Modeling Grain Boundary Structure and Mechanical Properties using LAMMPS* with EAM Potentials

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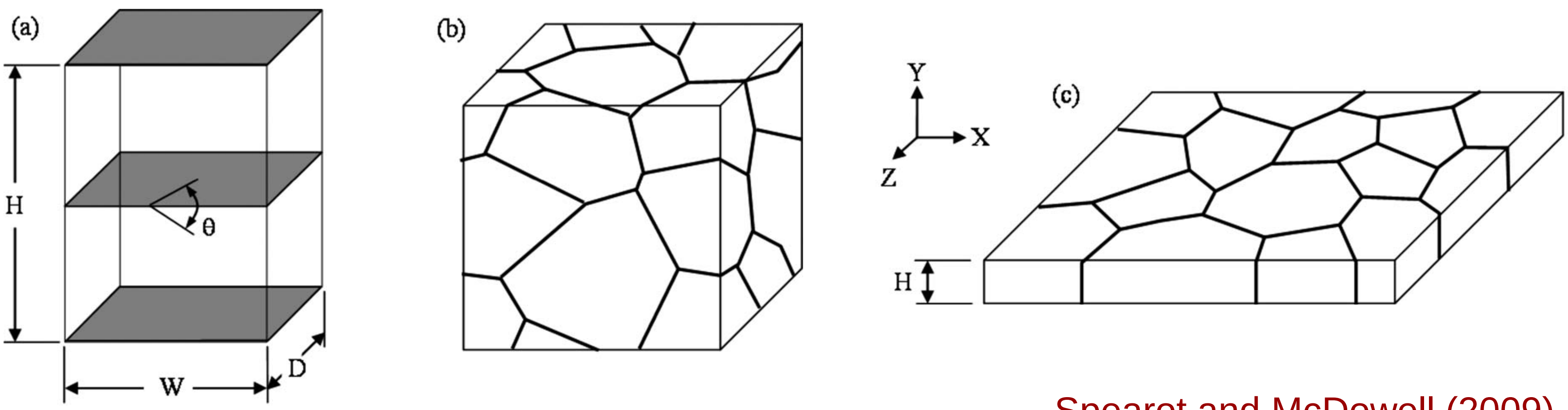
*Some calculations done with WARP

Constructing GB Models

- Grain boundary modeling
  - Bicrystal models allow for "isolation" of specific mechanisms
  - Nanocrystalline models allow for an analysis of triple junctions and deformation constrains imposed by opposing grains



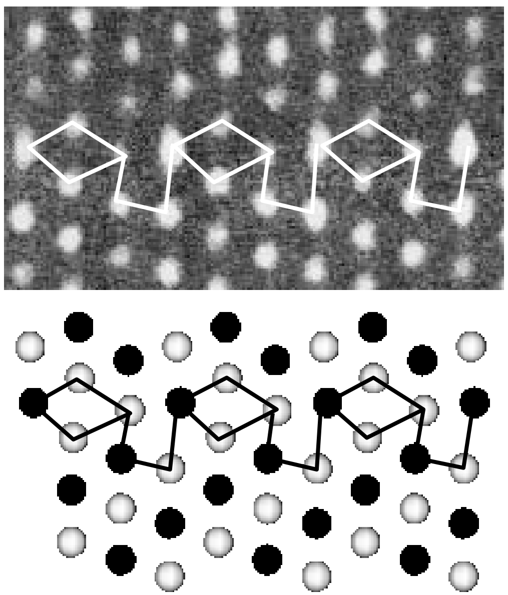
Spearot and McDowell (2009)

- Relevant LAMMPS commands
  - Bicrystal: region, lattice, orient, origin, delete_atoms (overlap)
  - Polycrystalline: read_data (created in matlab)

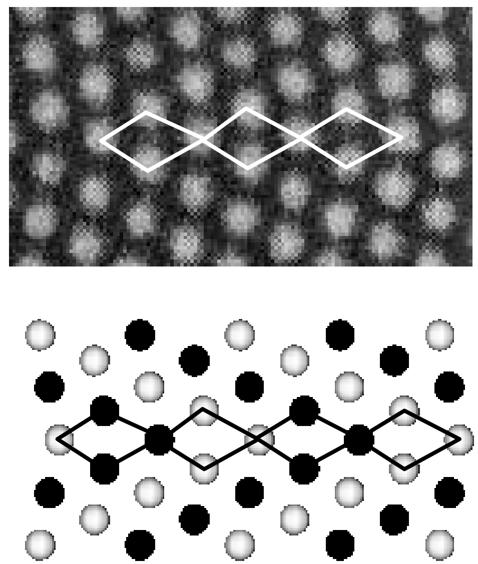
Grain Boundary Structures

- Energy minimization
  - ➢ Steepest decent or conjugate gradient method
  - ➢ Multiple starting positions must be used to probe energy landscape

