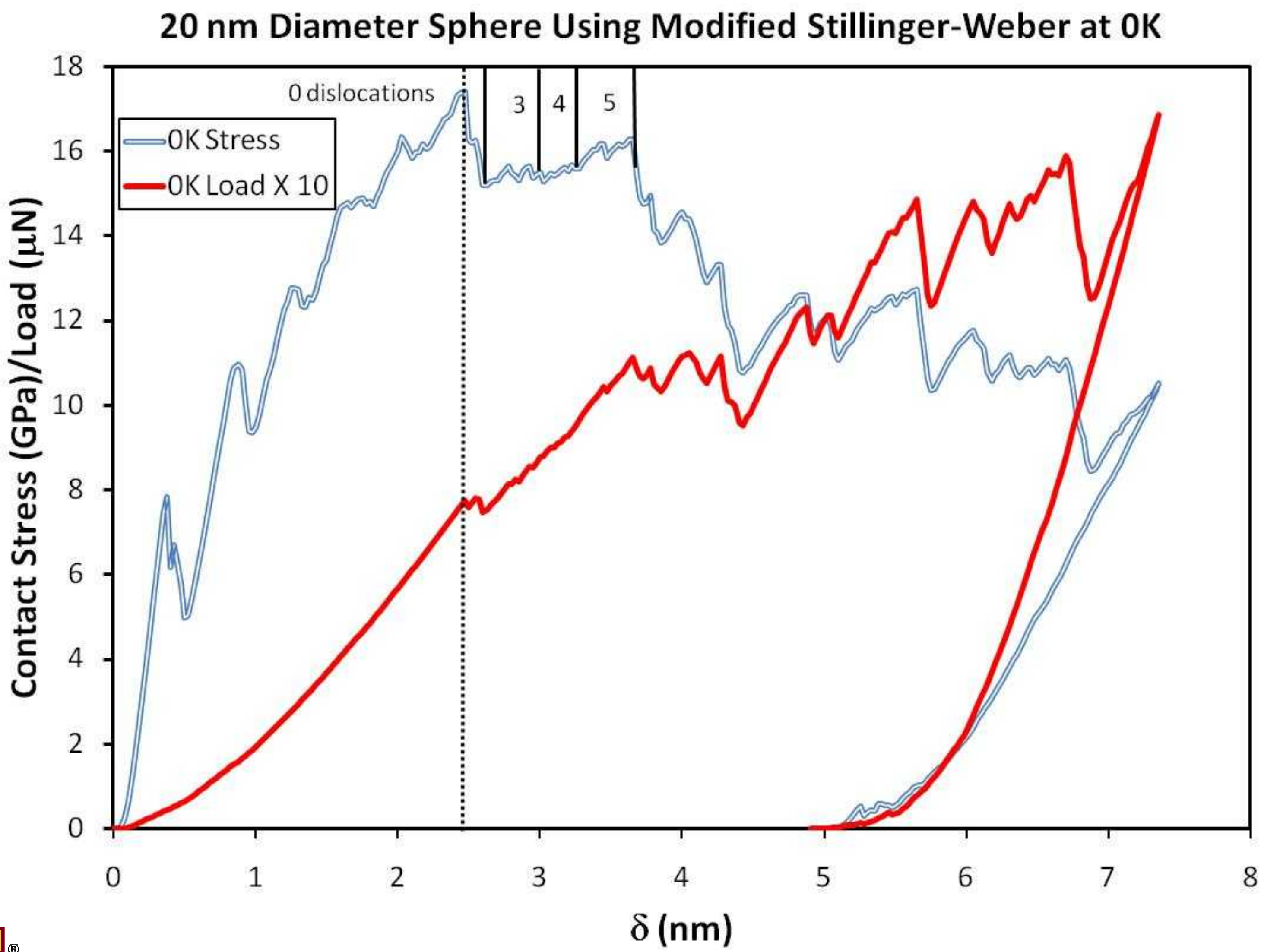
# Size Dependence



# Load and Stress

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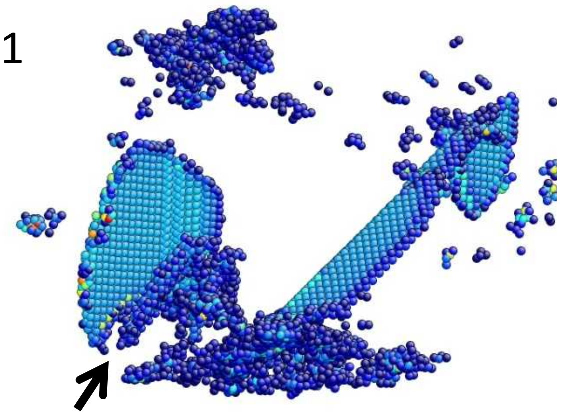
# Summary/Conclusions

- Tersoff
  - Hardening behavior independent of phase transformation
  - 0 K runs reach high loads due to high resistance to yield and increased stiffness
- Stillinger-Weber
  - Extensive dislocation yielding observed
  - Hardening possible through build-up of dislocations within sphere
