Statistics of Mechanics

or

Statistical modeling of plastic yielding at small length scales

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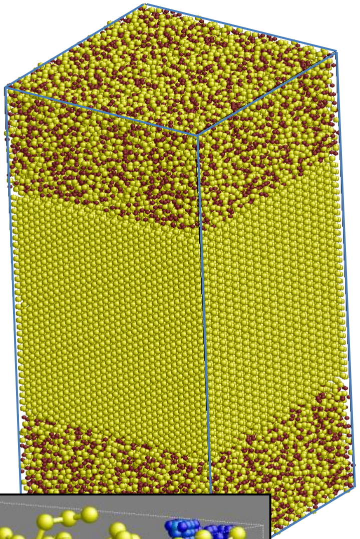
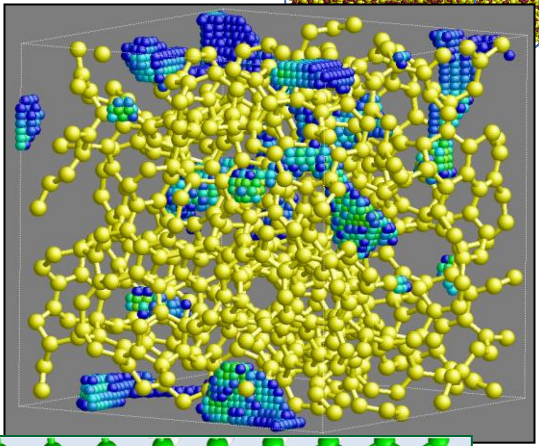
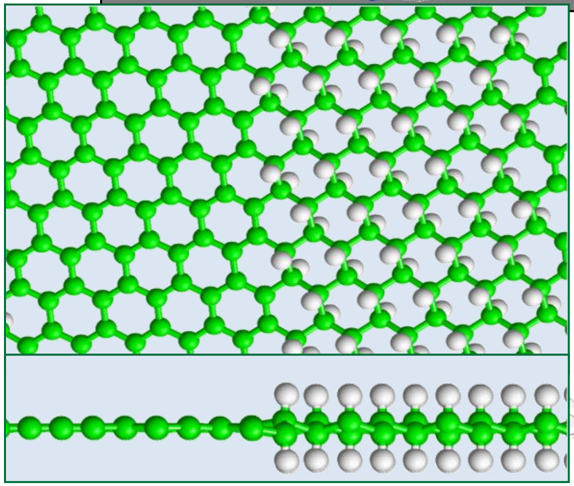
Sponsor: Materials Science and Engineering Division, Basic Energy Sciences, Department of Energy

Other projects:

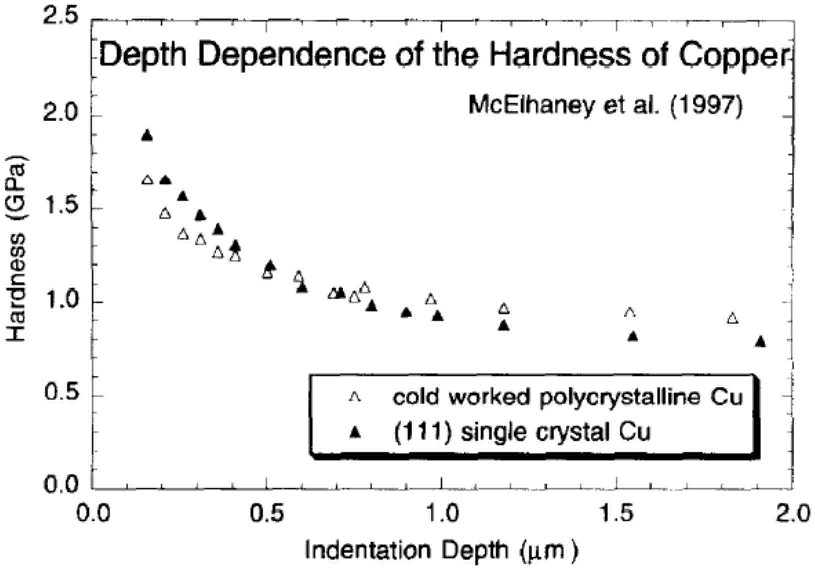


- Last CMSN meeting: metallic glasses & interfaces
- Traditional CMSN topic: solid-liquid interfaces, crystal nucleation (JCP 2010)
- H_2 storage in carbon structures (JPCC 2010)
- Hydrogenated planar structures and interfaces (PRB 2009)





“Conventional” length scale effects in nanoindentation



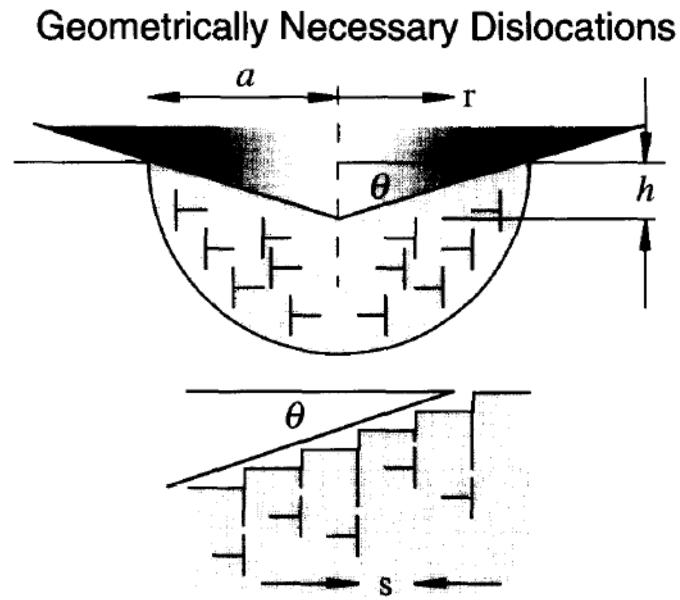


Fig. 2. Geometrically necessary dislocations created by a rigid conical indentation. The dislocation structure is idealized as circular dislocation loops.

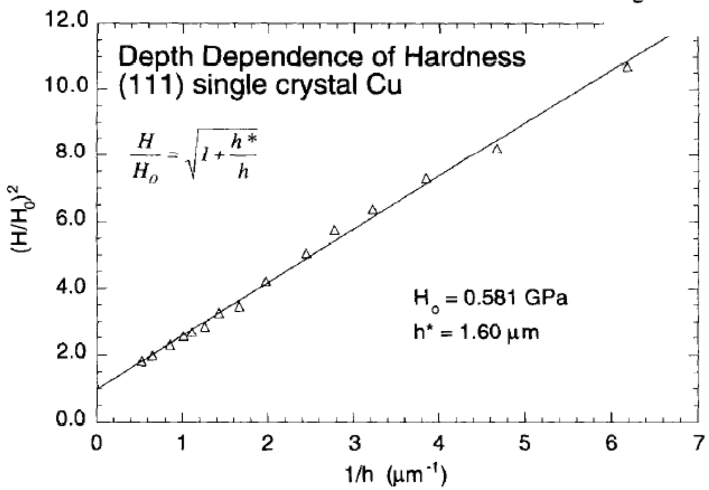


Fig. 3. Depth dependence of the hardness of (111) single crystal copper, taken from Fig. 1, plotted according to eqn (8).

