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Investigating the Role of Grain Boundaries during the Plastic Deformation of Bicrystalline Nanowires Using Molecular Dynamics

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Sandia National Laboratories

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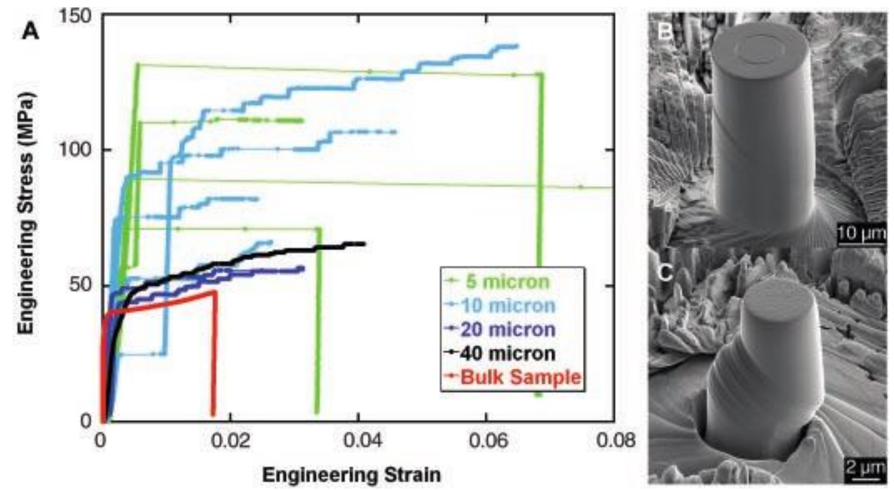
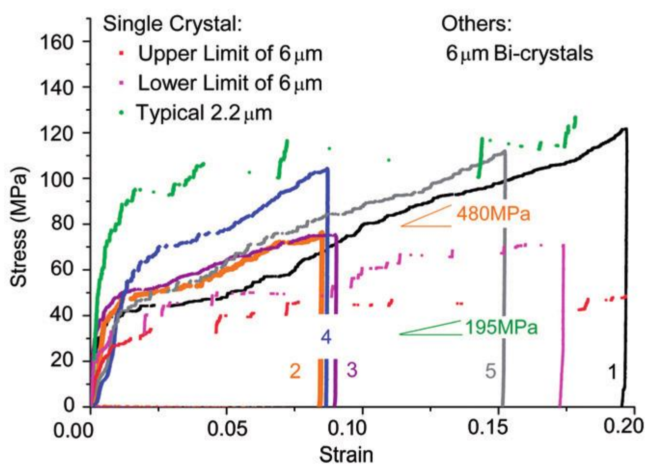
Micro-Mechanical Testing

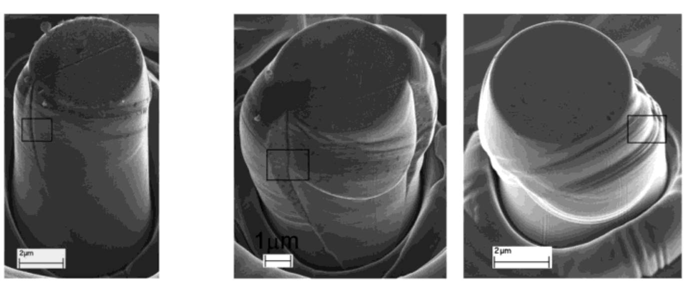
- Size-dependent plasticity
  - Strain `bursts'
  - Low work-hardening rates
  - Higher strength with smaller diameter (Power law)

→ Source-limited plasticity



Uchic et al., Science (2004)





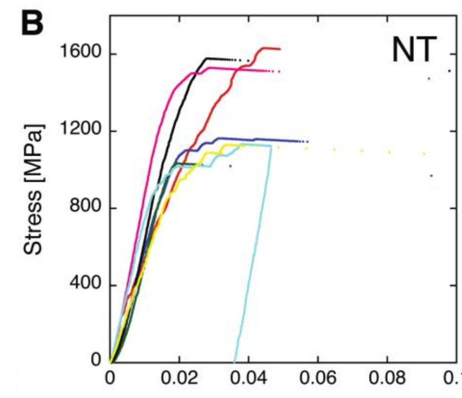
Ng and Ngan, Phil Mag (2009)

- Role of interfaces during deformation of bi-crystal pillars (*as compared to single-crystal specimens*)
  - Smaller strain bursts
  - Higher work-hardening and flow stress
  - Greater dislocation debris after deformation
  - GBs can trap lattice dislocations and lead to the alternative mechanical behavior

→ Internal GBs affect mechanical behavior and dislocation accumulation

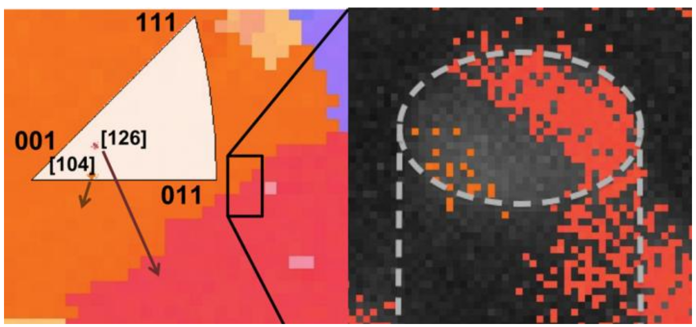
Nano-Mechanical Testing

- Size-dependence observed in nanopillars as well
  - Function of diameter and microstructure (i.e., presence of GBs, twin boundaries, and other internal features).
- GBs tend to weaken nanopillar, and twin boundaries tend to strengthen nanopillar.
- Possible changes to the bulk behavior and underlying deformation processes, due to GBs, surfaces, and sample dimensions.