- Compared to experimental (Future work)
  - Larger diameters = more dislocations
  - Oxide barrier to resist reaching the surface

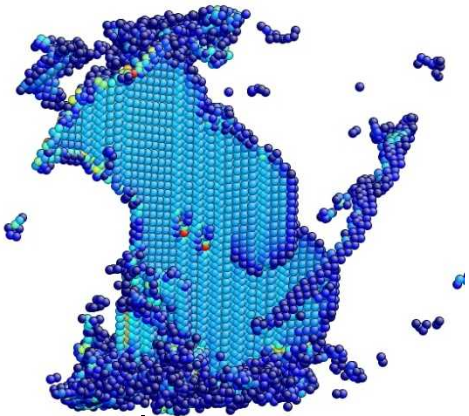
# Dislocation Motion and Interaction

1



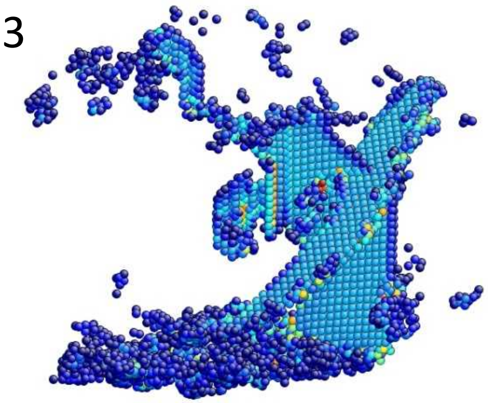
Nucleates and grows from base

2



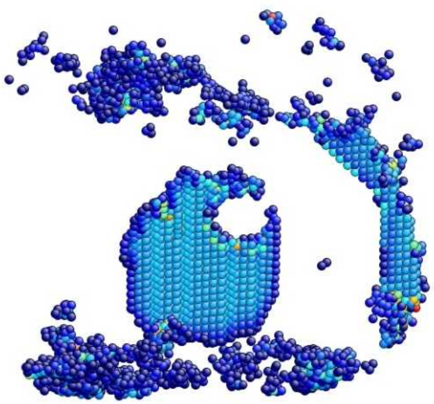
Grows and crosses previous dislocation – twist appears

3



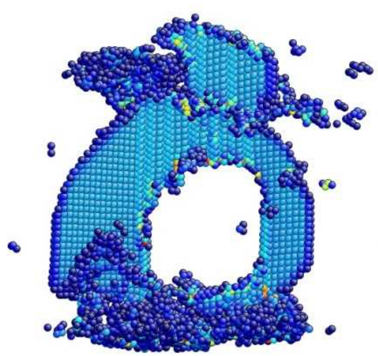
New dislocation nucleates from twist (center)

