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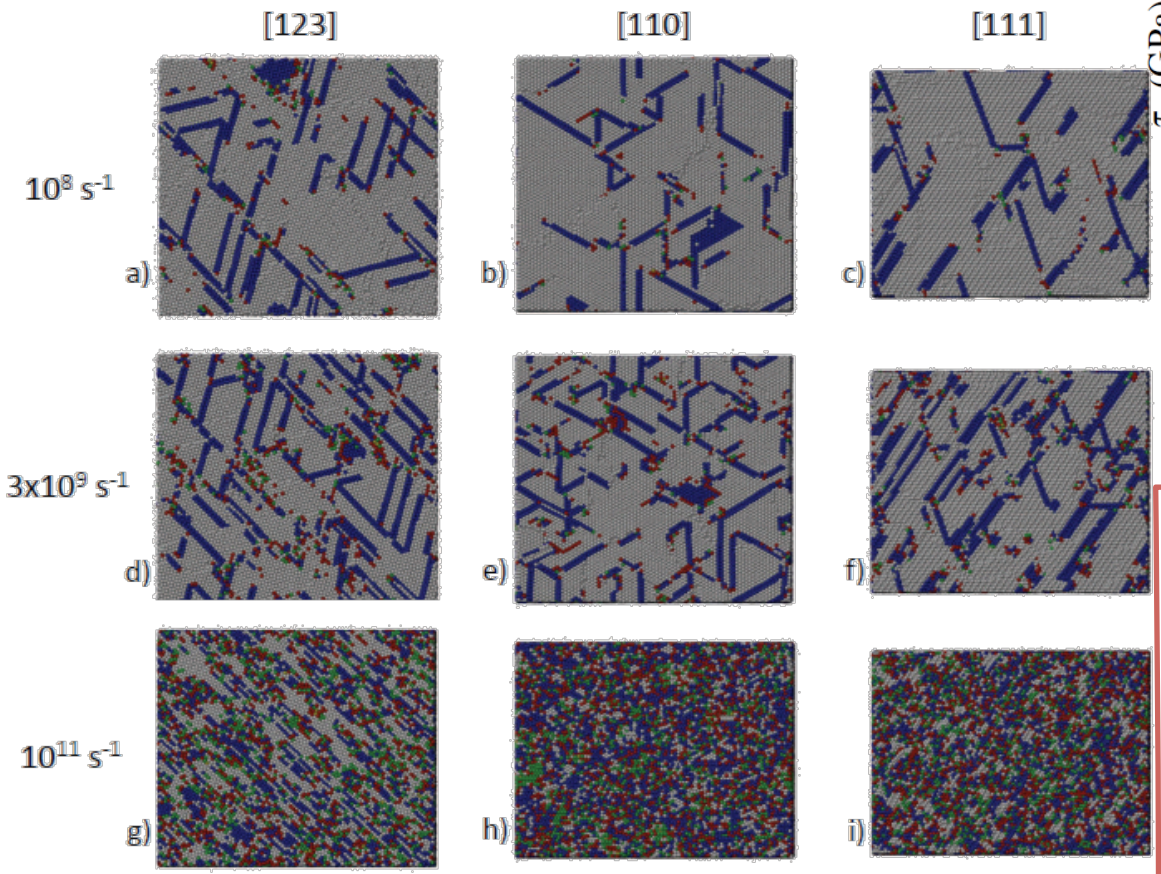
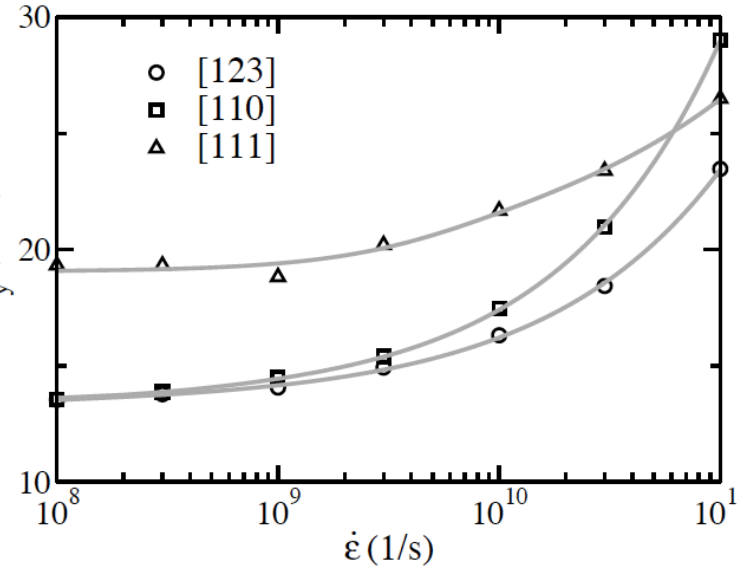
Institutional Computing Annual Report 2012