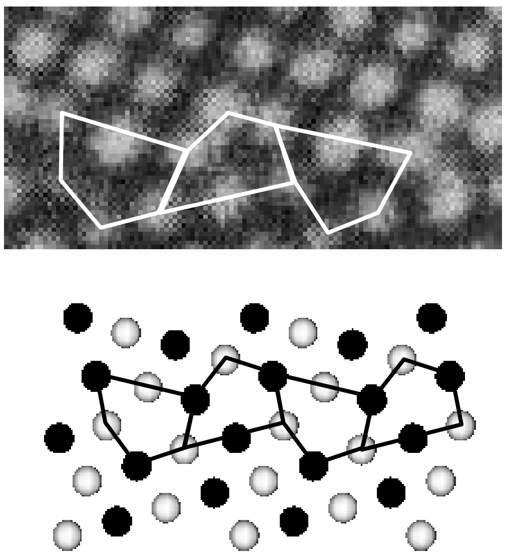
Mills et al. (1992); Medlin et al. (1993)



Σ3 (112) 70.5°



Σ11 (113) 50.5°



Σ9 (221) 141.1°

Spearot (2005)

- Relevant LAMMPS commands
  - ➢ minimize, min_style, min_modify

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Controlled Deformation Methods

- Uniaxial tensile deformation
  - fix_nept (N, strain rate, P, T)

$$\eta_{load} = \frac{\dot{h}}{h}$$

Prescribed to meet desired strain rate

$$\dot{\eta}_{nonload} = \frac{v_P^2}{NkT_o} V\left(P - P_o\right)$$

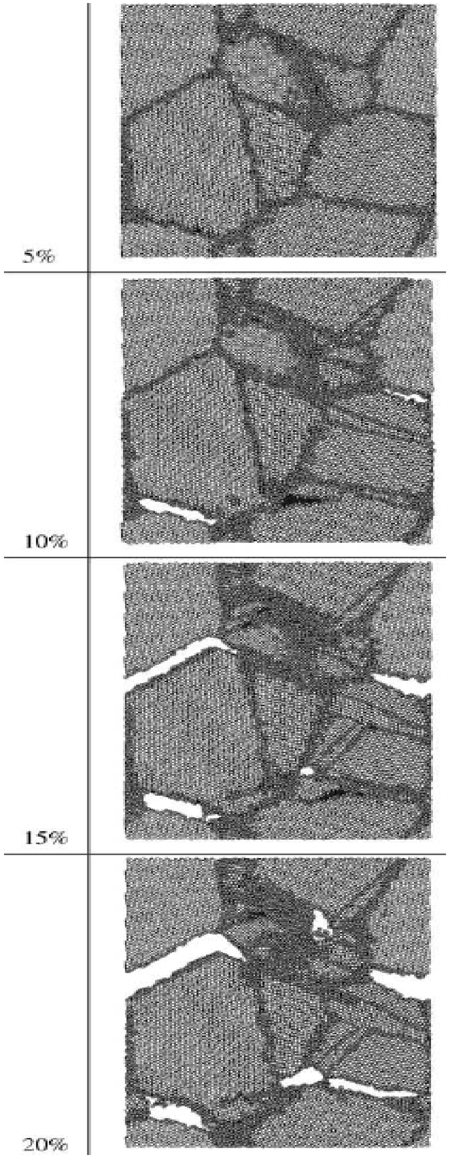
Boundary motion controlled by Melchionna *et al*. (1993) equations of motion