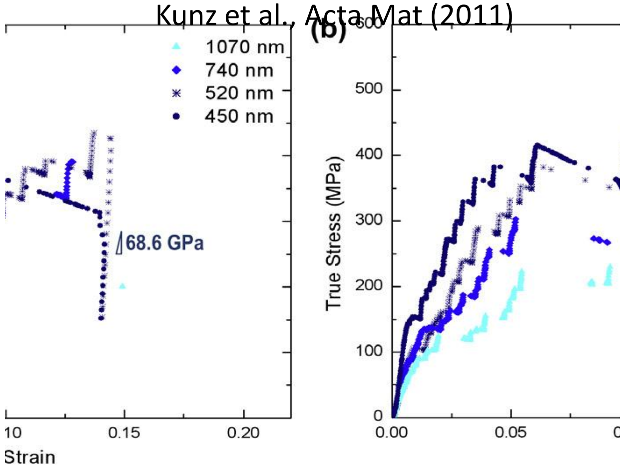


Jang et al., Nano Letters (2011)

Smaller is stronger



Kunz et al., Acta Mat (2011)



When compared to SC nanopillars

- Identical power-law behavior (yield strength)
- Lower hardening angles
- Larger strain bursts

→ Limited dislocation accumulation and GBs as a possible sink

How do GBs influence the mechanical behavior of nanowires?

→ source/sink/obstacle for dislocations

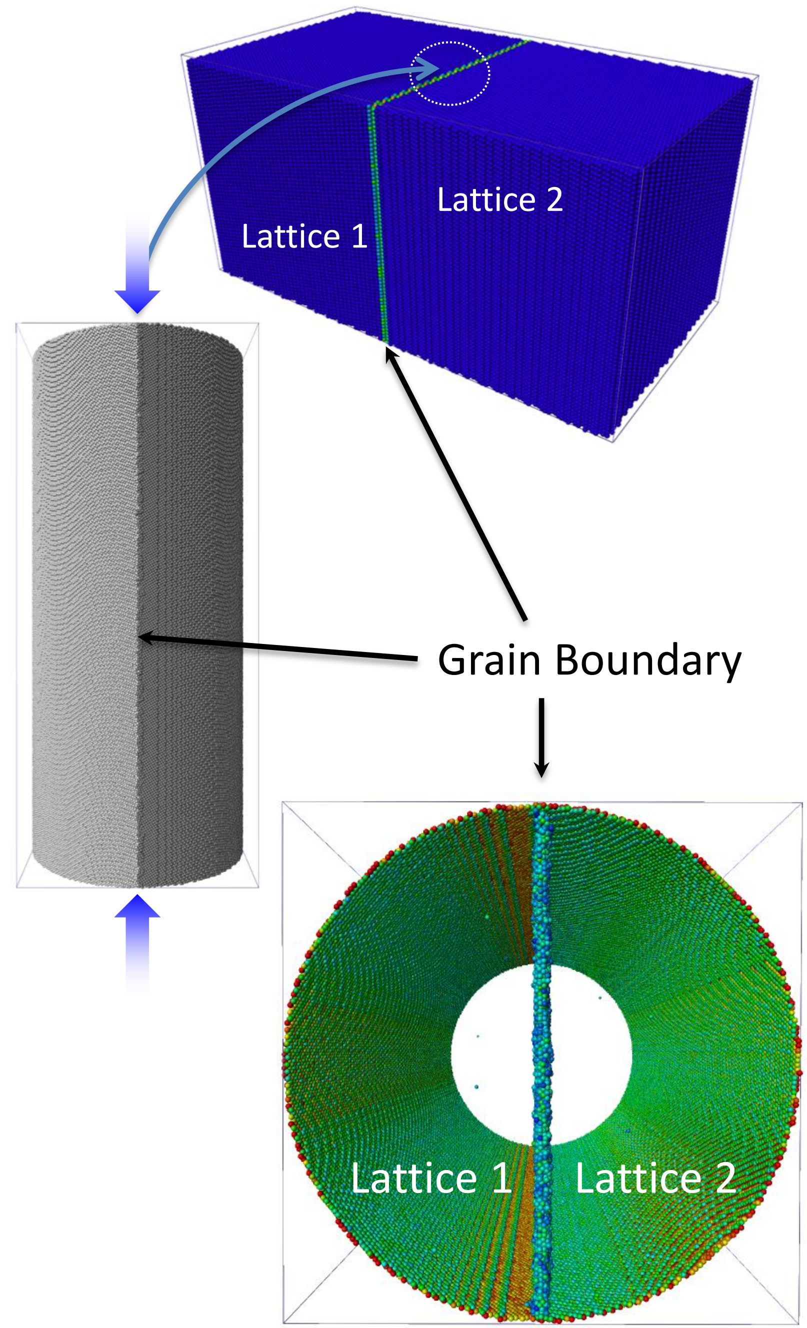
→ alter the deformation mechanisms

Methodology – creating nanowires

- Create 3D periodic bicrystalline structure
- Minimize energy and equilibrate to 300K for 100 ps.
- Extract nanowire from bulk structure with interface along vertical axis.
- Aspect ratio for each nanowire is at least 2:1
- After extraction, we then minimize energy and equilibrate to 300K for 100 ps

