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Author(s): Fensin, Saryu J.
Valone, Steven M.
Cerreta, Ellen K.
Gray, George T. III
Farrow, Adam M.
Trujillo, Carl P.

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Interfaces and Inclusions in Shock-Induced Damage in Two-Phase Metals: Copper-Lead

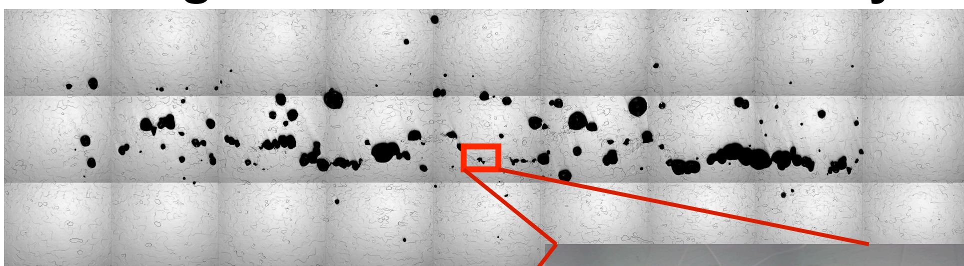
Saryu J. Fensin, <u>Steven M. Valone</u>, Ellen K. Cerreta, George T. Gray, Adam M. Farrow, Carl P. Trujillo

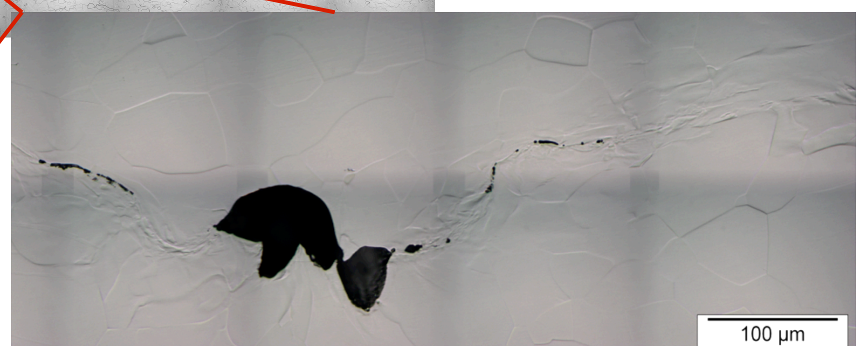
Materials Science and Technology Division
Los Alamos National Laboratory

U.S DOE Center for Materials at Irradiation and Mechanical Extremes, an Energy Frontier Research Center, Advance Simulation & Computing, Office of Basic Energy Sciences DOD/DOE Joint Munitions Program

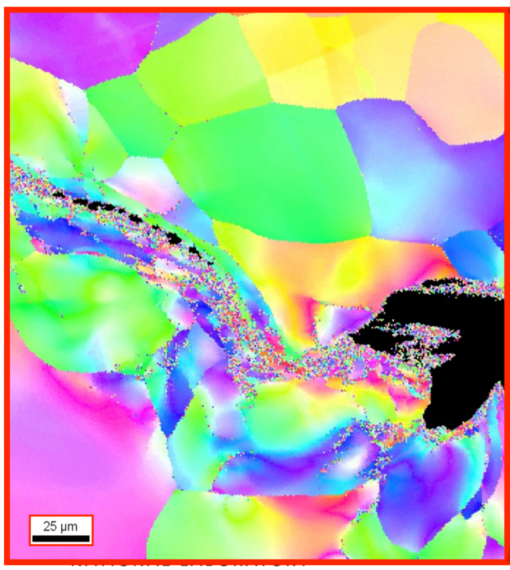
Motivation: Understand Role of a Soft, 2nd Phase on Damage Evolution

- 2^{nd}-phase particles, inclusions compared to grain boundaries, 1-xtal during defect nucleation under dynamic loading (shock in this case)





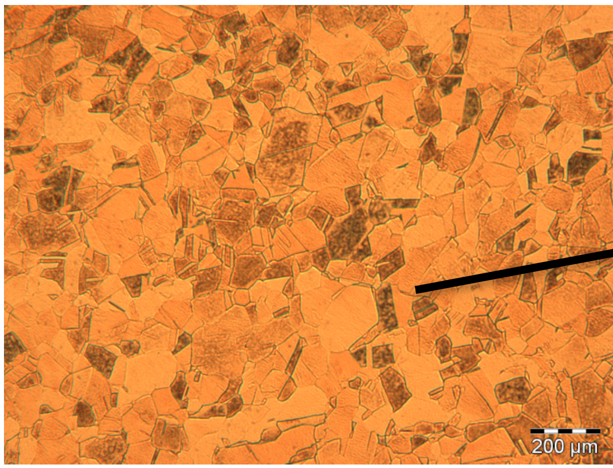
- Grain boundaries possible sites of nucleation