4

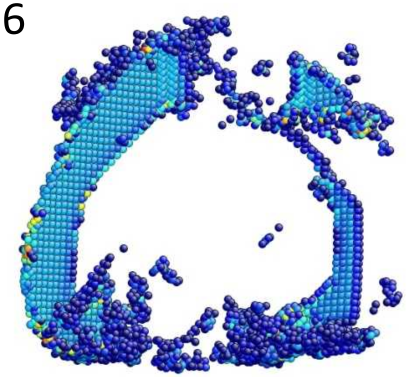


New dislocation grows as original reaches surface

5



6



Dislocation grows and reaches surface

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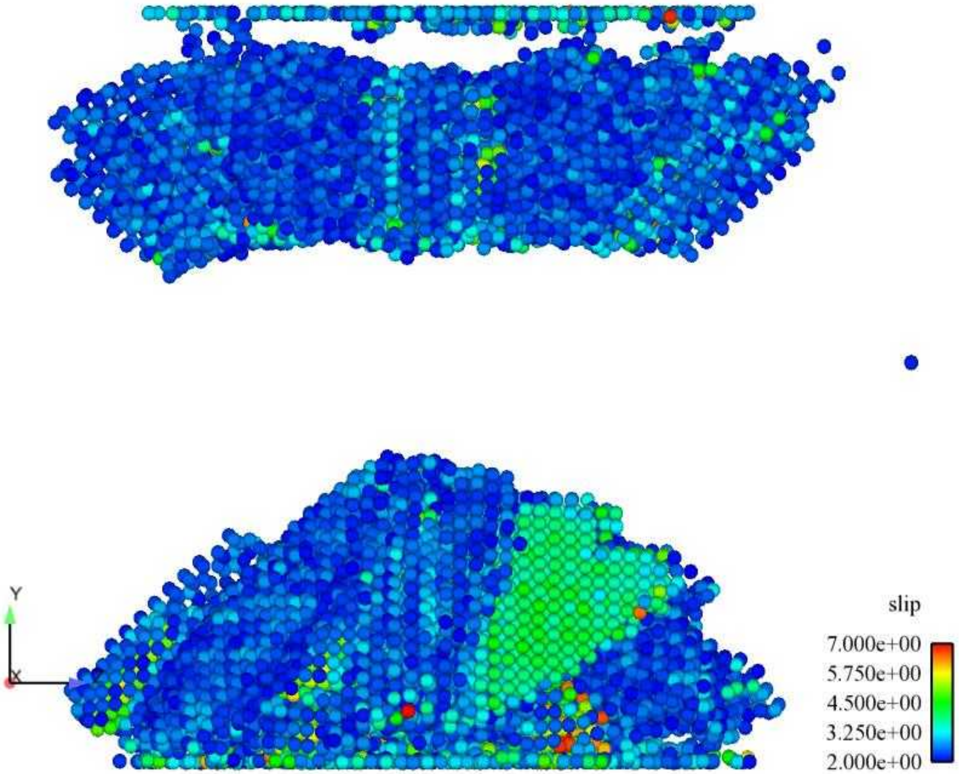
# Tersoff: Dislocations in 20 nm sphere

- Plane is {111}, slip direction is {110} and magnitude is around ½[110]a (perfect dislocation)
- Slip intersects surface
- 9 total found