Methodology – deforming nanowires

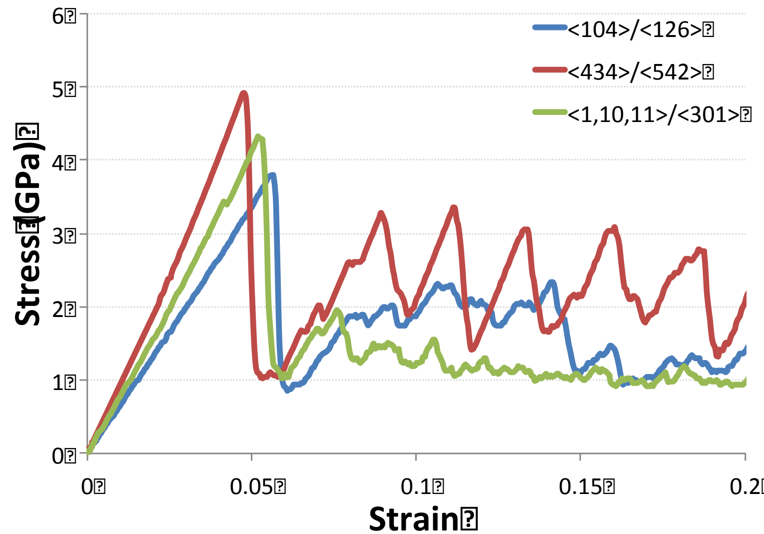
- Apply uniaxial compression at a constant strain rate of 10^8 s^{-1} along vertical axis of nanowire
- Deformation simulations are performed under NVT @ 300K until 20% uniaxial strain is achieved.
- Atomic snapshots are output every 0.005% strain containing full atomic stress tensor (virial), energy, centrosymmetry, etc…

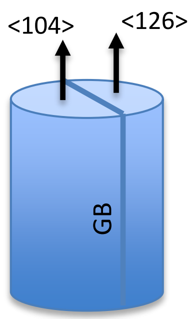


Nanowires containing random High-Angle Grain Boundaries (HAGBs)

Deformation of HAGB bicrystalline nanowires

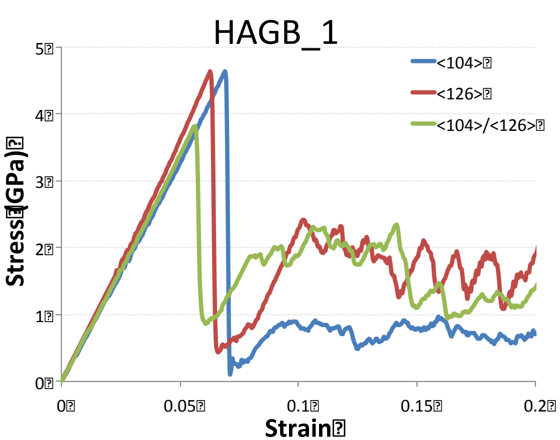
- 3 random HAGBs (defined by axis direction)
  - <104>/<126>
  - <434>/<542>
  - <1,10,11>/<301>
- Explore differences in the elastic deformation, peak compressive strength, and plastic flow regime.

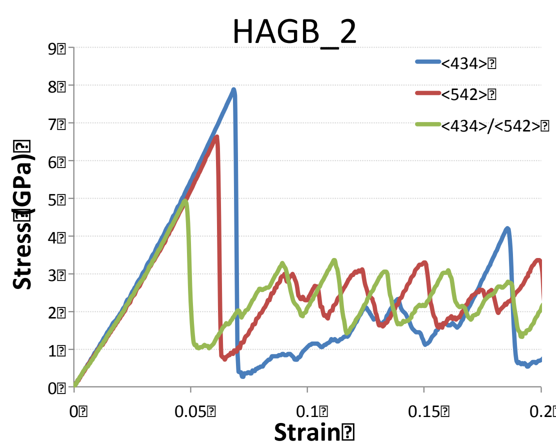


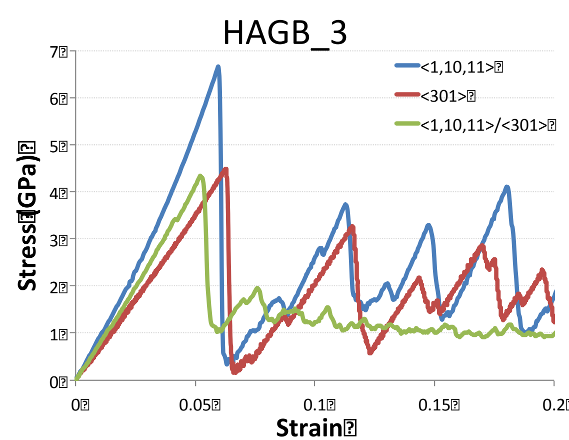


Bicrystalline nanowires can display both **smooth** and **jerky** plastic deformation at high uniaxial strains