$$\dot{r}^i = \frac{p^i}{m} + \eta\left(r^i - R_o\right)$$

$$\dot{p}^i = F^i - \left(\eta + \zeta\right) p^i$$

$$\dot{\zeta} = v_T^2\left(\frac{T}{T_o} - 1\right)$$

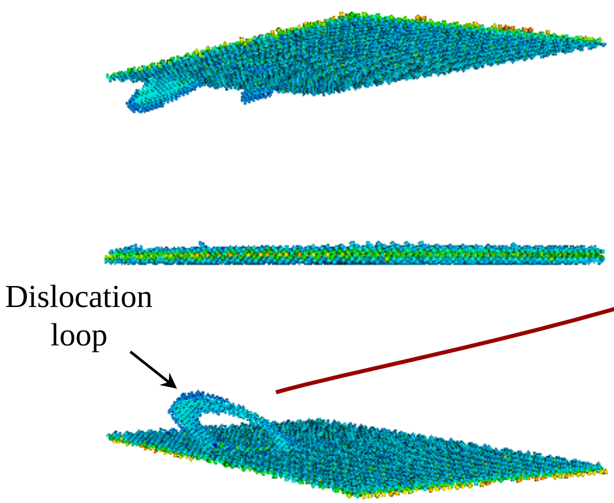
  - fix_deform
    - Essentially the same idea when "NULL" used as the pressure in the loading direction in fix_npt

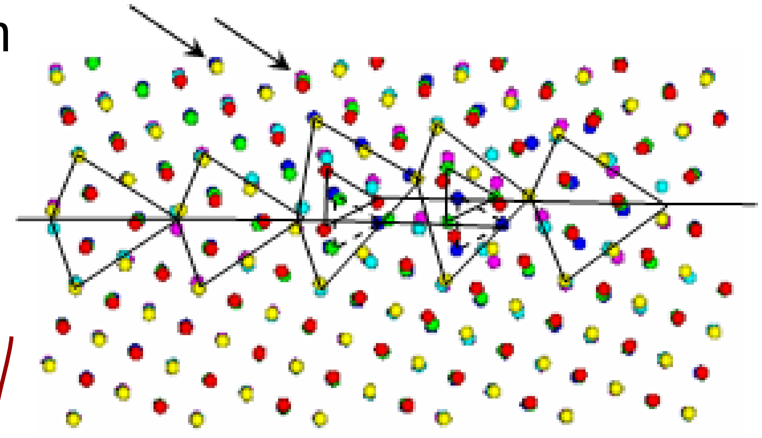


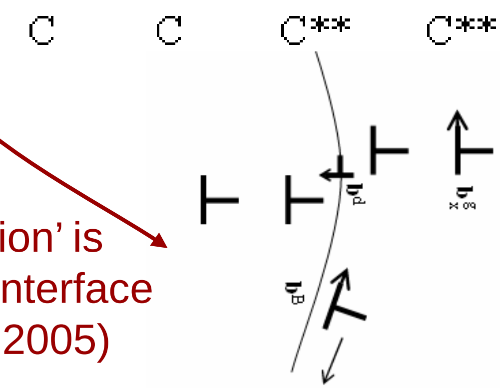
Frederiksen et al. (2004)

Dislocation Nucleation from GBs

- Emission of interface dislocations in bicrystals
  - Σ5 (310) <100> interface in aluminum
  - Calculations are performed at 10 K







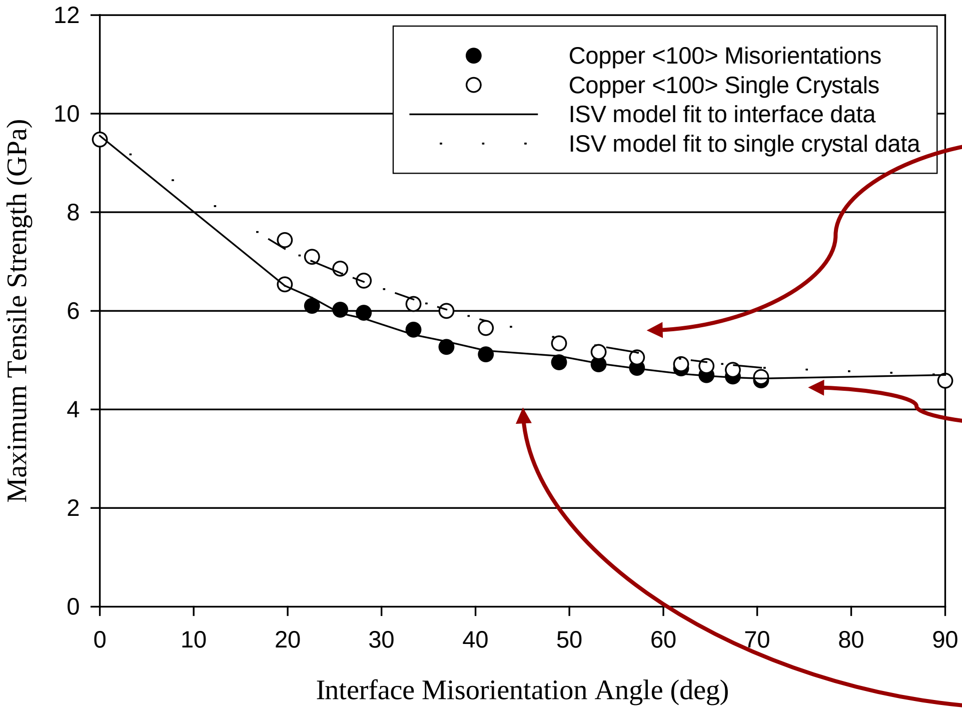
'Disconnection' is formed at the interface (Hirth et al., 2005)