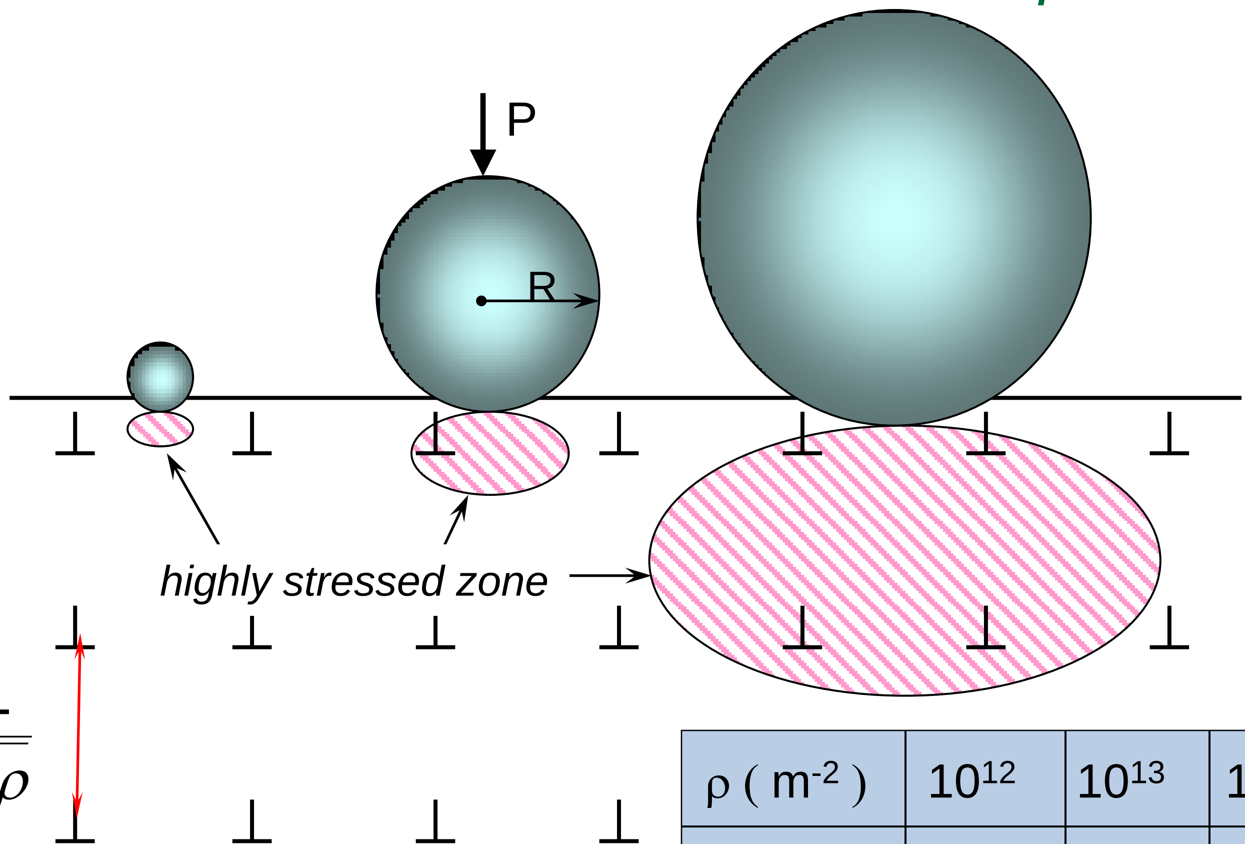
- H_0 = hardness due to pre-existing dislocations
- h^* = characteristic length scale arising from geometry, pre-existing dislocations

Nix & Gao

J. Mech. Phys. Solids, 1998

What happens as indenter becomes small? (Focus on spherically tipped indenters)

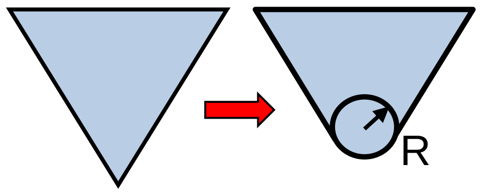
- a large indenter samples *many defects* (bulk limit)
- a small indenter likely samples *no defects* (theoretical limit)
- *Intermediate size is much more variable in response.*

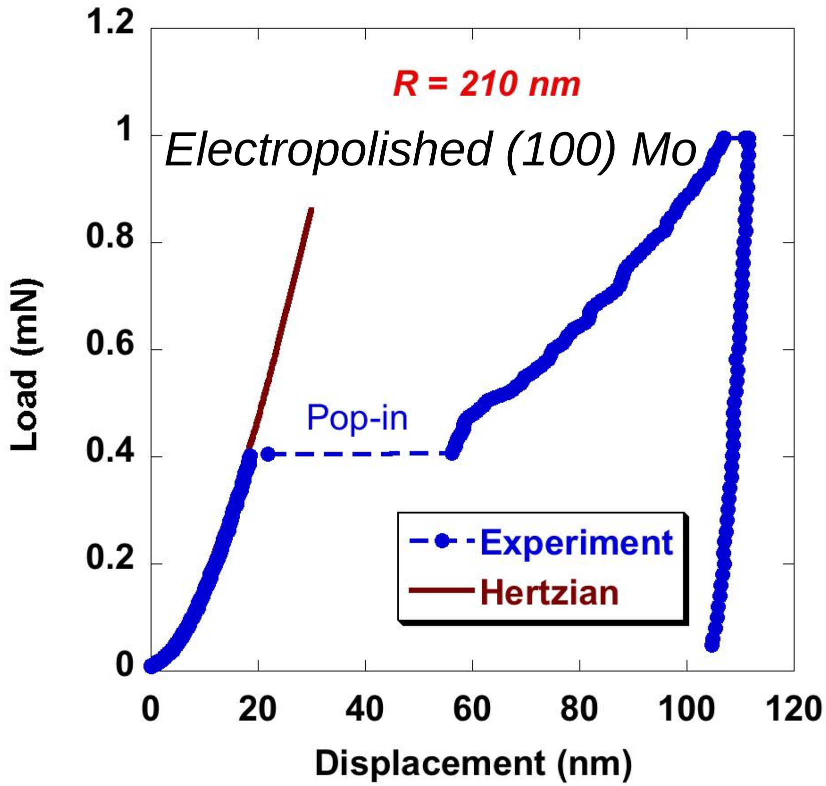


$$L \cong \frac{1}{\sqrt{\rho}}$$

ρ (m^{-2})	10^{12}	10^{13}	10^{14}
L (μm)	1.0	0.3	0.1

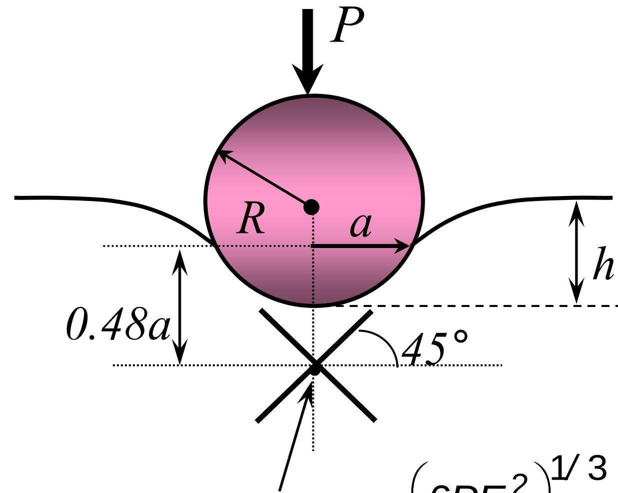
- For very small indentors, there is a sharp transition from elastic to plastic behavior.
- Usually assumed to be due to homogeneous formation of dislocation loops