→ GB structure influences mechanical behavior



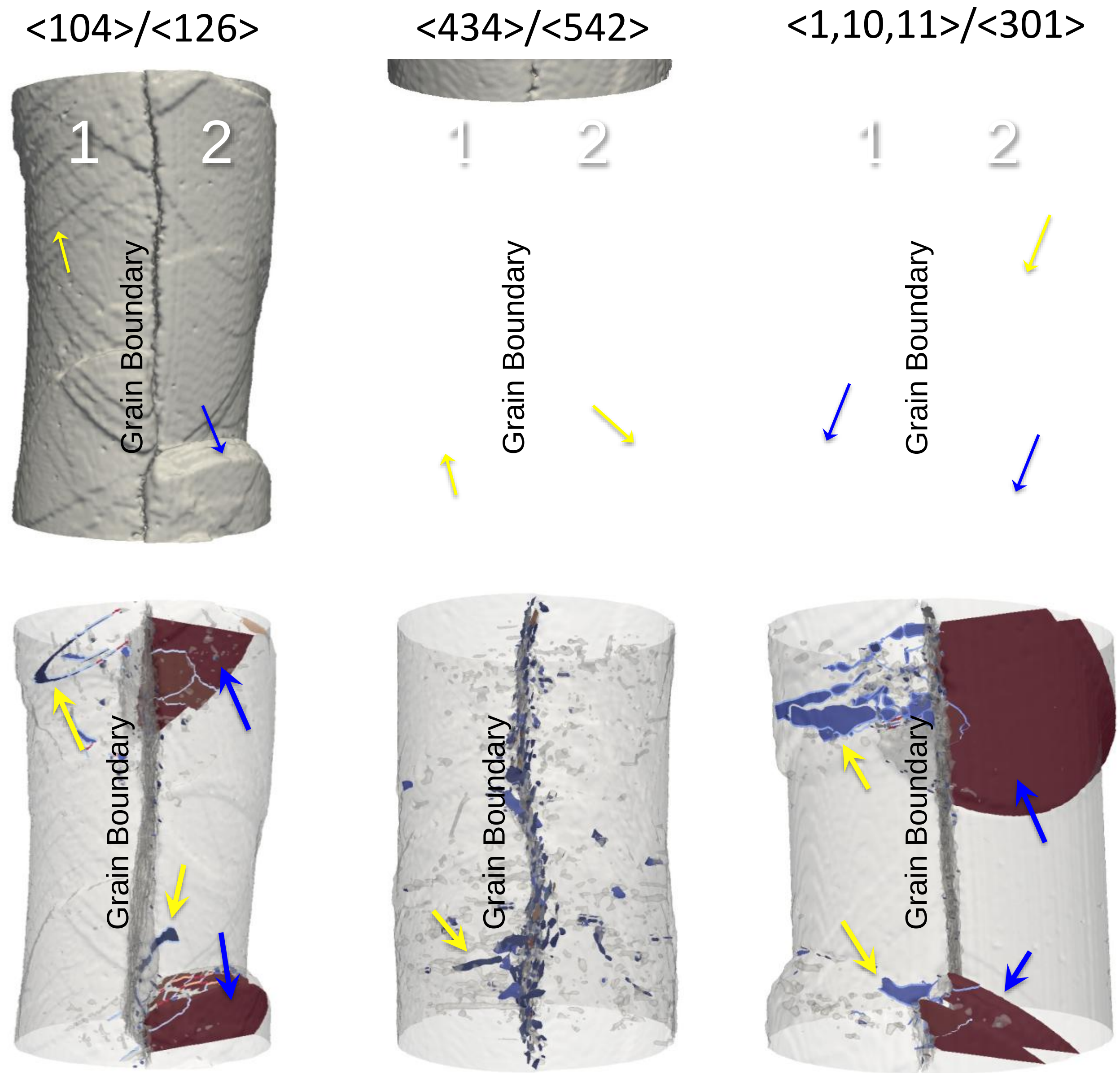




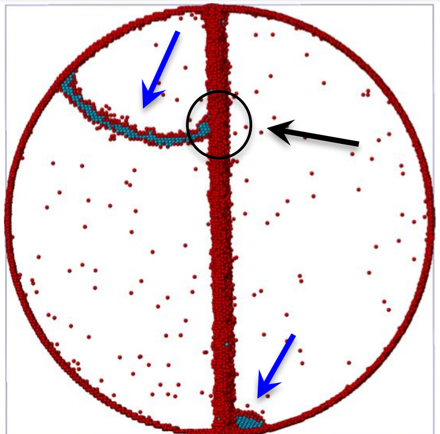
Deformed HAGB Bicrystalline Nanowires

Surface Ledges:
- Dislocation Slip
- Twin Boundaries

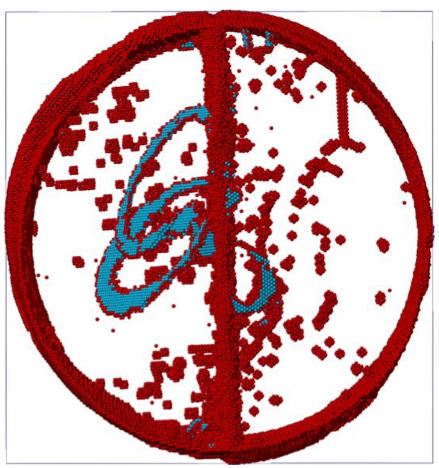
Deformation Mechanisms:
- Dependent on structure
- Multiple mechanisms active simultaneously (e.g., <104>/<126>)
- Twin boundaries influence plastic behavior at high strains



Do GBs act as a source or sink for dislocations?