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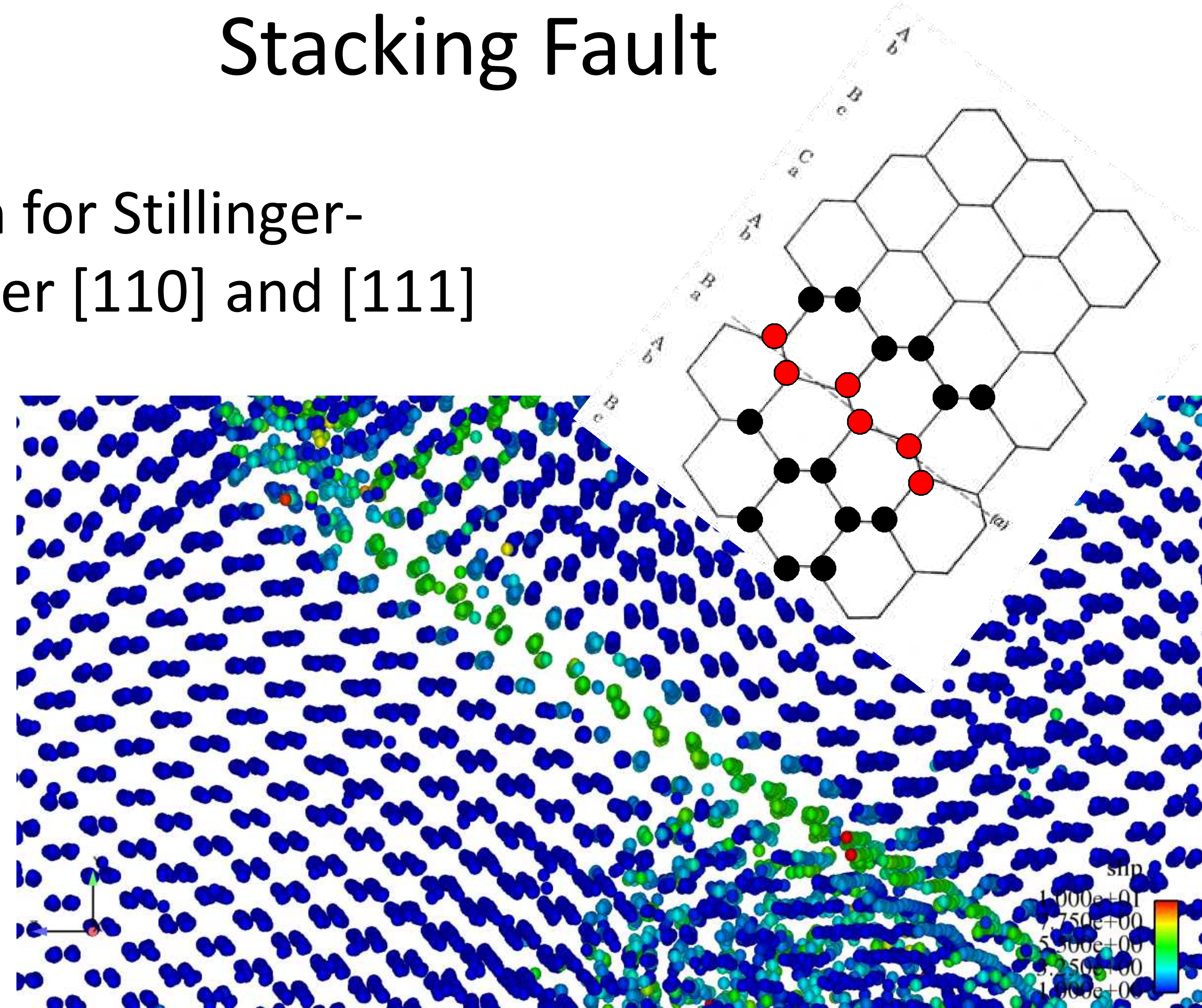
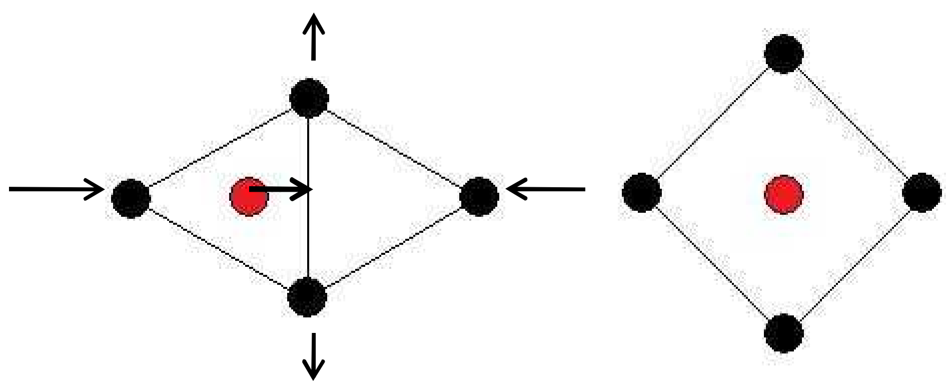
# Stacking Fault

- Seen for Stillinger-Weber [110] and [111]