A ledge is formed at the interface after the nucleation of the trailing partial dislocation without atomic shuffling along the interface plane

Spearot et al., Acta Materialia (2005)

Dislocation Nucleation from GBs

- Stress required for dislocation nucleation
  - ➢ Symmetric tilt copper <100> bicrystal interface models



Orientation of the adjoining lattice regions plays a strong role in the tensile strength of the interface for many boundary misorientations

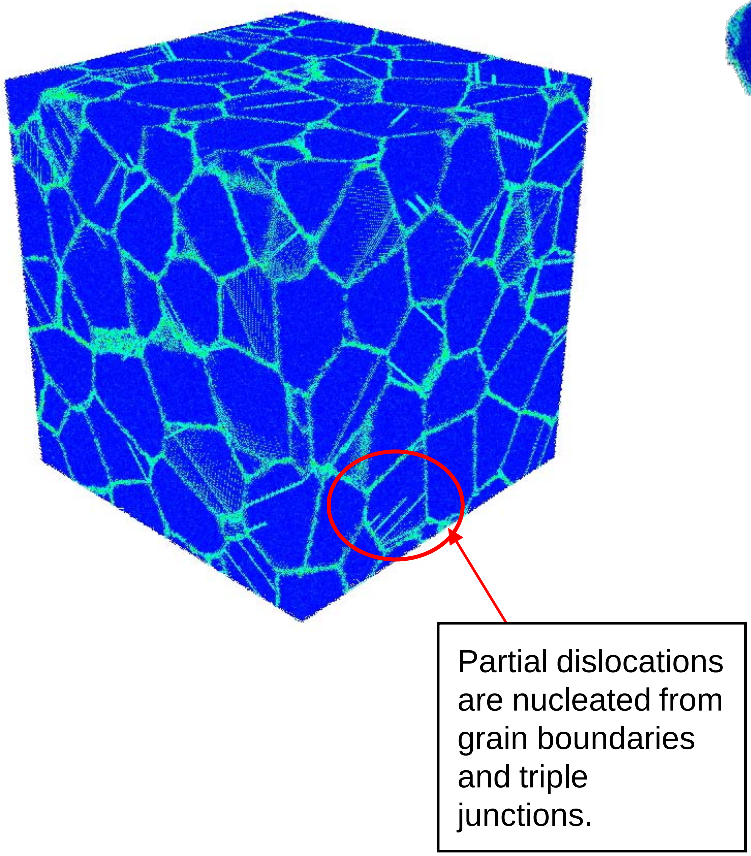
Dislocation nucleation shows significant non-Schmid behavior in agreement with *ab initio* calculations by Ogata *et al*. (2002)

