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W12\_copperstrength

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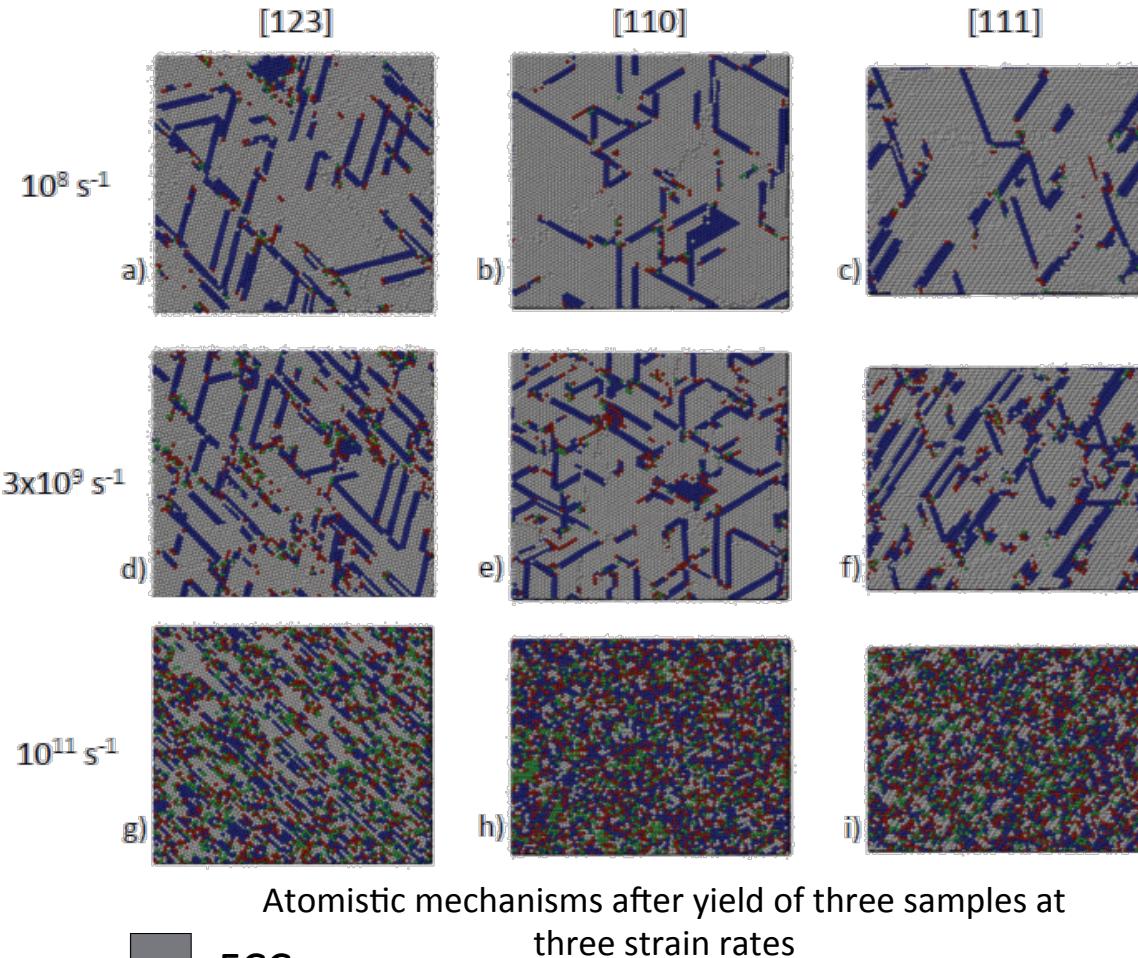
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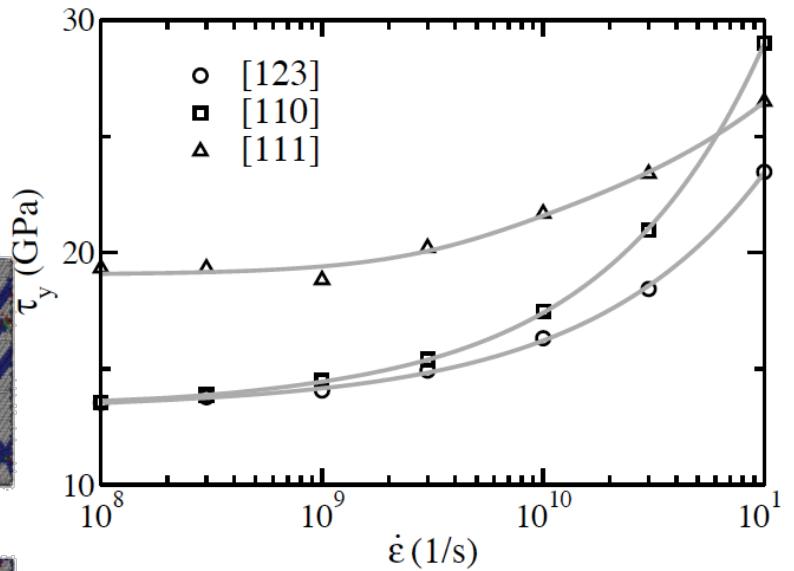
# Institutional Computing Annual Report 2012