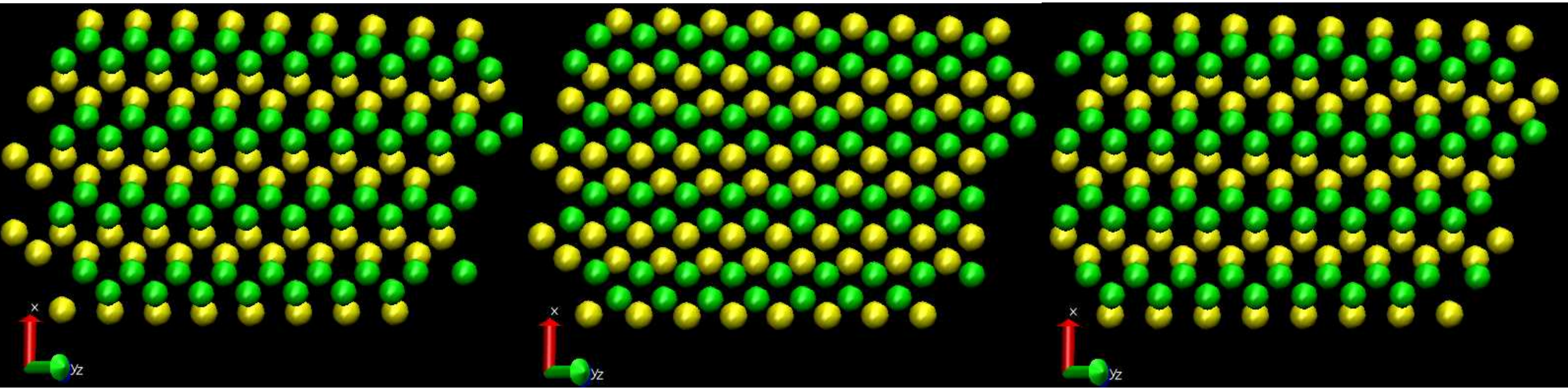
# BCT5 Nucleation

- Diamond cubic's tetrahedral bonding changes to  a 5 CN bonding
  - Best seen as a deformation of a {111} plane from a hexagonal to square shape



# Dislocation Nucleation

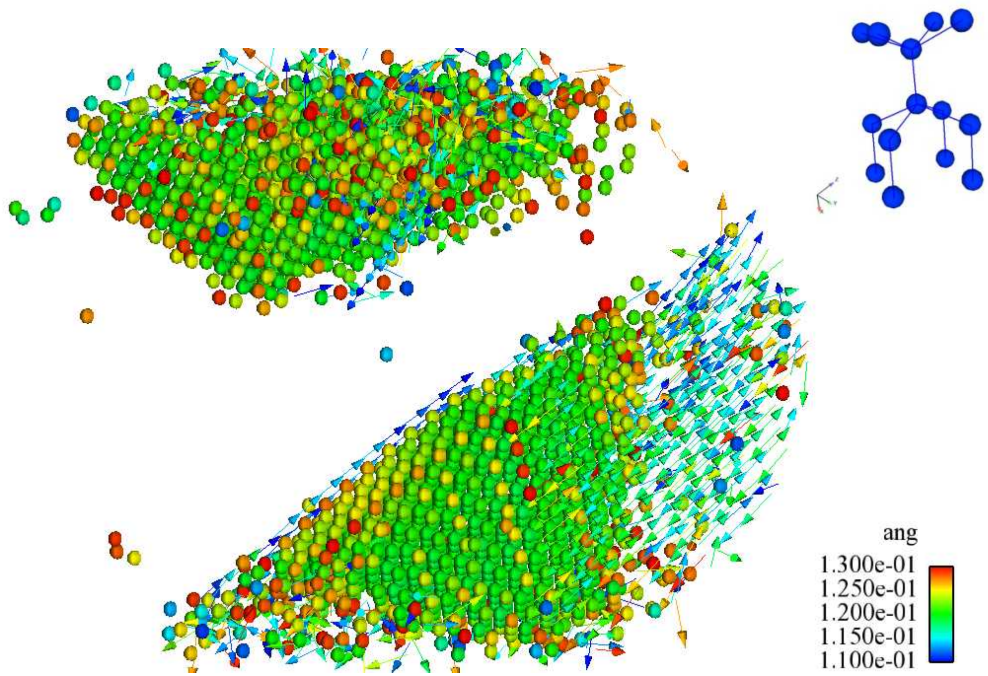
- "Partials" appear before full dislocations
  - Slip between $\{01\,\bar{1}\}$ planes