$P_{pop\text{-}in} = 0.4$ mN

Hertzian Analysis



$$\tau_{max} = 0.31 p_m = 0.31\left(\frac{6PE_r^2}{\pi^3 R^2}\right)^{1/3}$$

R = 178 nm; *E* = 322 GPa; ν =0.30

τ_{max} = 16.3 GPa

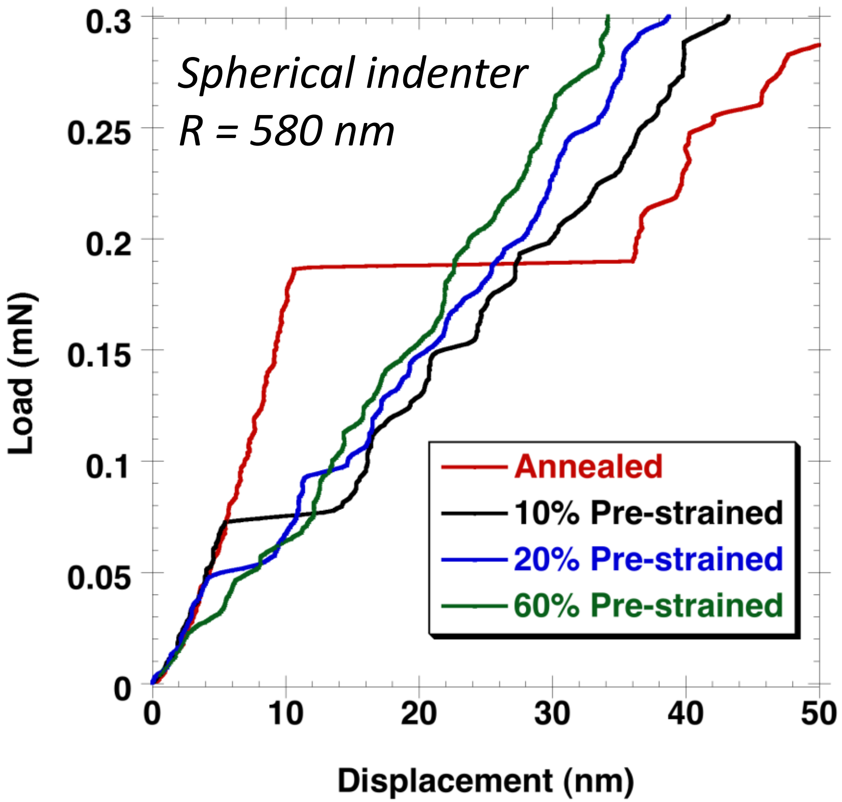
~ *G/8*

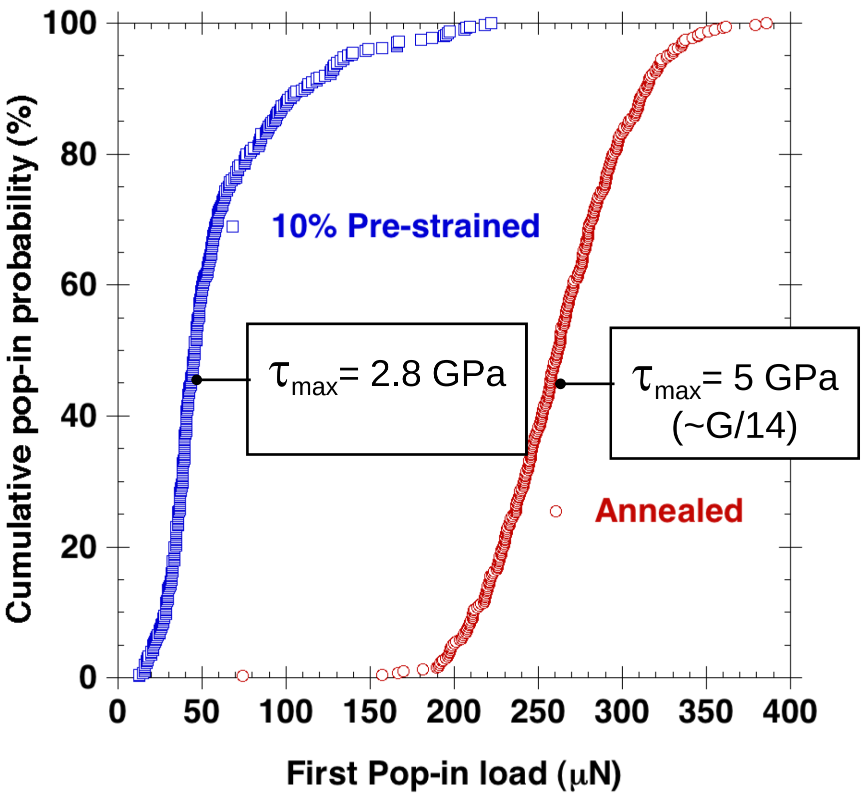
DFT: τ_{theo} = 15 GPa
(Ogata et al, *PRB*, 2004)

Not necessarily "homogeneous" dislocation nucleation:

Depends on processing!

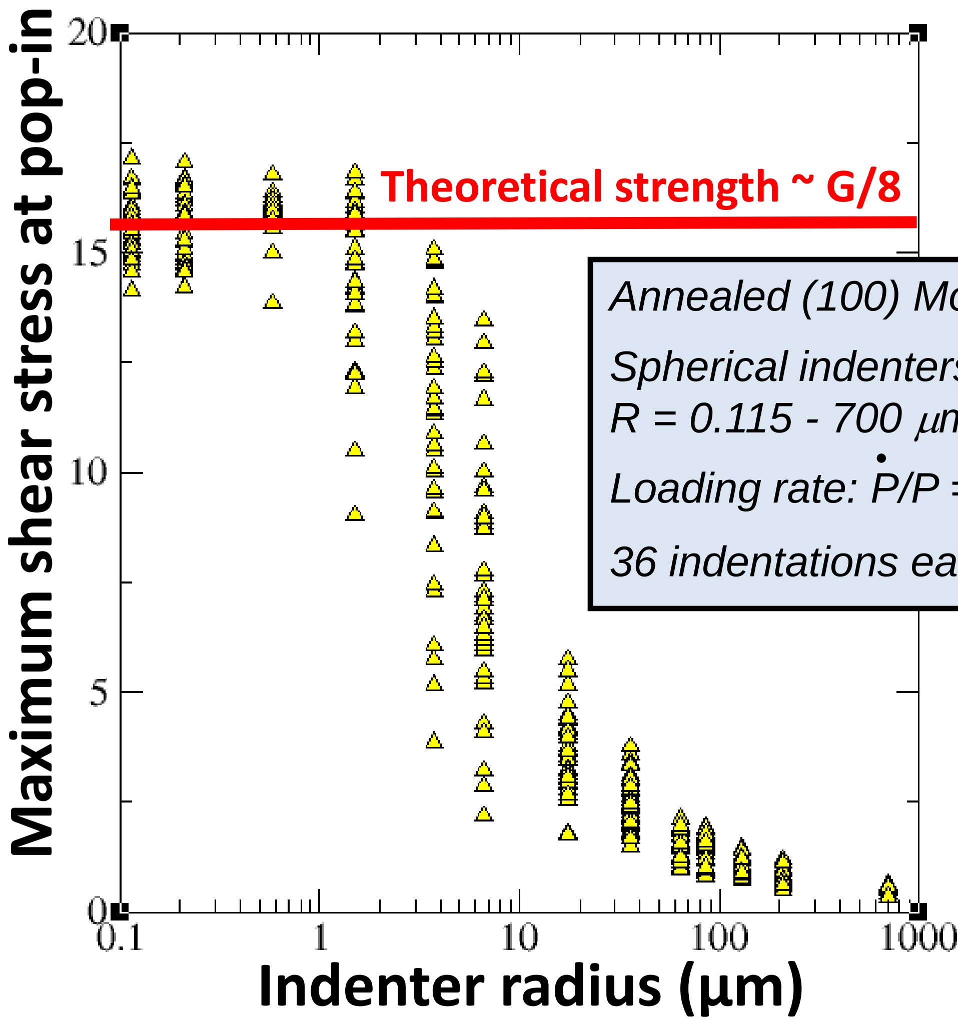
Highly annealed vs. pre-strained (100 Ni)





100 indentations

New nanoindentation size effect:
Pop-in stress varies with both indenter size and dislocation density

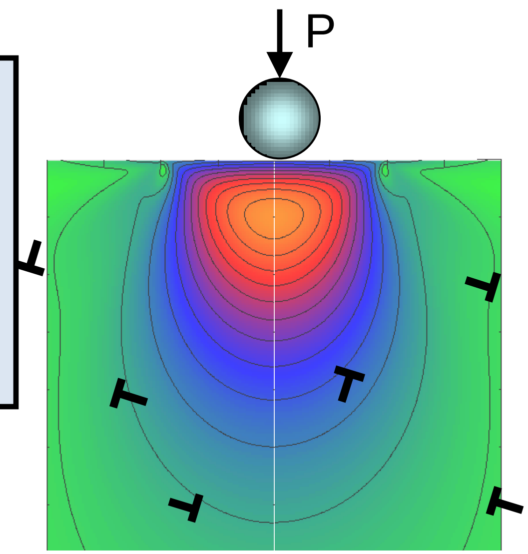


Annealed (100) Mo (pure)

