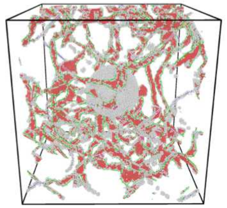
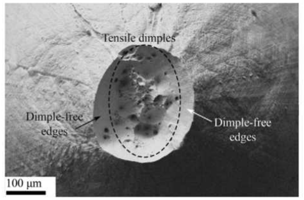
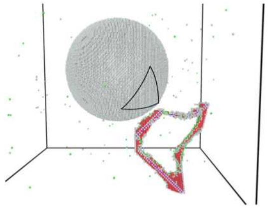
SAND2018-14088C

# Void Growth by Dislocation Adsorption During Ductile Rupture





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# The Standard Theory of Ductile Rupture


Ductile rupture = failure by. microvoid coalescence

Three steps:

1. Voids nucleate at "inclusions" or other hard particles
2. Void grow via plastic deformation
   - Grow rate typically described in terms of Rice-Tracey

$$\frac{\dot{R}}{R} = \alpha \exp\left(\frac{3\sigma^H}{2\sigma_Y}\right)\dot{\epsilon}^{eq}$$

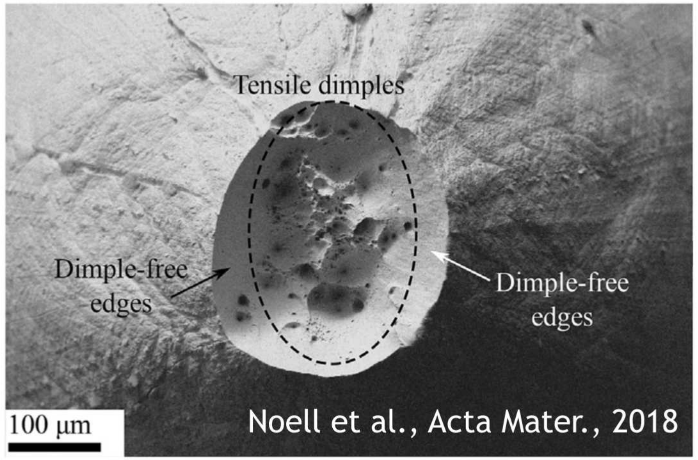
3. Rupture occurs when microvoids coalesce

Wildly successful, but still outstanding questions and unexplained observations:

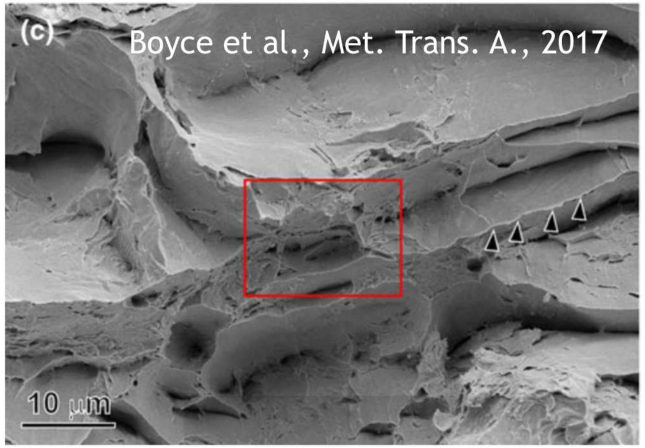
- How do voids nucleate in pure metals?
- How do voids nucleate in shear-dominated loading?
- What micromechanical processes underlie void growth? How do we expect the micromechanics of growth to affect the rupture process?