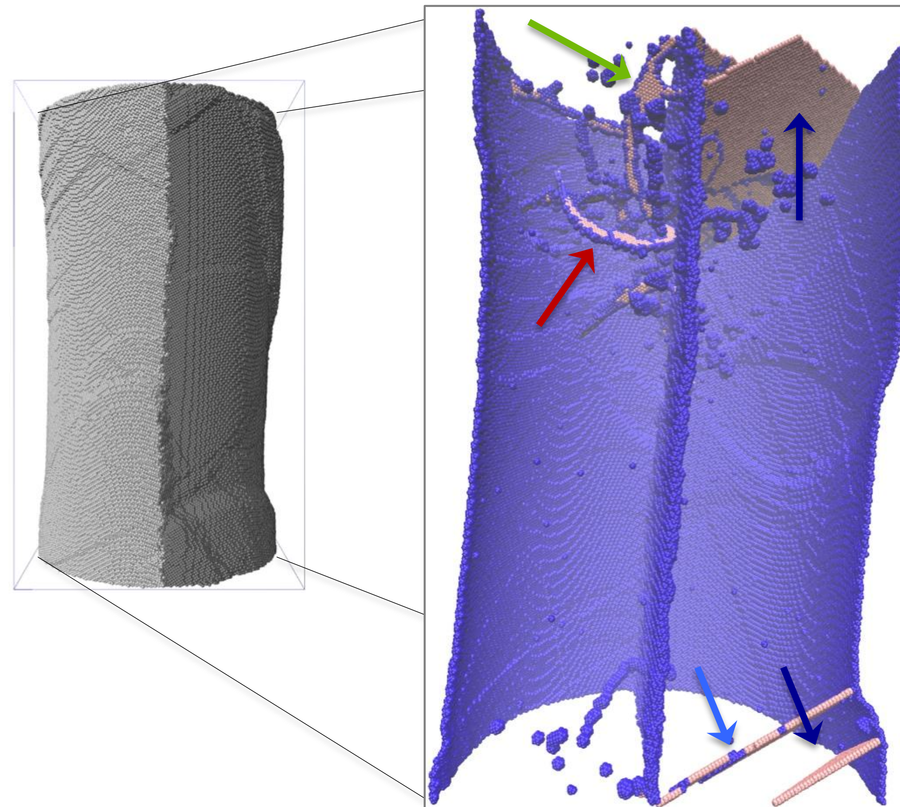
Nucleation from surface/interface



Nucleation from interface

GBs can act as both a source or sink for dislocations

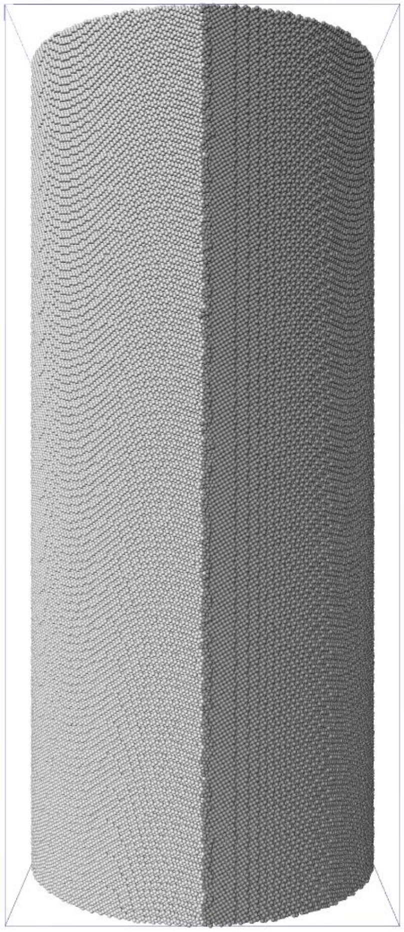
What mechanisms are observed?



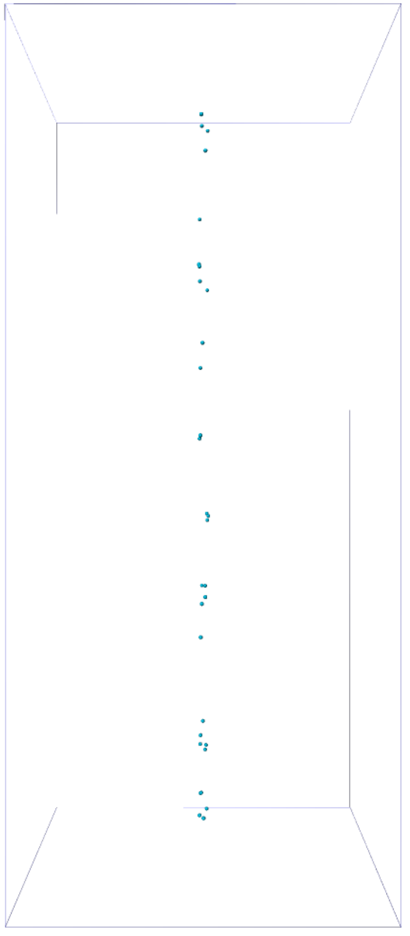
- Surface dislocation nucleation
- GB dislocation nucleation
- Twinning
- Twin boundary partial dislocations