Spherical indenters:
R = 0.115 - 700 µm

Loading rate: $\dot{P}/P = 0.05\ s^{-1}$

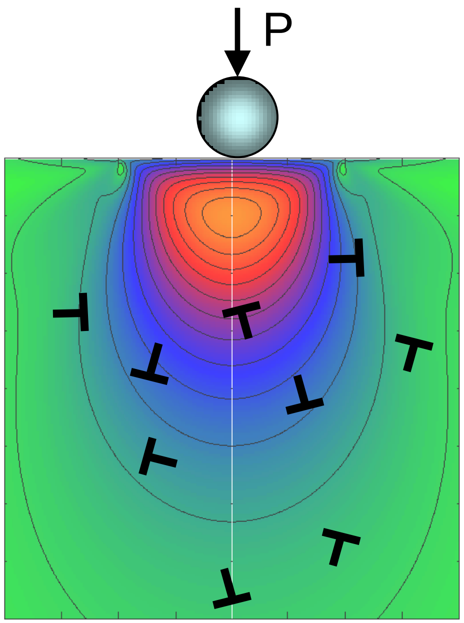
36 indentations each



Resolved shear stress distribution under indenter

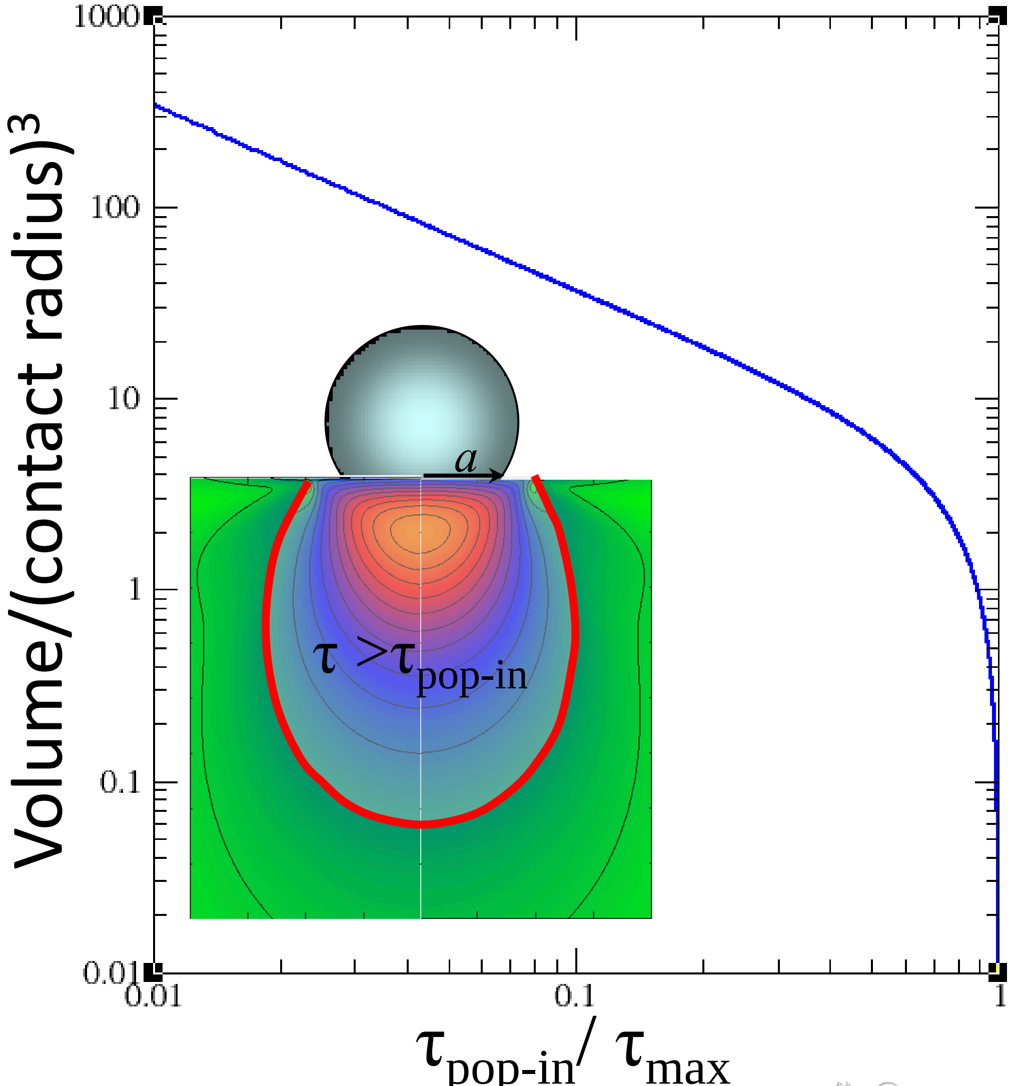
A statistical model for pop-in statistics:

- Assume a defect density $\boldsymbol{\rho}$ (per volume).
- Assume the defects are *perfectly randomly distributed.*
- Assign a pop-in stress $\boldsymbol{\tau_{pop\text{-}in}}$ associated with each defect.
  - For simplicity, assume this is identical for each defect.
- What is the probability that a given load *P* samples does not affect any defects?
  - Determined by the volume where $\tau > \tau_{pop\text{-}in}$
  - Poisson statistics: Prob(no defect) = exp(- ρV)



Scaling of volume in Hertzian contact theory

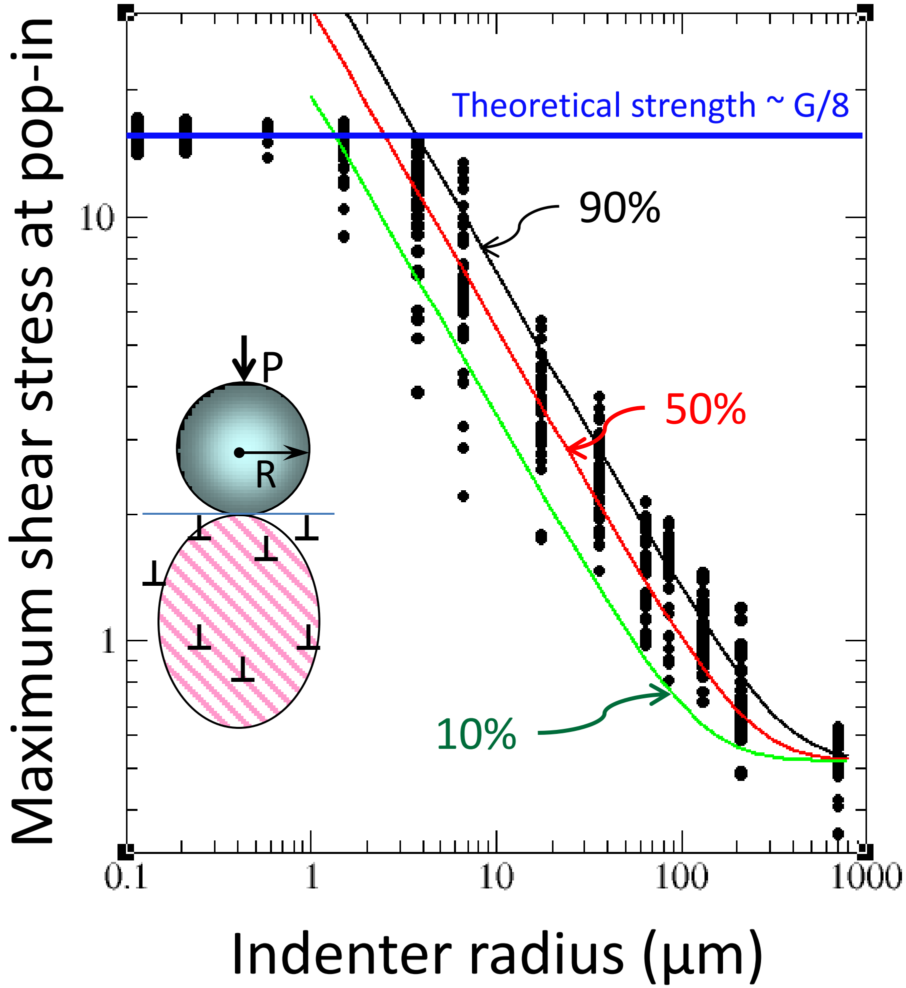
- Elastic solution from Hertzian contact theory
- Length scale set by *contact radius a*
- Stress scale is set by *mean pressure* or equivalently by the *peak shear stress under the indenter.*
- V/a^3 is a function of $\tau_{pop\text{-}in} / \tau_{max}$