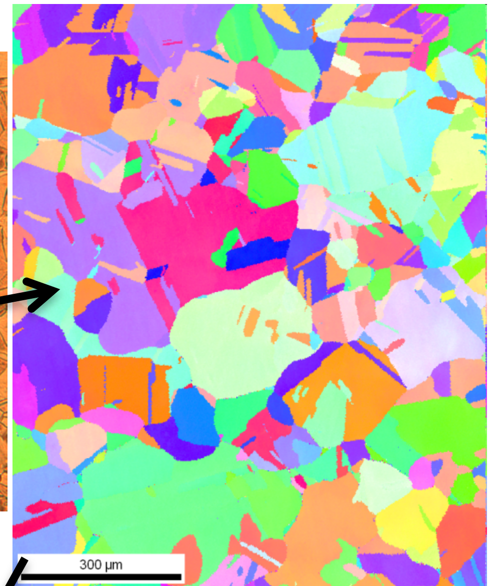


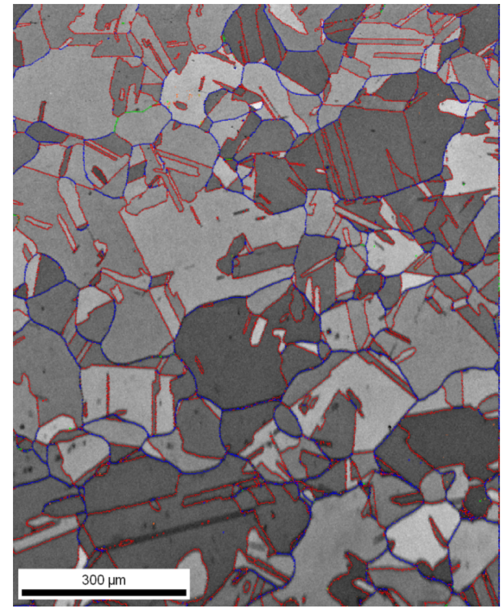
- During shock release, voids nucleate, grow and coalesce to produce spall failure

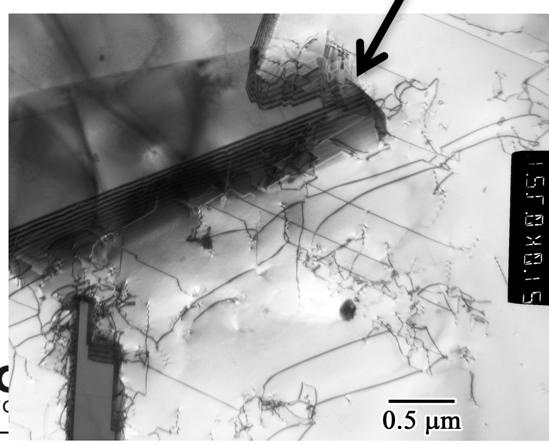
Material Microstructure Characteristics Span Multiple Length Scales

Copper









Typical Features in High Purity Metals:

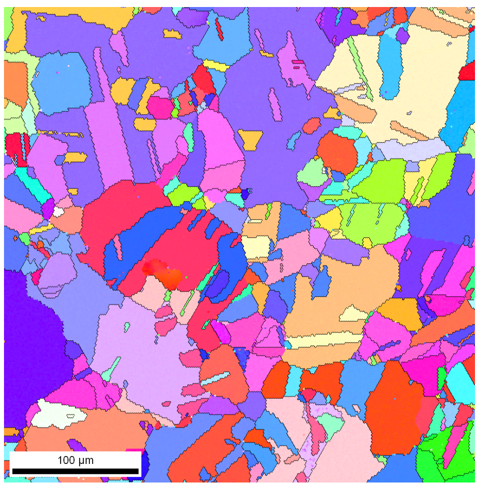
- Grain size, orientation
- Grain size, orientation of neighbors
- Grain Boundaries

Complex physics occurring through a range of length scales

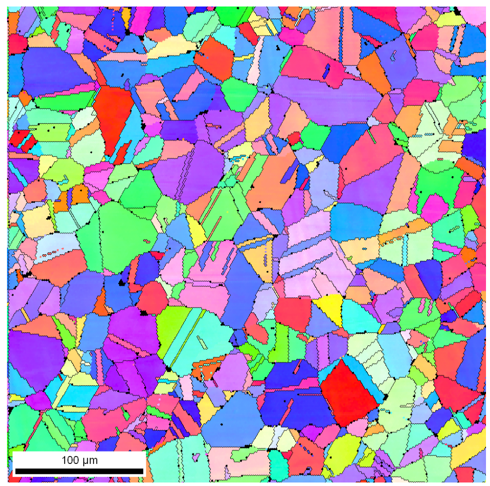
Cu–1 wt-% Pb As Model Material

As-annealed Cu Chemistry (wt-%)