Project: W12_copperstrength

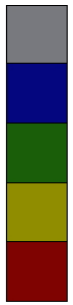
PI: Timothy C. Germann (T-1, tcg@lanl.gov, 5-9772)



Atomistic mechanisms after yield of three samples at three strain rates



Evolution of the yield stress as a function of strain rate for the same samples.



Main findings for **single crystals**:

- [111] is stronger at low strain rates and yields at higher strains; strain rate has the least effects on these samples (above)
- 3 deformation regimes observed: homogeneous nucleation of dislocations, amorphization, intermediate regime where disorder is relaxed by nucleation of dislocations (left)
- Criterion based on the critical resolved shear and normal stresses is not enough to predict yielding at all strain rates

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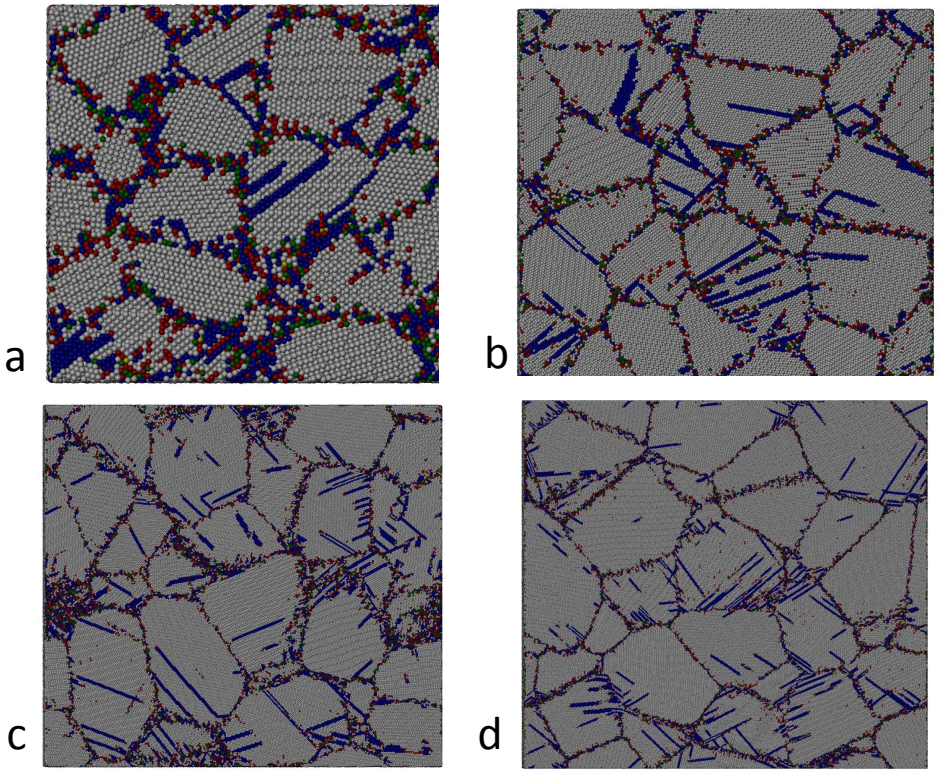
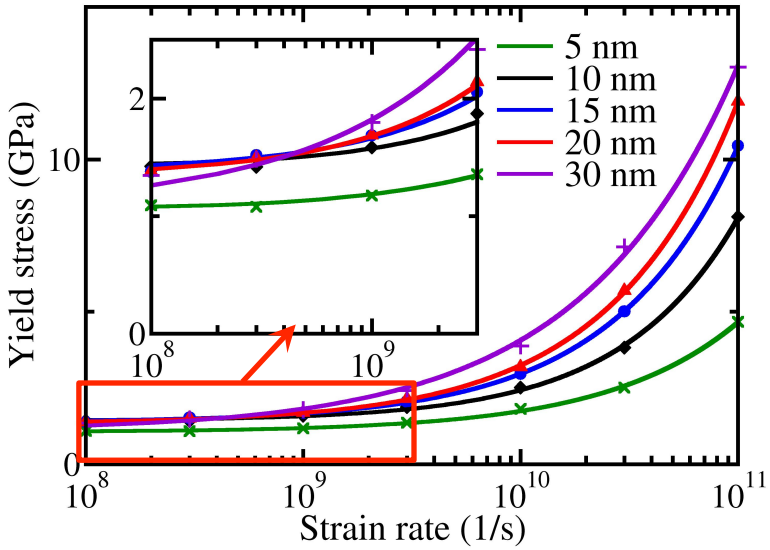