GB structure and sample dimensions influence mechanical behavior

Surface Atoms



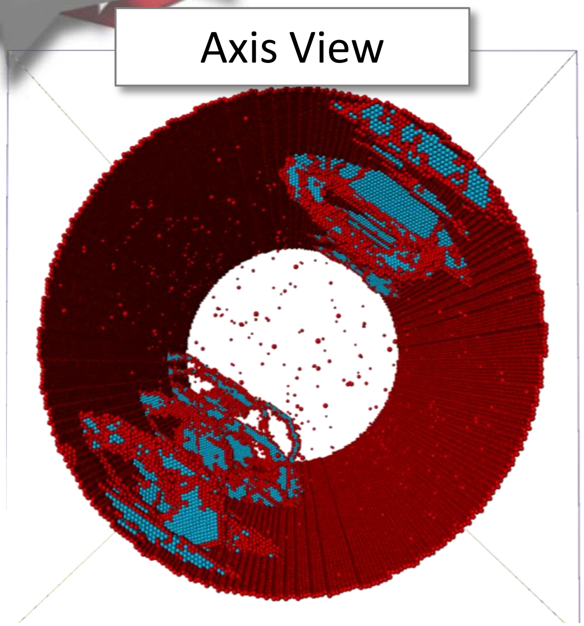
HCP Atoms

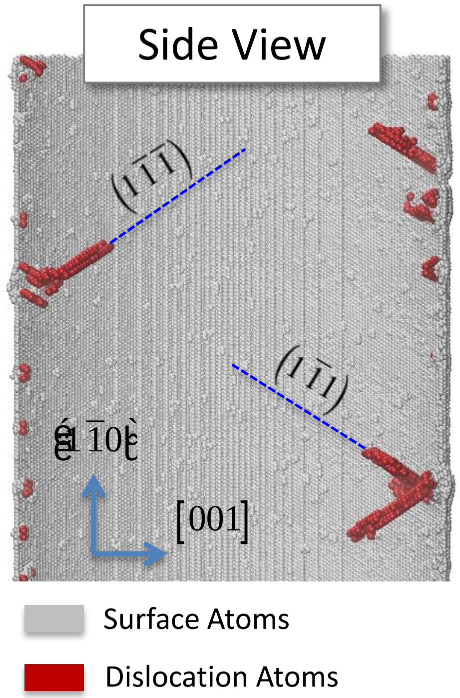


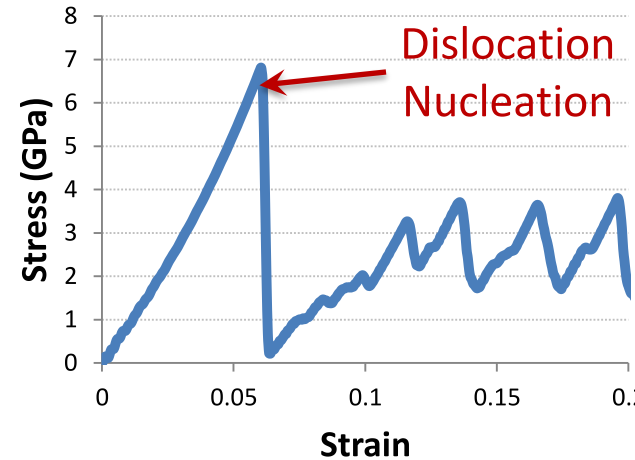
PLAY MOVIE!

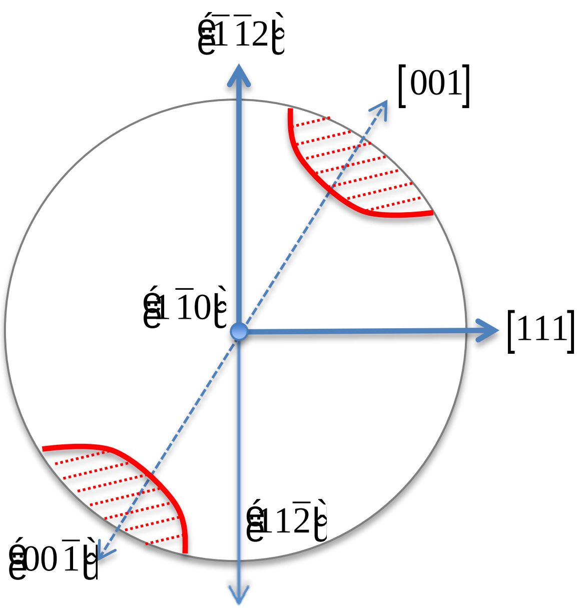
Nanowires containing <110> Symmetric Tilt Grain Boundaries (STGBs)