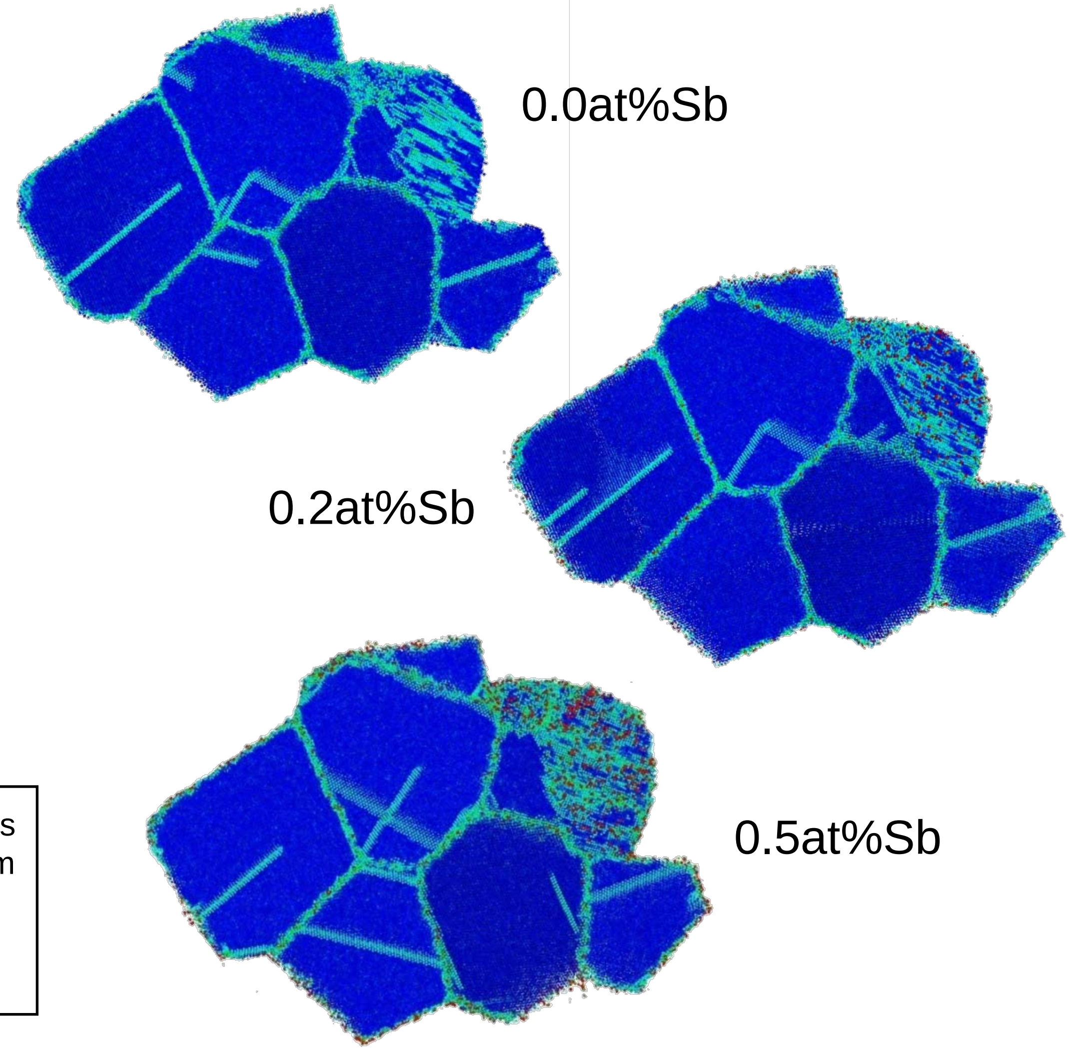
No special behavior is observed at low-order CSL <100> boundaries, GB energy and dislocation nucleation stress are not correlated

$$\sigma_{\max}^{\mathrm{int}} = (1-\xi D_c)\sigma_{\max}^{\mathrm{sc}} = (1-\xi D_c)\frac{\tau_{ideal}}{\mu_s SF + \mu_n NF + \mu_p PF}$$

Spearot et al. (2007) Acta Materialia, 55, 705-714.