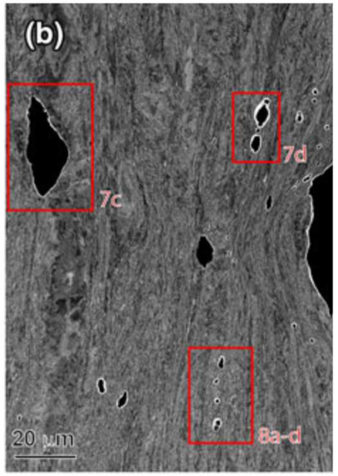
# Void nucleation in pure metals

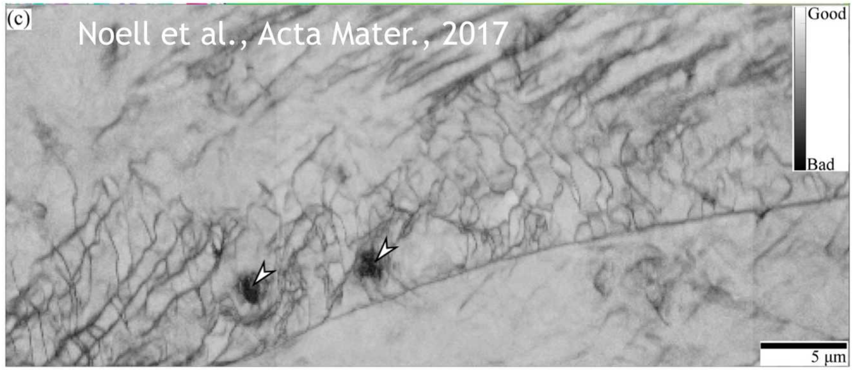
99.999% Cu



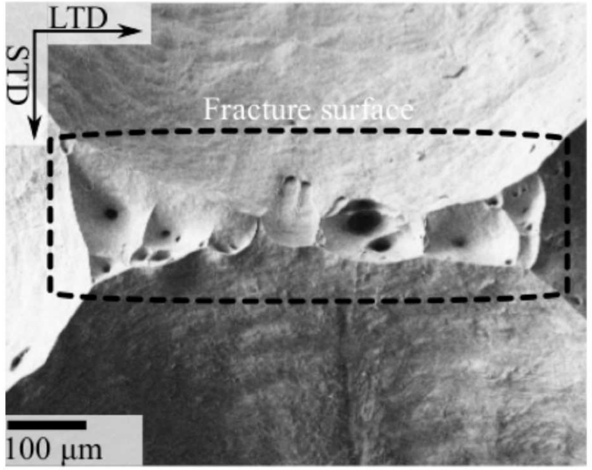

99.9% Ta

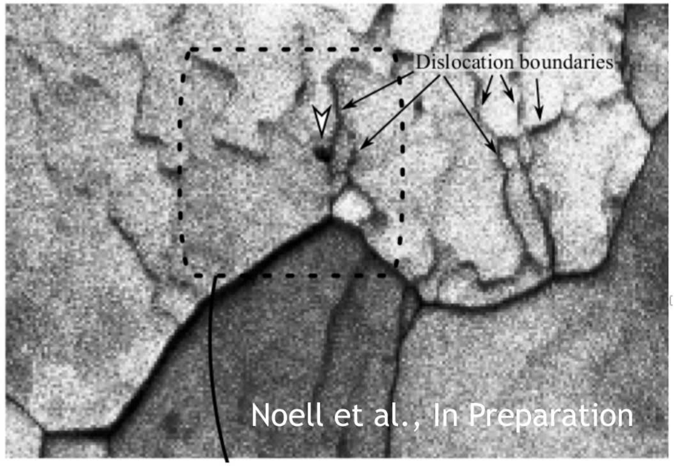


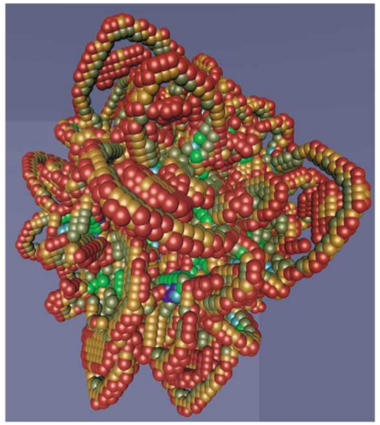

99.99% Al



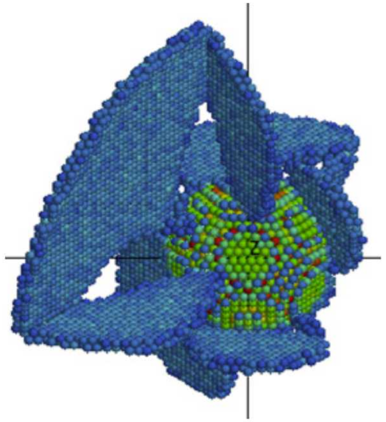




*Consistent feature*: voids tend to nucleate at dislocation boundaries/cell walls, but not those with the high misorientation