<110> Single-Crystalline Nanowire



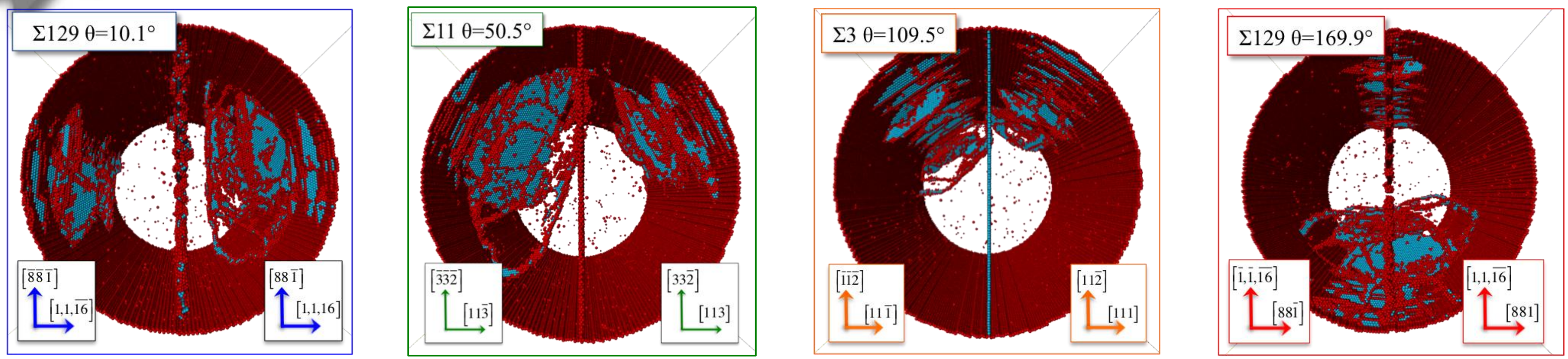




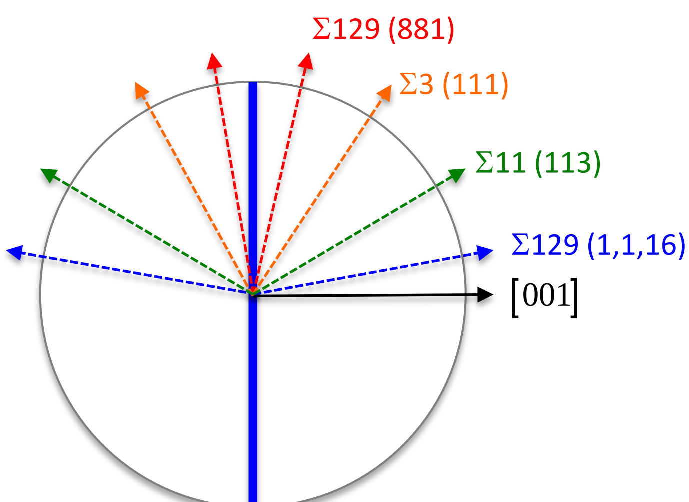


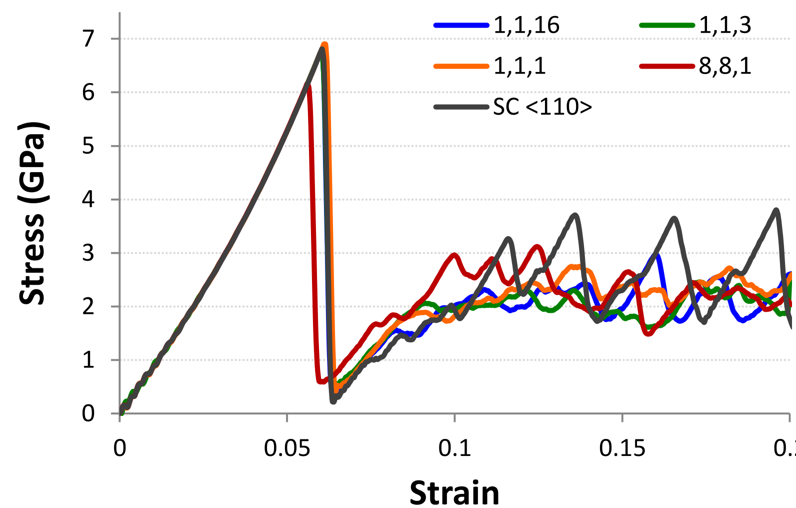
- <110> single-crystalline nanowire deforms by surface dislocation nucleation near peak compressive stress
- Full dislocation loops are nucleated from the 001 surface facets and migrate along {111} slip planes
- At nucleation stress, multiple dislocations are nucleated, but only a few dislocations are eventually emitted from the 001 surface facets
- Emitted dislocations tend to traverse the entire nanowire before exiting and leaving a surface step, leading to the stick-slip behavior at higher strains

Influence of Misorientation Angle on Dislocation Nucleation



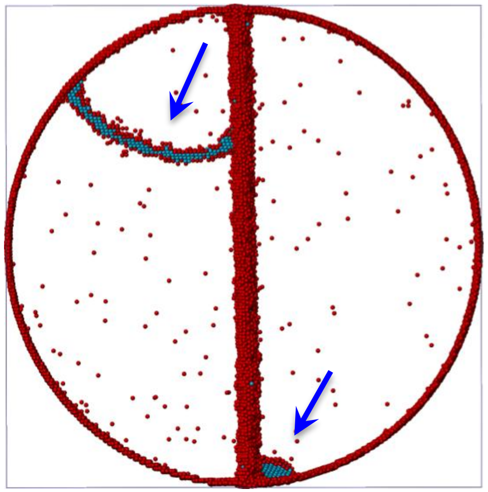
- Different misorientation angles of <110> symmetric tilt GBs
- Schematic shows the relative position of the [001] direction in each bicrystalline nanowire



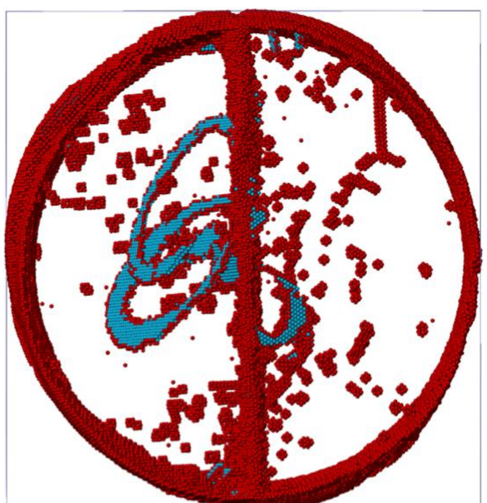


- Identical elastic response for all <110> nanowires
- Identical peak stress, except for the (881) bicrystalline structure (nucleation from interface/surface location).
- Similar flow response for all bicrystalline nanowires, but different from the <110> single crystalline nanowire