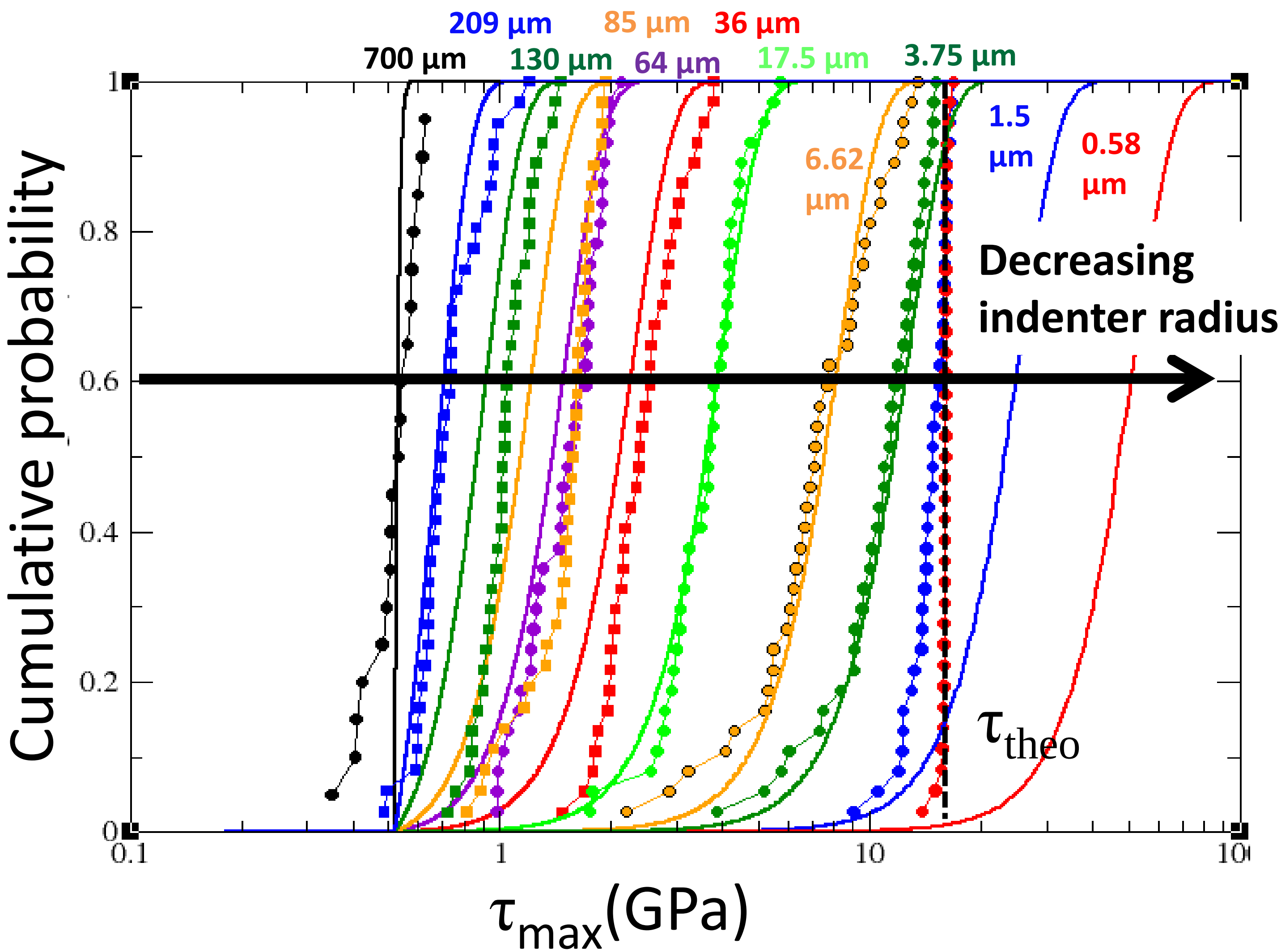
Statistical model of defect-driven pop-in:

Simplest model:

- Assume a *completely random* distribution of defects.
- Only 2 parameters:
  - Defect activation stress = 0.52 GPa
  - Defect density = $2x10^{16}$ / m^3
- Fit shown at right.
  - Red line indicates a 50% *cumulative* probability of pop-in.
  - Green, black lines show 10% and 90% values.

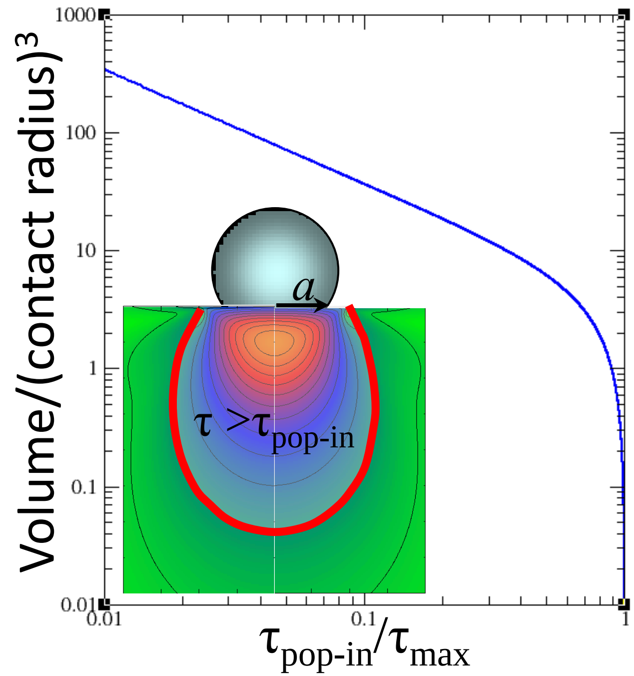


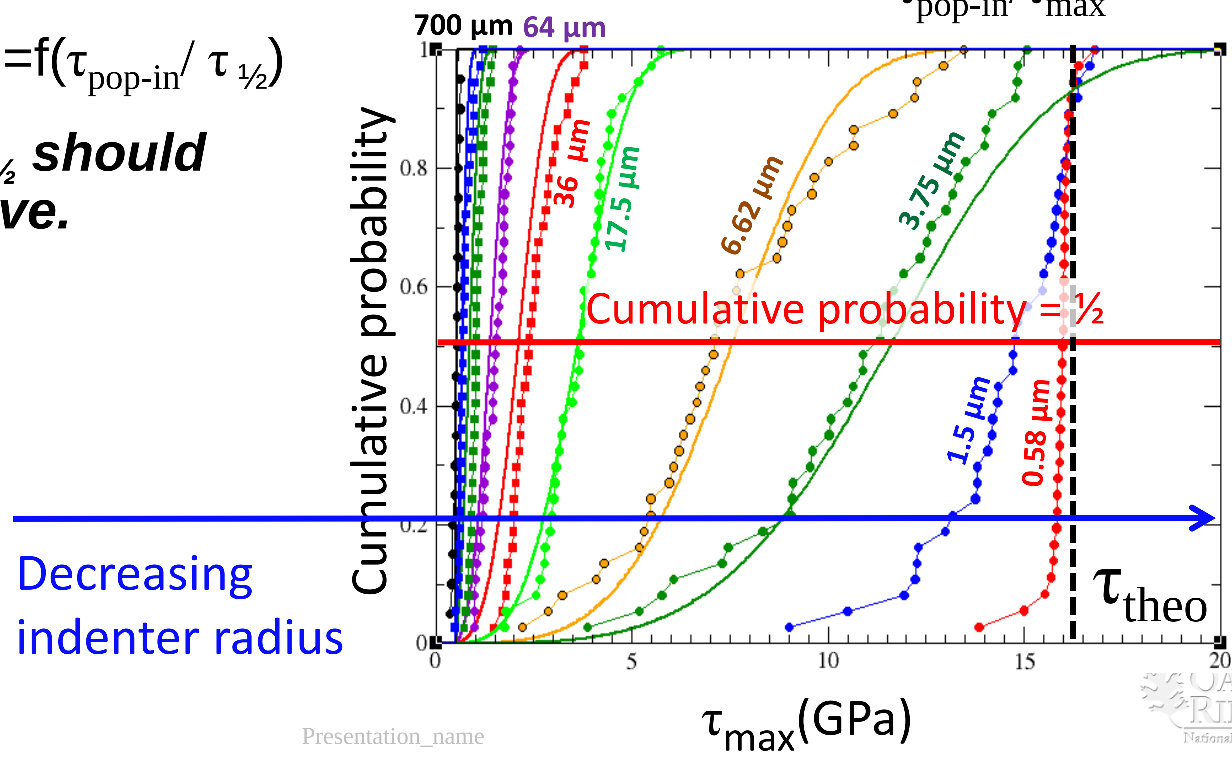
Can compare with full probability distribution:



Scaling theory:

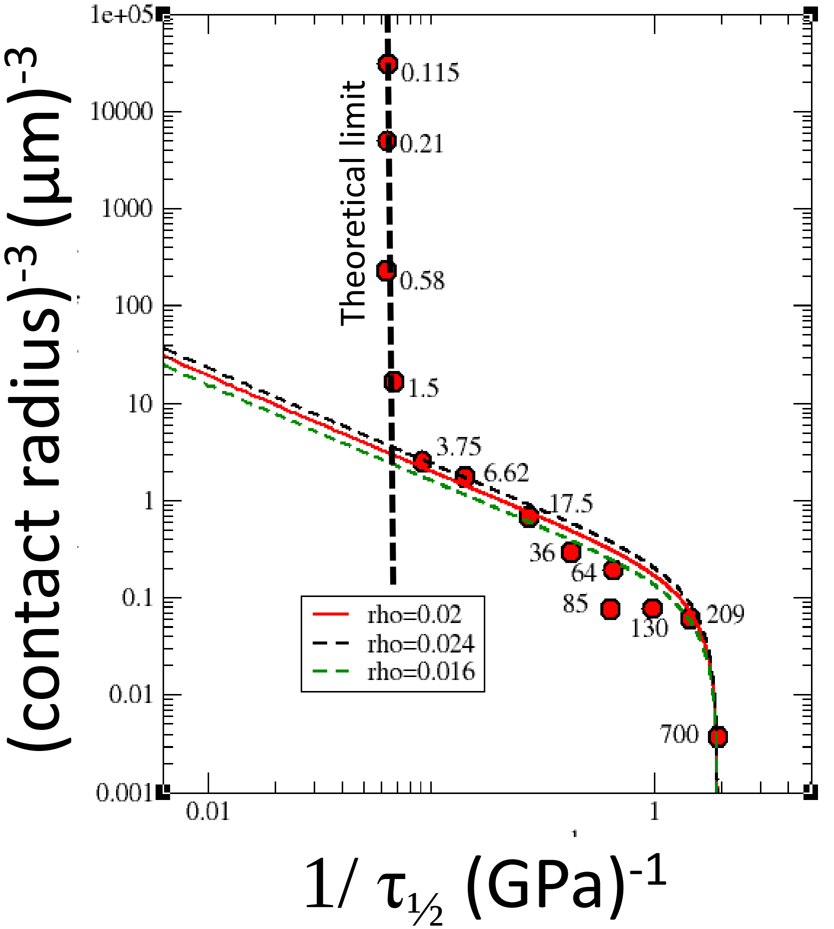
- From before,the high-stress region has a scaled volume $V/a^3 = f(\tau_{pop\text{-}in}/\ \tau_{max})$
- Define $\tau_{½}$ to be value of τ_{max} when cumulative probability = ½
  - Theory predicts $\rho V = \ln(2)$ at this stress.
- $(\rho V)/(\rho a^3) = \ln(2)/(\rho a^3) = f(\tau_{pop\text{-}in}/\ \tau_{½})$
- ***Plotting $1/a^3$ vs. $1/\tau_{½}$ should give a universal curve.***





Behavior of experiments closely matches predicted scaling law when $\tau_{½} < \tau_{theo}$:

- Solid red curve shows fit to theory.
- Only two parameters in fit: the defect density, and the defect strength.
- $\tau_{\text{pop-in}} = 0.52$ *GPa*
- $\rho = 0.02 / \mu m^3$
- Dashed lines examine sensitivity to dislocation density.



Is the defect density reasonable?

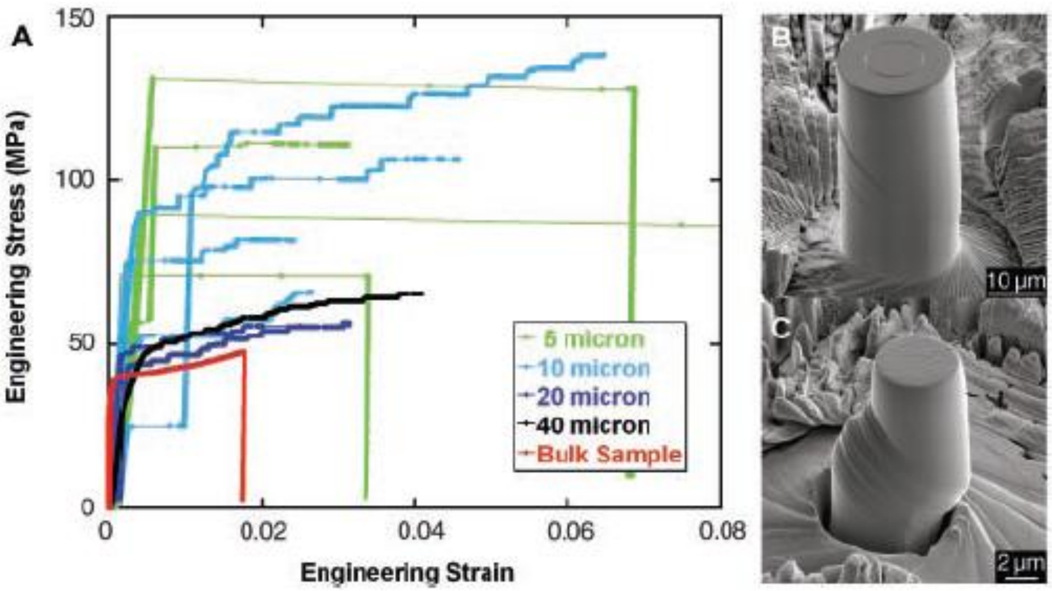
- Defect density = ρ_{defect} = $0.02/(\mu m)^3$ = $2x10^{16}/m^3$
  - Characteristic distance between defects ~ $\rho_{disl}^{-1/3}$ = 3.7 μm
  - Corresponds to a dislocation density of $2x10^{11}/m^2$
- For our annealed Mo single crystal:
  Dislocation density ρ_{disl} = $10^{11}/m^2$ = $0.1/(\mu m)^2$
  - Coarse estimation from x-ray line broadening
  - Characteristic distance between dislocations ~ $\rho_{disl}^{-1/2}$ = 3.2 μm
  - → *reasonable estimate of spacing between defects*
- Or: ρ_{disl} ~$10^{11}/m^2$ = $0.1/(\mu m)^2$ = $100\ nm/(\mu m)^3$
  - 1 defect per 50 nm of dislocation length

What about "Wires & whiskers?"
Size effects without strain gradients

Sample Dimensions Influence Strength and Crystal Plasticity

Michael D. Uchic,[1]* Dennis M. Dimiduk,[1] Jeffrey N. Florando,[2] William D. Nix[3]