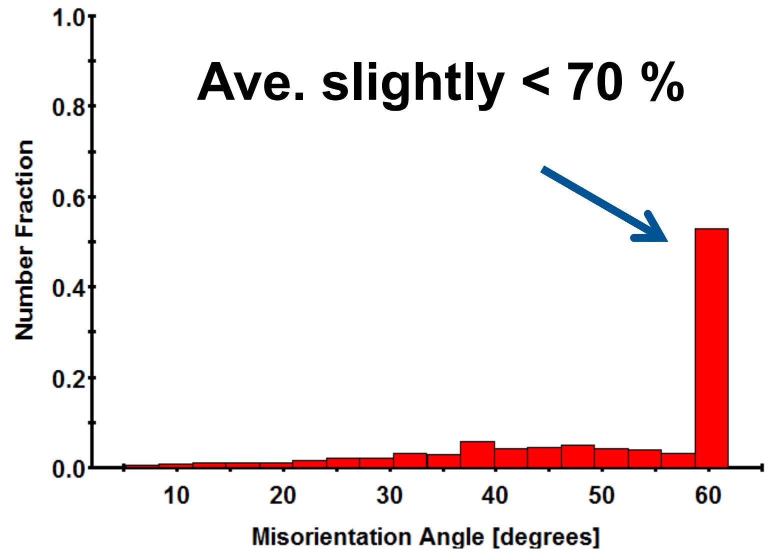
Cu	Ni	Ag	Pb	Sn	Zn	Fe
98.75	0.01	0.01	1.24	0.01	0.01	0.01