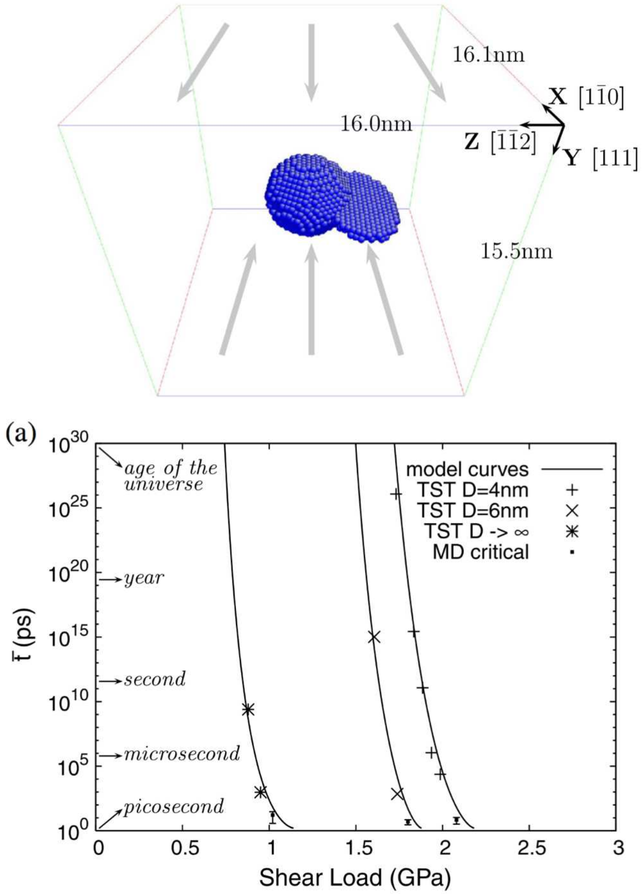
# Micromechanics of void growth



Marian et al., PRL, 2004



Bringa et al., Acta Mater., 2010

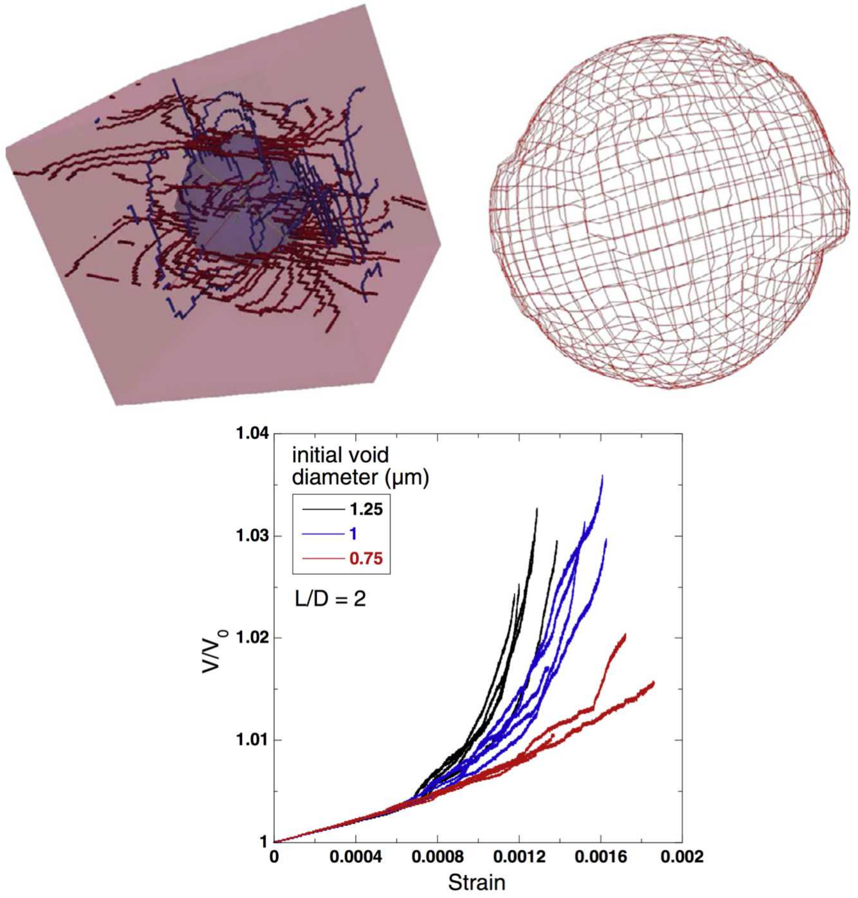



Nguyen and Warner, PRL, 2012

Only relevant for high stress loading!

Dislocation nucleation

Chang et al., Scripta Mater. 2015



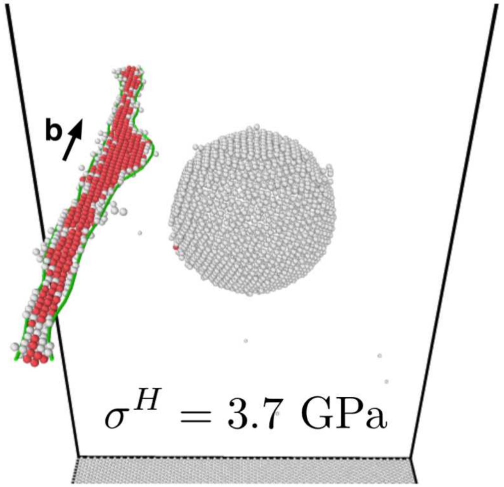

Dislocation adsorption

*Major outstanding questions:*