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



FCC  
 HCP  
 BCC  
 ICO  
 Other



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

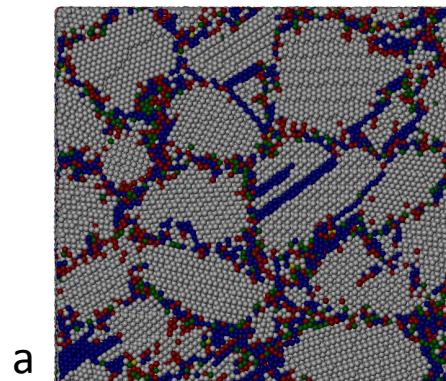
regime where disorder is relaxed by nucleation of dislocations (left)

- Criterion based on the critical resolved shear and normal stresses is not enough to predict yielding at all strain rates

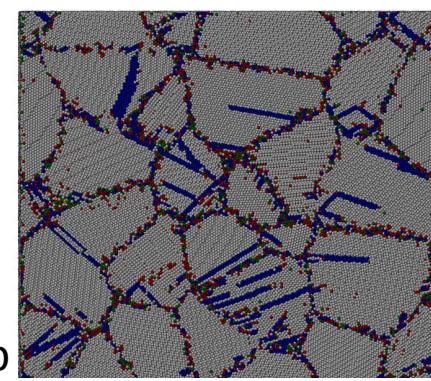
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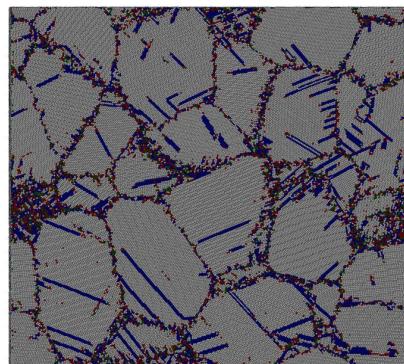
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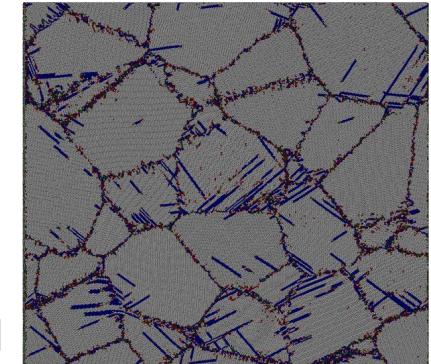
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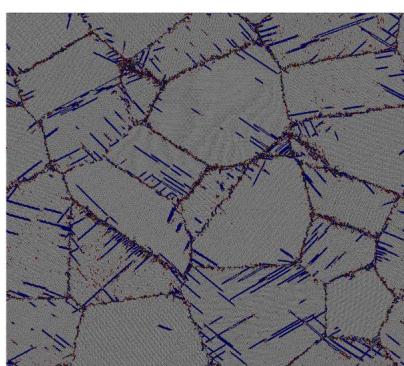
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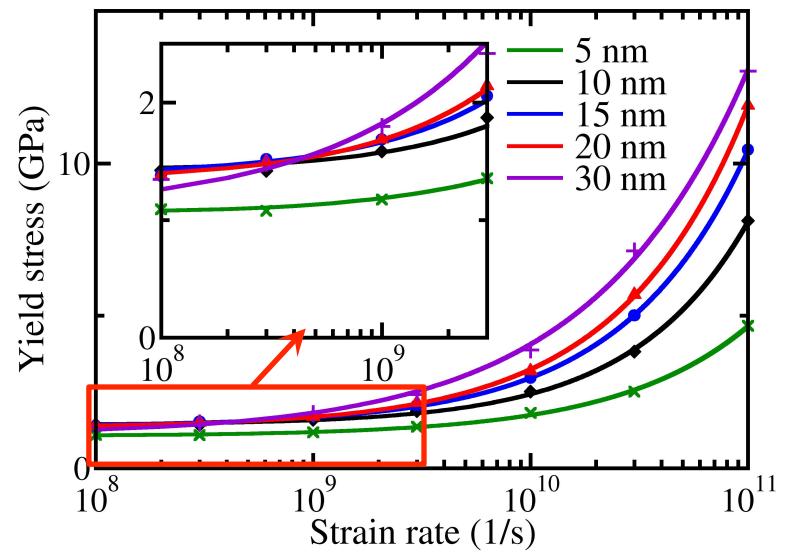
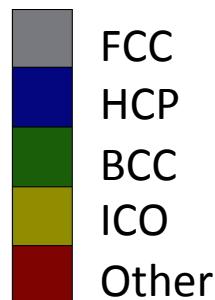


d



e

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 ( $\dot{\epsilon} = 10^{10} \text{ s}^{-1}$  and  $T = 300 \text{ K}$ ).