Plastic Deformation of NC Cu-Sb

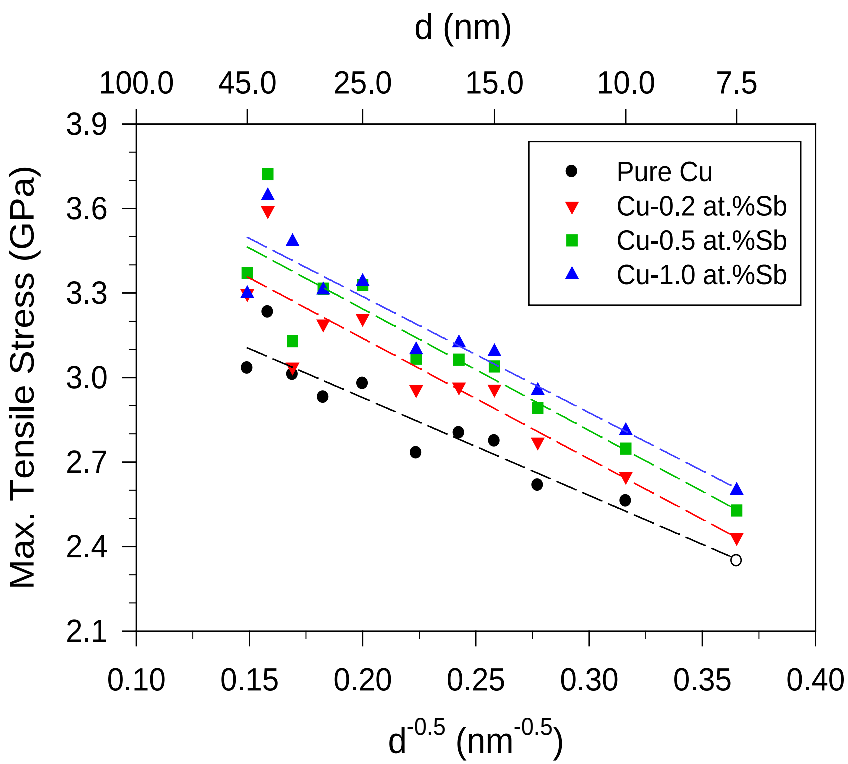


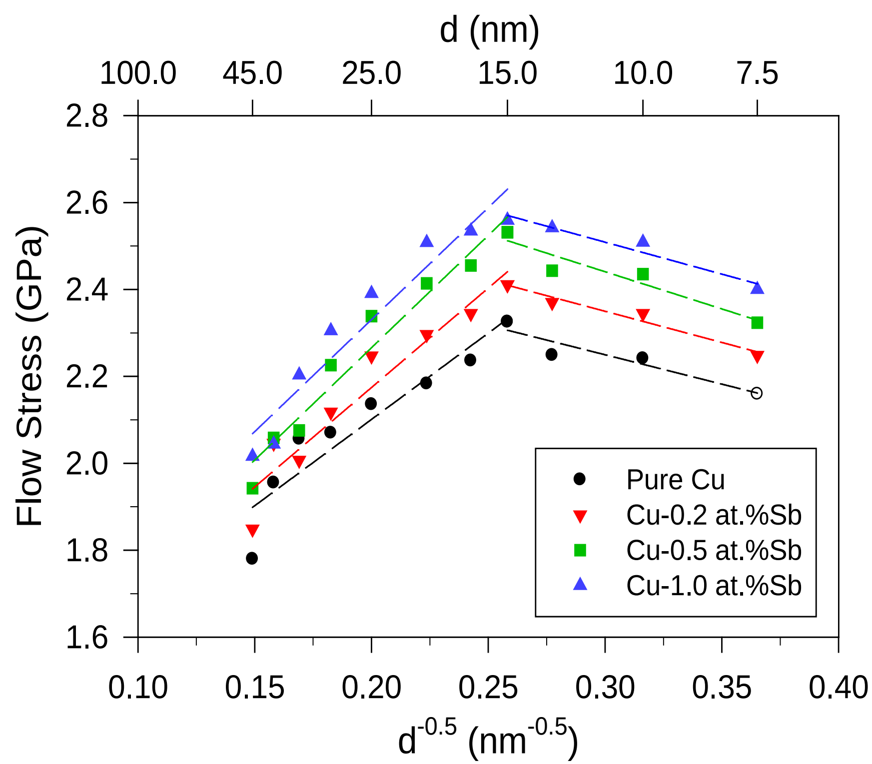


Rajgarhia et al. (2010) Journal of Materials Research, in press.

Plastic Deformation of NC Cu-Sb

- Nanocrystalline Cu with Sb at grain boundaries
  - ➢ Uniaxial tensile deformation at 300 K





Small concentrations of Sb at the grain boundaries increases the flow stress, but does not shift the grain diameter associated with peak strength

Rajgarhia et al. (2010) Journal of Materials Research, in press.

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Challenges / Opportunities

- Rendering / moving large dump files
  - Ensight (www.ensight.com)
  - Ovito (www.ovito.org) – still beta release
  - Paraview (www.paraview.org) – distributed rendering at TACC
- Modeling triple junctions
  - Incompatibility with “classical” periodic boundary conditions?
  - May require flexible border boundaries (Cai et al., Kurtz et al.)
- Linking bicrystal and nanocrystalline data
  - Incorporating bicrystal properties/mechanics into constitutive models for polycrystalline behavior
  - Sampling and statistics? (Foiles, Olmsted and Holm)

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