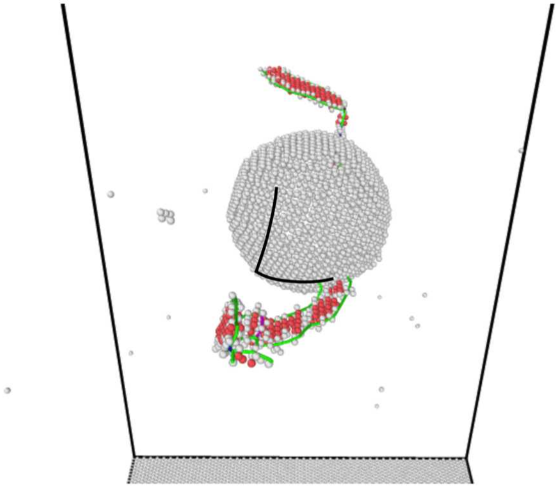
- Fundamental dislocation-void interactions?
- Relationship to nucleation-mediated growth?
- Growth rate as a function of stress?

# Dislocation-void interactions under hydrostatic stress

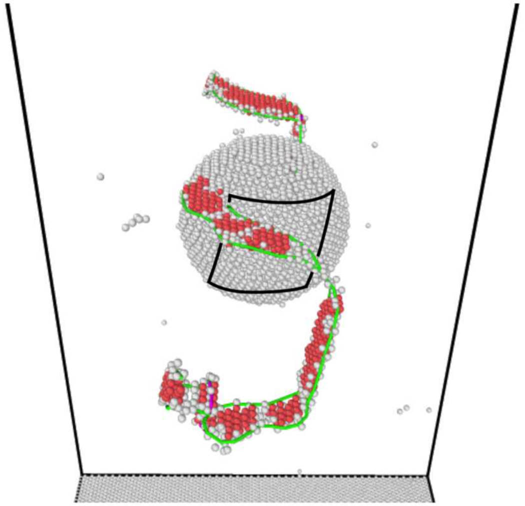
Graphics made with OVITO




Screw dislocation in FCC Al



Glides, cross-slips, glides,…



…cross-slips, glides, cross-slips…

No volume change to insert a screw dislocation!