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

## Main findings for polycrystals:

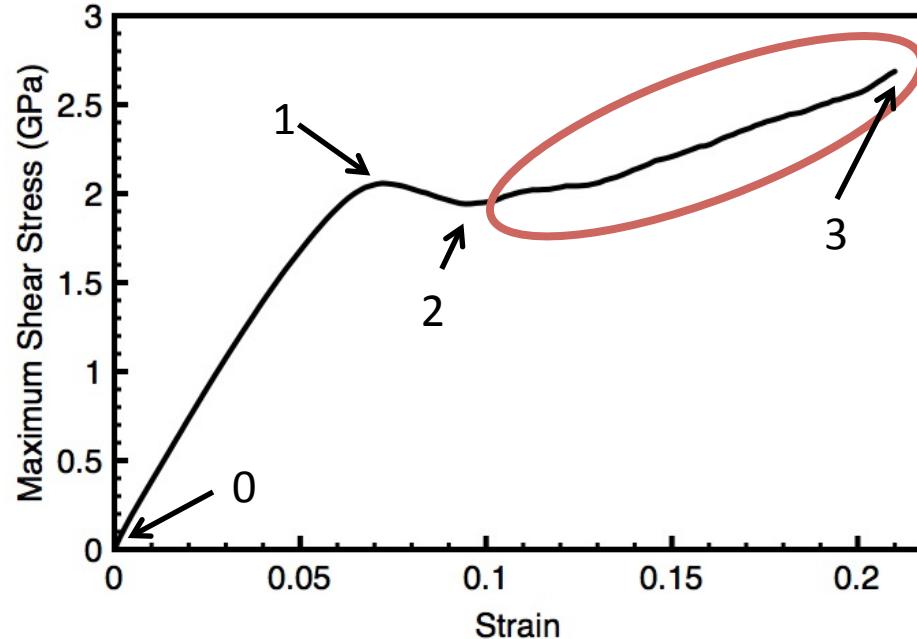
- Preliminary results indicate that strongest grain size is strain rate dependent (above)
- Deformation mechanisms change from boundary sliding to dislocation nucleation with increasing grain size (left) and increasing strain rate

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

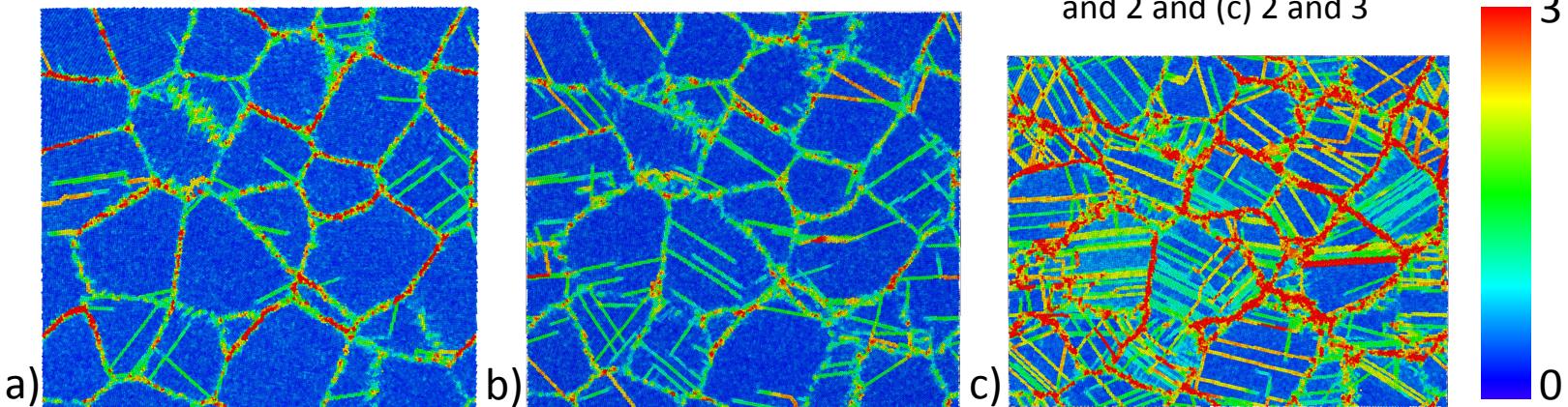
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(Above) Stress-strain curve for 15-nm grain size polycrystal at 300 K and  $3 \times 10^9 \text{ s}^{-1}$ .



## We are currently investigating:

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