Uchic *et al.* *Science 2004*



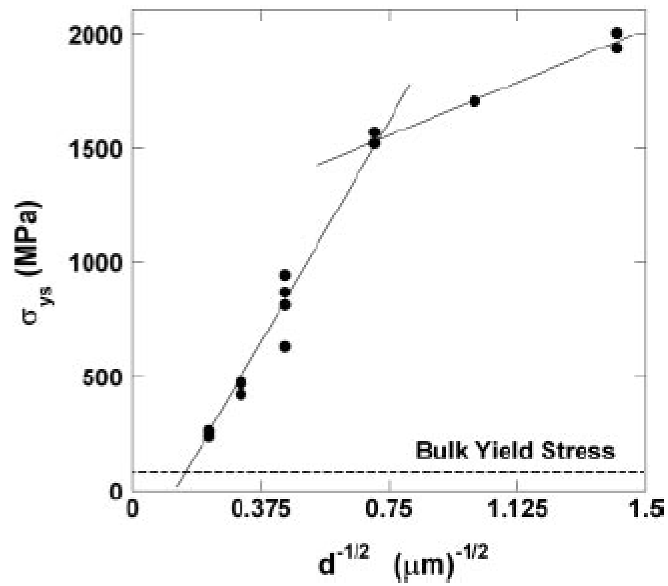
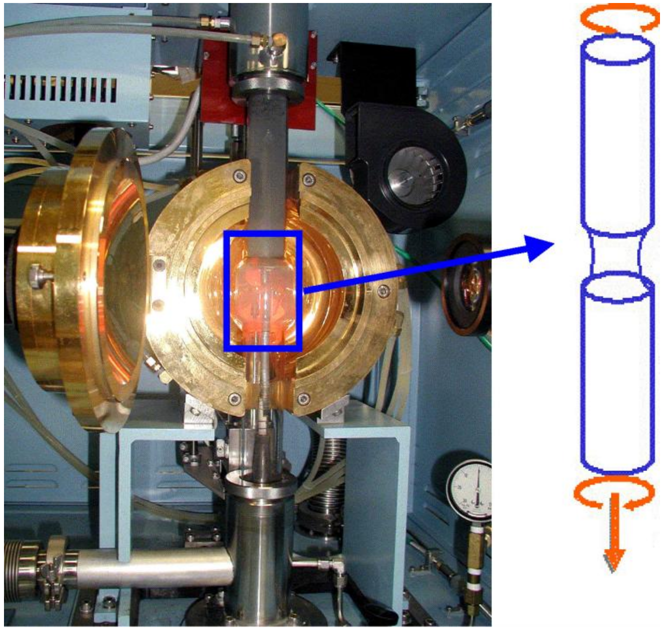


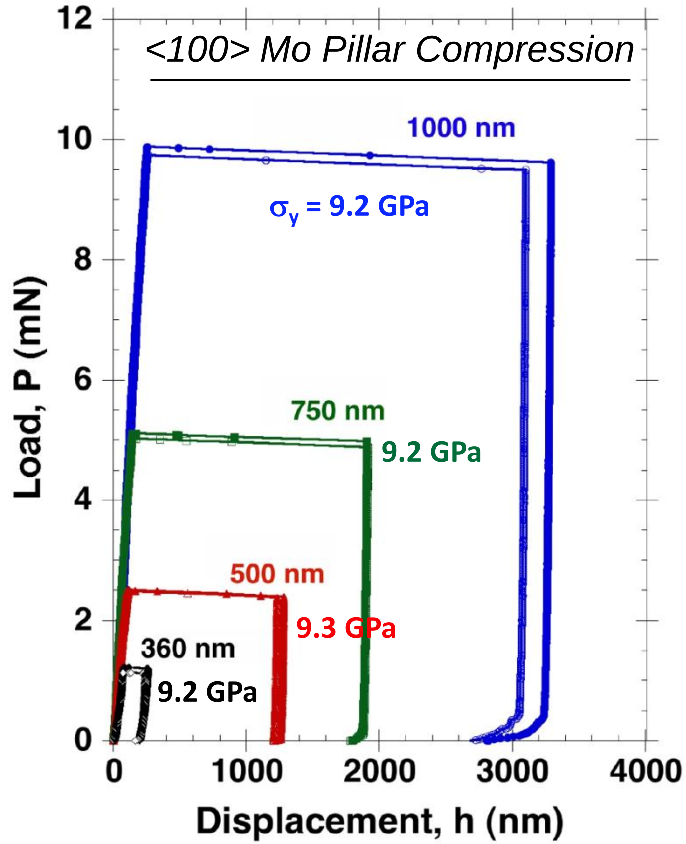
Fig. 3. Dependence of the yield strength on the inverse of the square root of the sample diameter for Ni_3Al-Ta. The linear fit to the data predicts a transition from bulk to size-limited behavior at ~42 µm. σ_{ys}, the stress for breakaway flow.

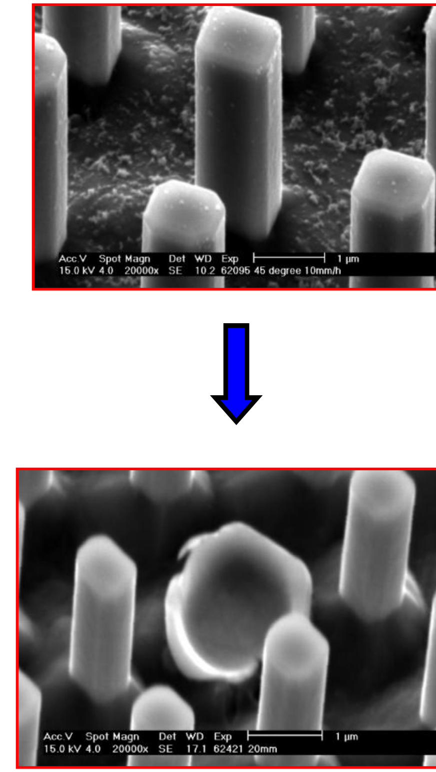
- Defect-free Mo pillars grown by directional solidification
- Yield at the theoretical strength independent of size



Directional solidification of Mo-NiAl eutectic

Bei et al, *Scripta Mater.* (2007)



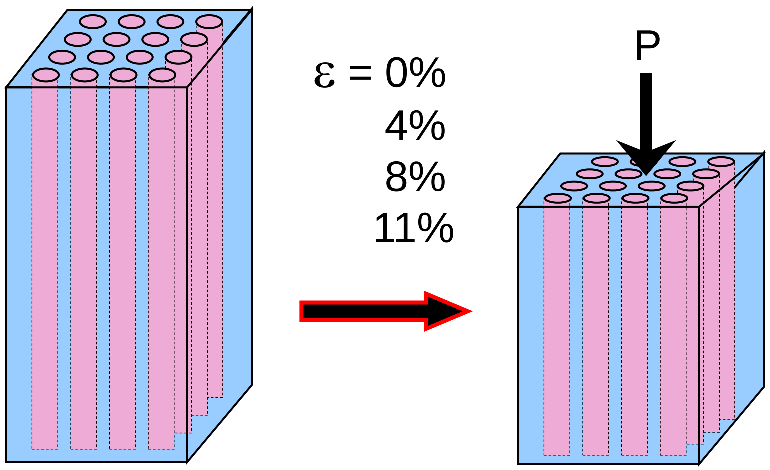


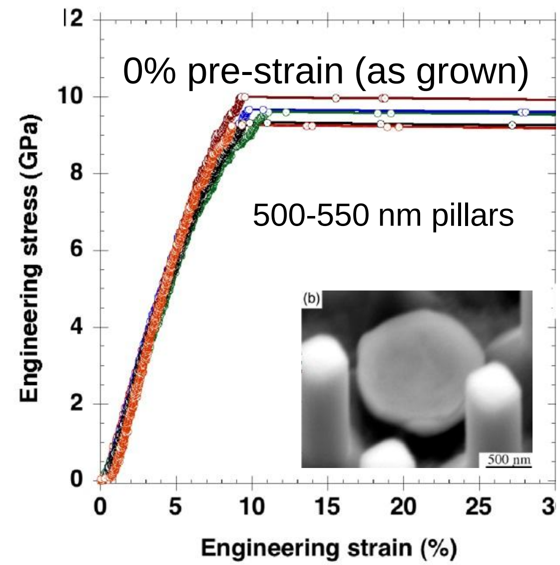
Important Observations:

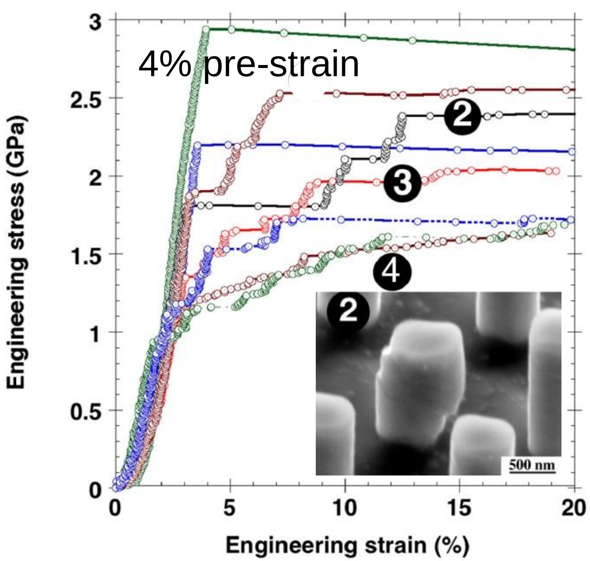
1. Pillars yield at ~9.2 GPa, independent of size
2. τ_y is ~G/26 (in the range for τ_{theo})
3. Plastic deformation is unstable (work softening)

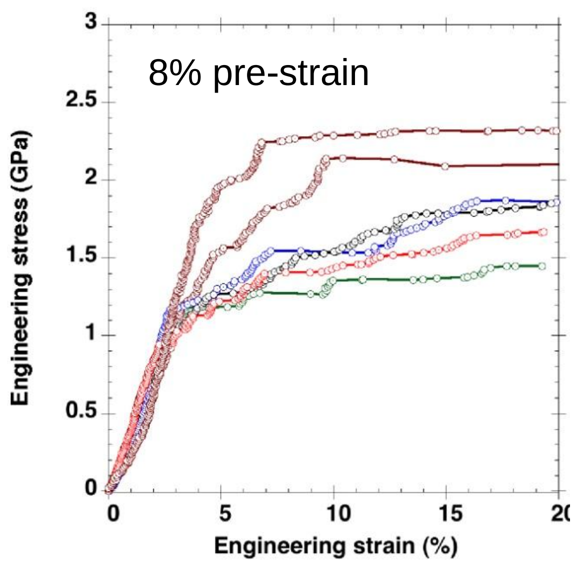
Preliminary experiments show that pre-straining can indeed be used to vary the material length scale

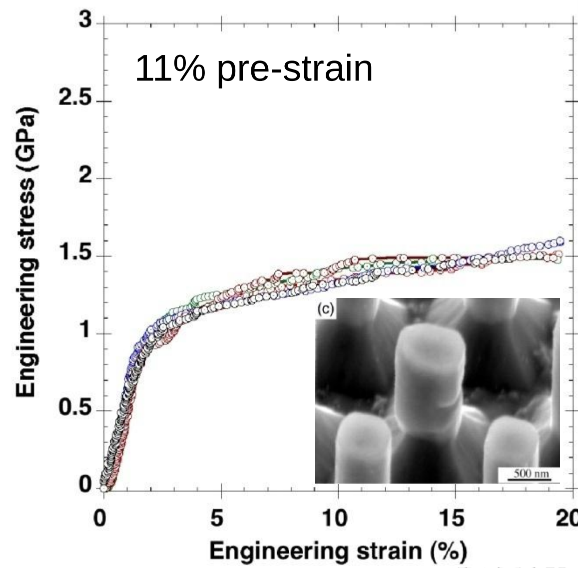
Bei, Shim, Pharr, & George, *Acta Mater.* (2008)











Effects of FIB damage on mechanical properties of nanopillars

Shim et al., *Acta Mater.* (2009)

Compressive load

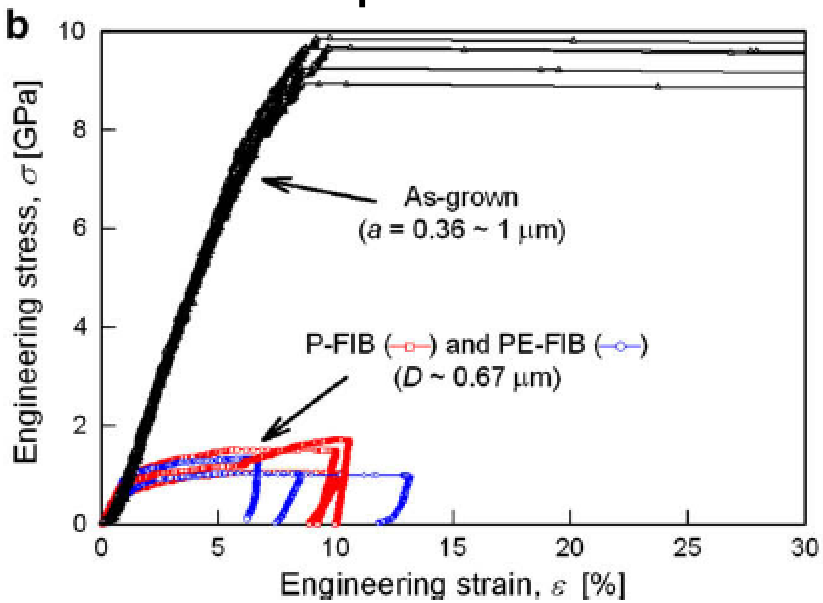


Fig. 5. (a) Compressive load–displacement curves for FIB-milled micro-pillars and (b) stress–strain curves for as-grown (directionally solidified) and FIB-milled pillars. Note that *a* is the edge length of square cross-section as-grown pillars and *D* is the diameter of circular cross-section FIB-milled pillars.

Nanoindentation behavior

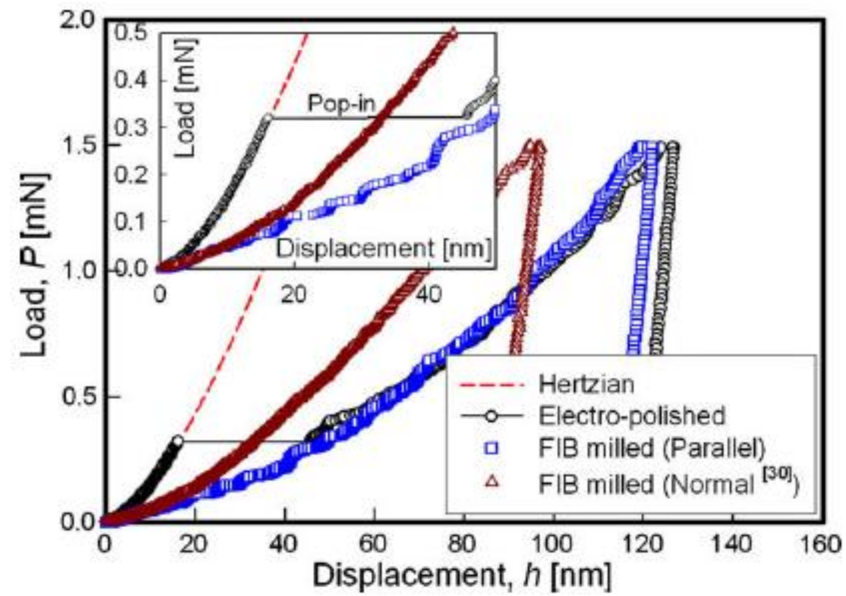


Fig. 9. Nanoindentation load–displacement curves obtained from electropolished and FIB-milled surfaces. The Hertzian elastic solution follows closely the curve for the electropolished surface below the pop-in.

Conclusions:

- A new, exactly solvable model shows that statistics of defects in small volumes affect size-dependent nanoindenter pop-in.
- The ***same*** two parameters in the model describe the experimental results for ***all*** indenter sizes (700 μm down to 3.75 μm):
    - the defect *strength* and the defect *density.*
- A scaling theory agrees nicely with the experimental results.
- Crossover from bulk (determinative) behavior to stochastic pop-in occurs when the defect density ρ is on order of $1/V_{stressed}$. This volume may be much greater than (contact radius)^3.
- Similar effects seen experimentally in deformation of pristine and pre-deformed pillars. Small amount of FIB damage hides the effects.

On-going work:

- Same model applied to pillar compression
- Examination of *distribution* of defect strengths