$$\delta V = \int_S \mathbf{b} \cdot d\mathbf{A}$$

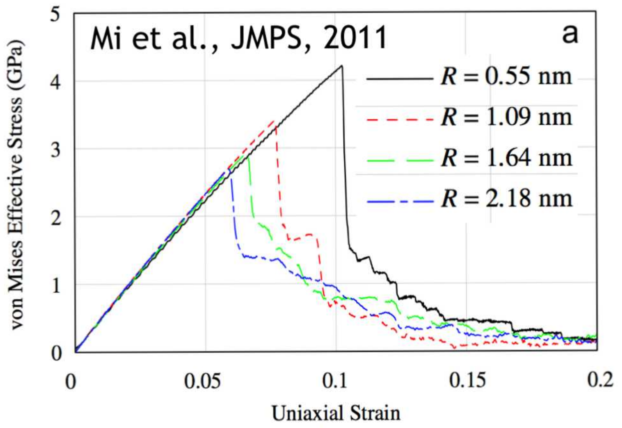
Hirth and Lothe, 1992
Bulatov et al., Scripta Mater., 2010

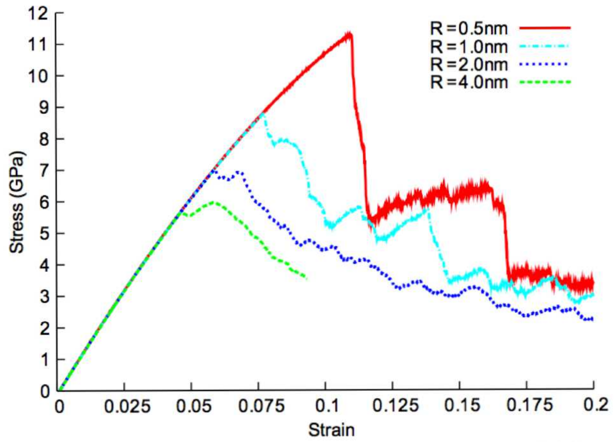
Growth is controlled by glide and cross-slip of pre-existing dislocations

- Enables growth without high stresses

# Influence of pre-existing dislocations on stress-strain curve

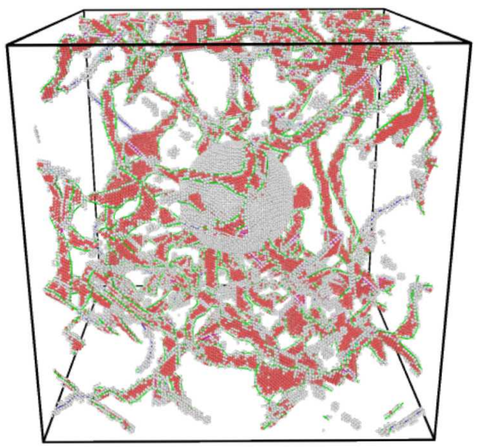
## No pre-existing dislocations



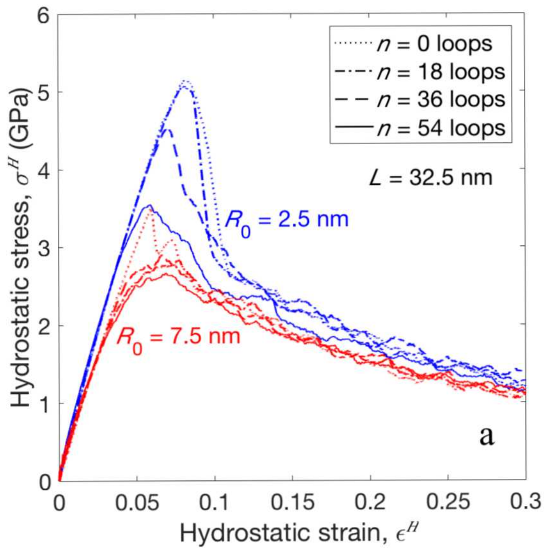




Traiviratana et al., Acta Mater., 2008

*Initial configuration*



18 loops ≈ 3.8 x $10^{16}$ $m^{-2}$




Stress drop associated with dislocation nucleation goes away as the initial dislocation density increases