Atomistic mechanisms at 10% deformation in the samples with a grain size of: a) 5 nm; b) 10 nm; c) 15 nm; d) 20 nm and e) 30 nm ($\dot{\varepsilon} = 10^{10}$ s^{-1} and T = 300K).



Evolution of the yield stress as a function of strain rate.

Main findings for **polycrystals**:

- Preliminary results indicate that strongest grain size is strain rate dependent (above)
- Deformation mechanisms change from boundary sliding to dislocation nucleation with increasing grain size (left) and increasing strain rate

V. Dupont and T. C. Germann, *Phys Rev B* **86**, 134111 (2012)

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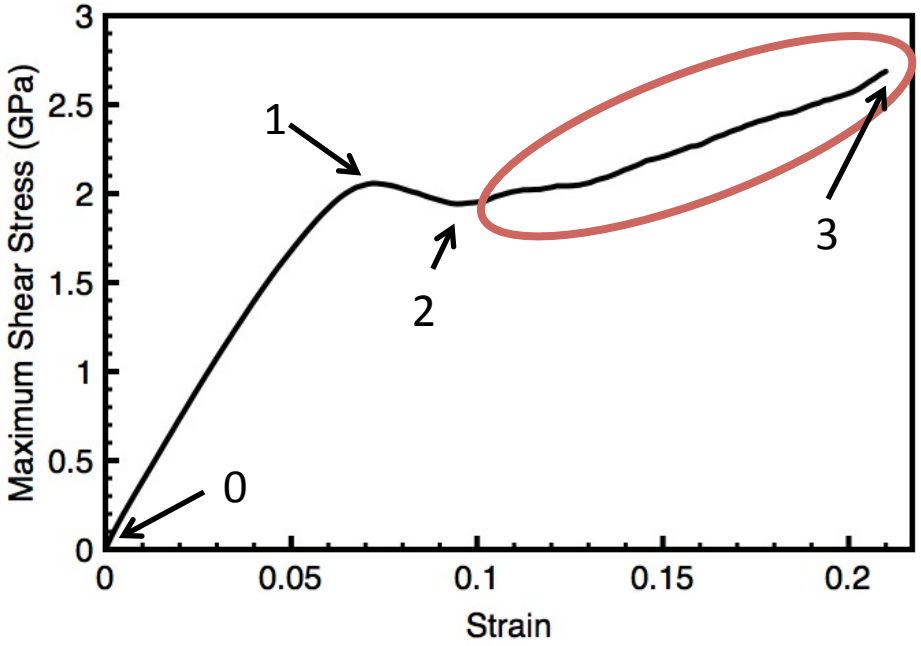

(Above) Stress-strain curve for 15-nm grain size polycrystal at 300 K and $3 \times 10^{9} s^{-1}$.

We are currently investigating:

- the strengthening effect observed in polycrystals (left); and
- methods for quantifying the competition between intergranular and intragranular slip (below)

(Below) Slip sustained by sample between (a) point 0 and 1 on graph; (b) 1 and 2 and (c) 2 and 3