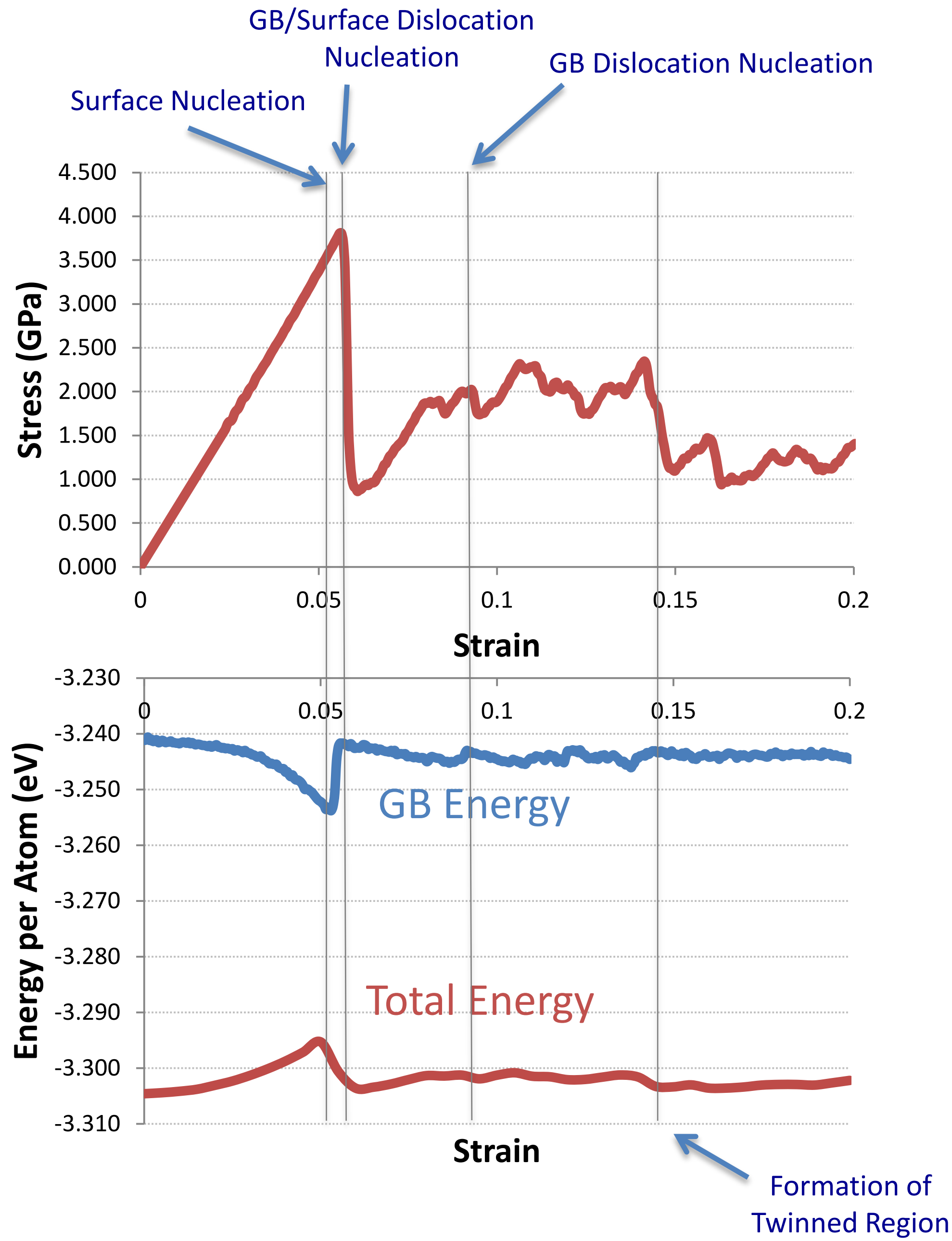
GB Energy Evolution and Dislocation Nucleation



Nucleation from surface/interface



Nucleation from interface



Conclusions

- MD simulations suggest that GBs do in fact influence the mechanical behavior of 30nm nanowires, but GB structure is important.
- Internal GBs can act as **both a sink and source for dislocations**, and simulations do not show the presence of dislocation pile-ups in 30nm nanowires under uniaxial compression at 300K.
- Surface dislocation nucleation is still observed in nanowires containing well-ordered or low-angle GBs, as compared to general HAGBs.
- The GB structure is influential on the bicrystalline nanowire mechanical behavior and underlying deformation.
- Insight into the **dual role of the GB** is provided by the evolution the the interfacial atomic energy – both GB dislocation nucleation and absorption.

Future Work

- ✧ Study the influence and response of single-arm sources, and the absorption of lattice dislocations in GBs.
- ✧ Compare various GB structures and metastable configurations for tailored properties.
- ✧ Explore tension-compression asymmetry and dependence of sample size in nanowires.

Acknowledgements

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