- Post-yield, results converge together…

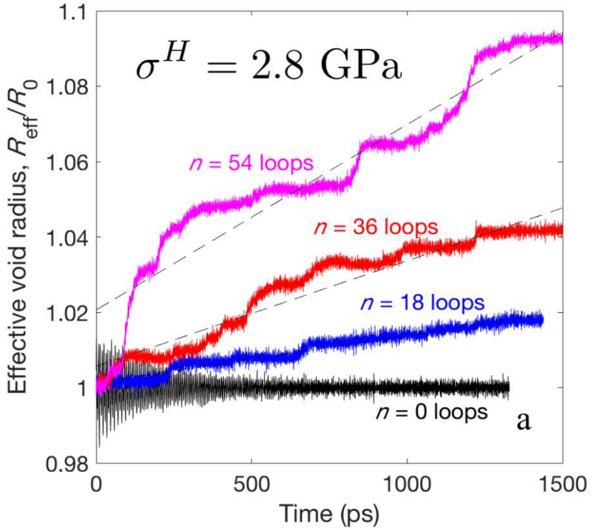
Even when system is initially dislocation-free, growth is controlled by dislocation adsorption!

# Void growth rates

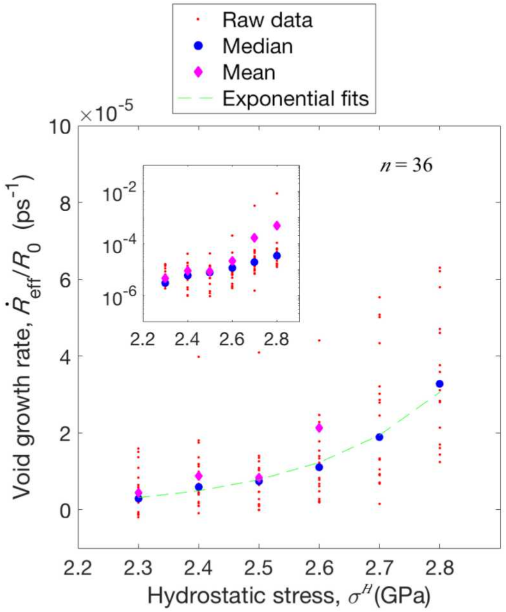
$$\frac{\dot{R}}{R} = \alpha \exp\left(\frac{3\sigma^H}{2\sigma_Y}\right)\dot{\epsilon}^{eq}$$

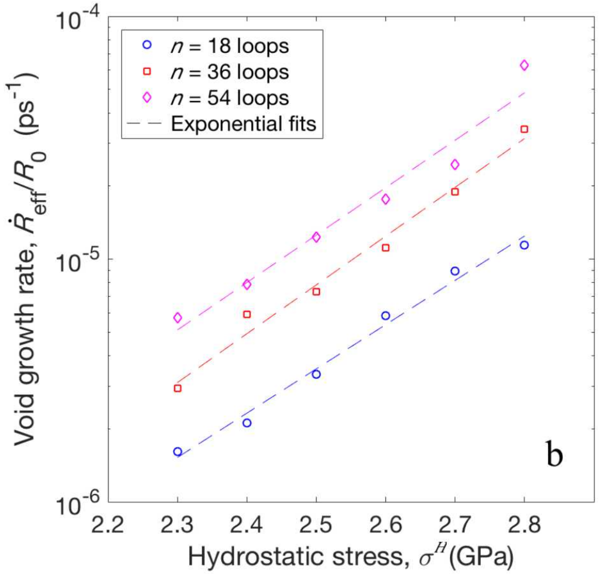
Can we make a meaningful comparison with Rice-Tracey?