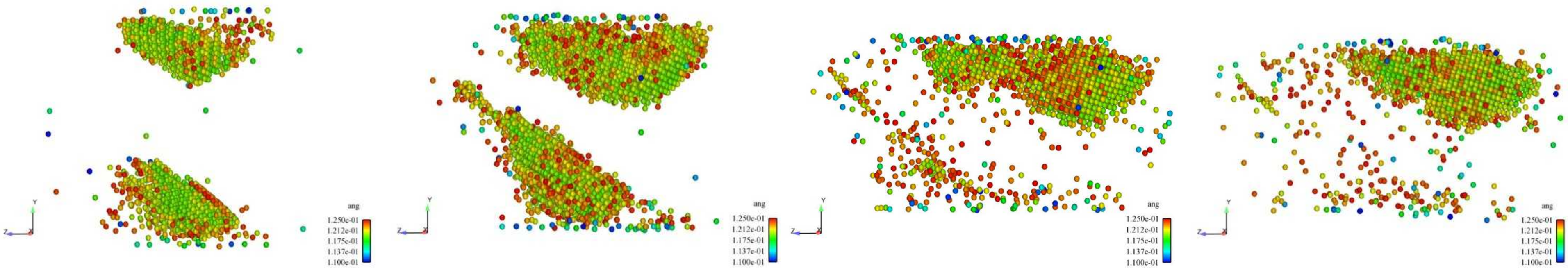



- ¼ <011>  displacement – Not a true crystalline minimum (not a stacking fault)

# 10nm SW [100] 0K (SW0 300K)

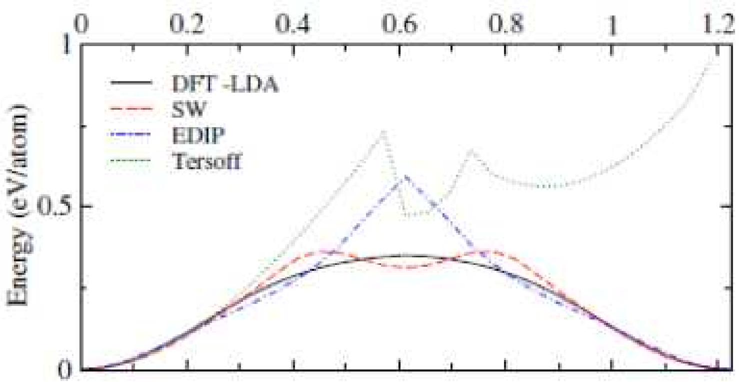
- Regions of BCT5 form
  - Top conical
  - Bottom pseudo-planar
- Dislocations form at edge of BCT5 and grow through DC
- Bottom region of BCT5 disappears as dislocations grow, top region shifts

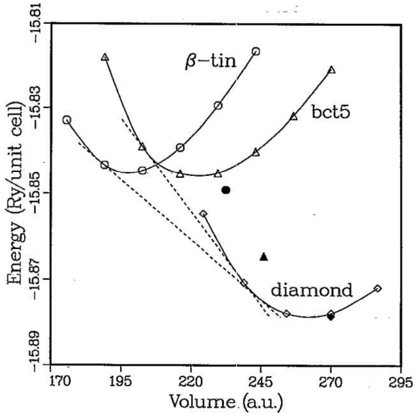


# ¼ <011>?

- Partially slipped plane has CN of 5
- Potential energy vs. <110> {111} Shuffle shearing shows dip at halfway point for Stillinger-Weber




- During initial shear process, crystal reaches midpoint and forms bonds similar to BCT5