- Can't do a one-to-one comparison because of boundary condition issues, but…




Repeat 20 times for each stress and dislocation density




Adsorption-mediated growth obeys exponential scaling!

$$\frac{\dot{R}}{R} = A(\rho)\exp\left(4.4\sigma^H\right)$$

# Implications and future work

Lower dislocation densities require higher hydrostatic stresses

- Recent experiments show that dynamic recrystallization in Al suppresses rupture (Noell et al., In Preparation)

Voids should exist in regions with enough dislocation content to accommodate growth

- Observe that voids most commonly appear in dislocation boundaries/walls

*Even in materials with inclusions*, local dislocation content will affect void nucleation/growth

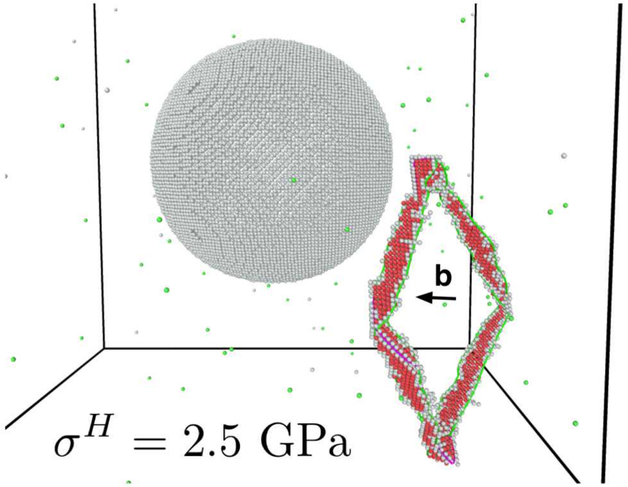
Coupling adsorption-mediated growth with vacancy condensation (Cuitino and Ortiz, Acta Mater., 1995) may explain void nucleation in pure metals

Future work:

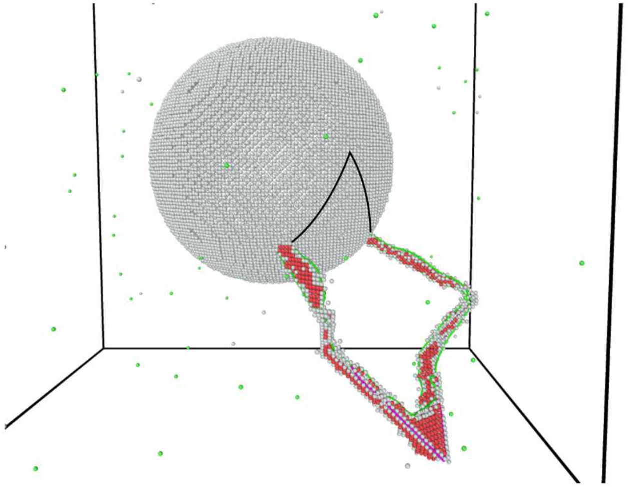
- Extend findings to lower stresses, lower dislocation densities – DDD collaboration with Wei Cai at Stanford
- Quantify influence of various dislocation processes (bulk cross-slip, surface cross-slip, glide, climb)

# Back up slides

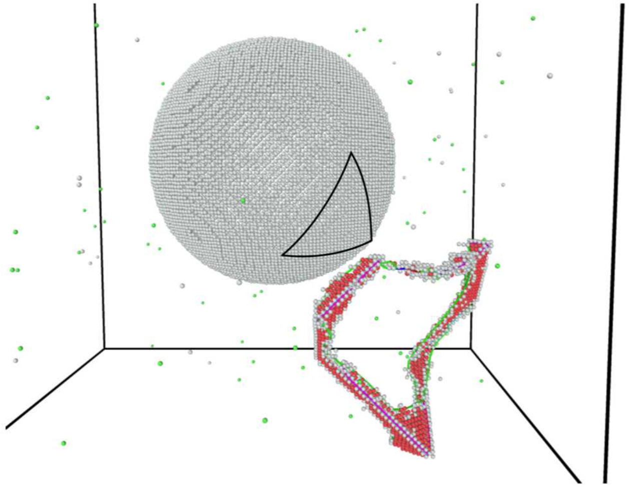
# MD case study 2




Prismatic loop in FCC Al



Glides towards and collides with void



Cross-slips, recombines, and glides away

# Universal stress-strain curve

Simulation with fixed number of atoms