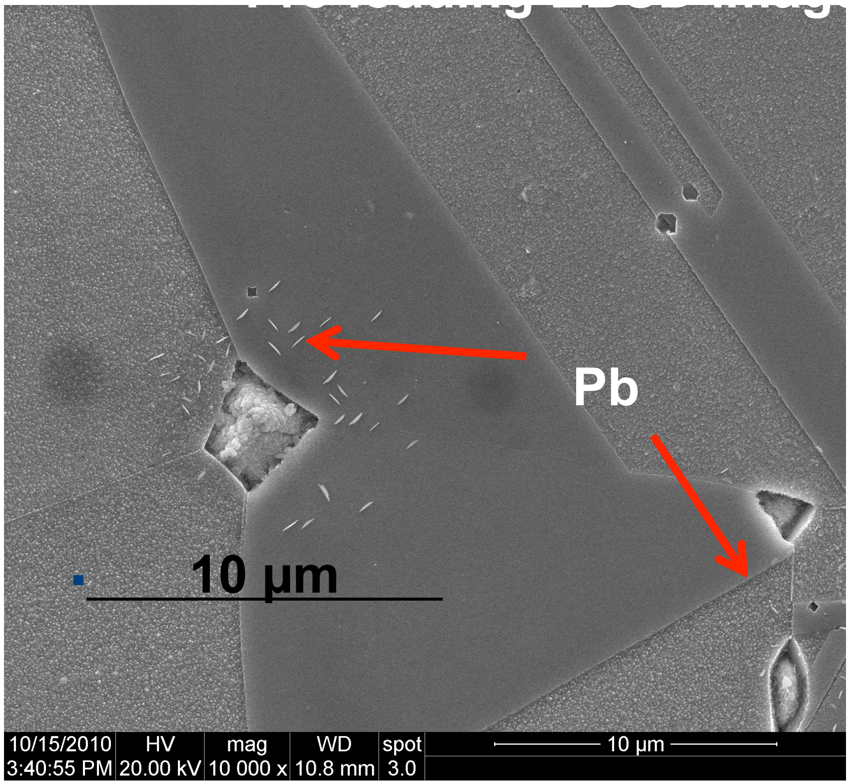
1hr 600 C
Grain Size = 60 µm

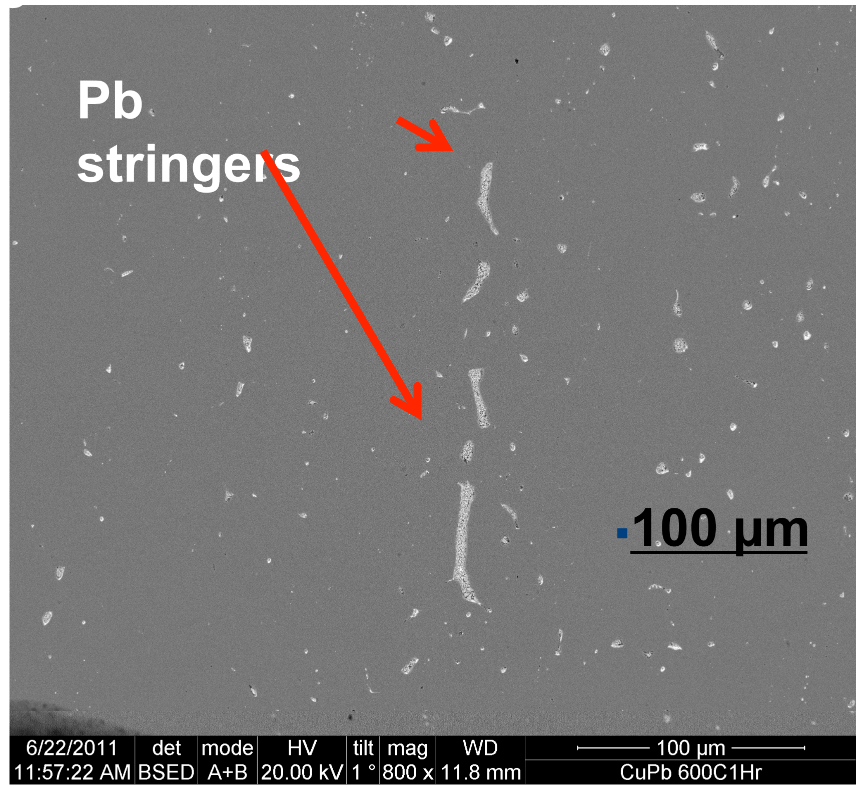


1 % Pb, 1 hr 600 C
Grain Size = 60 µm



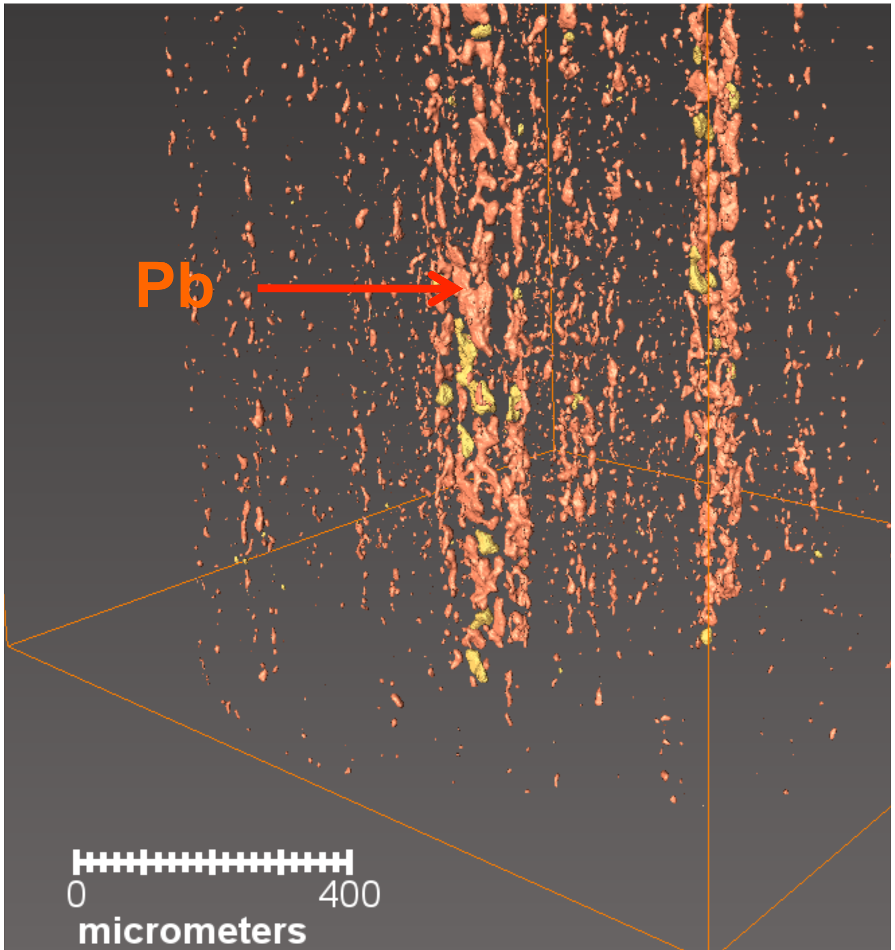
Lead Distribution Inhomogeneous

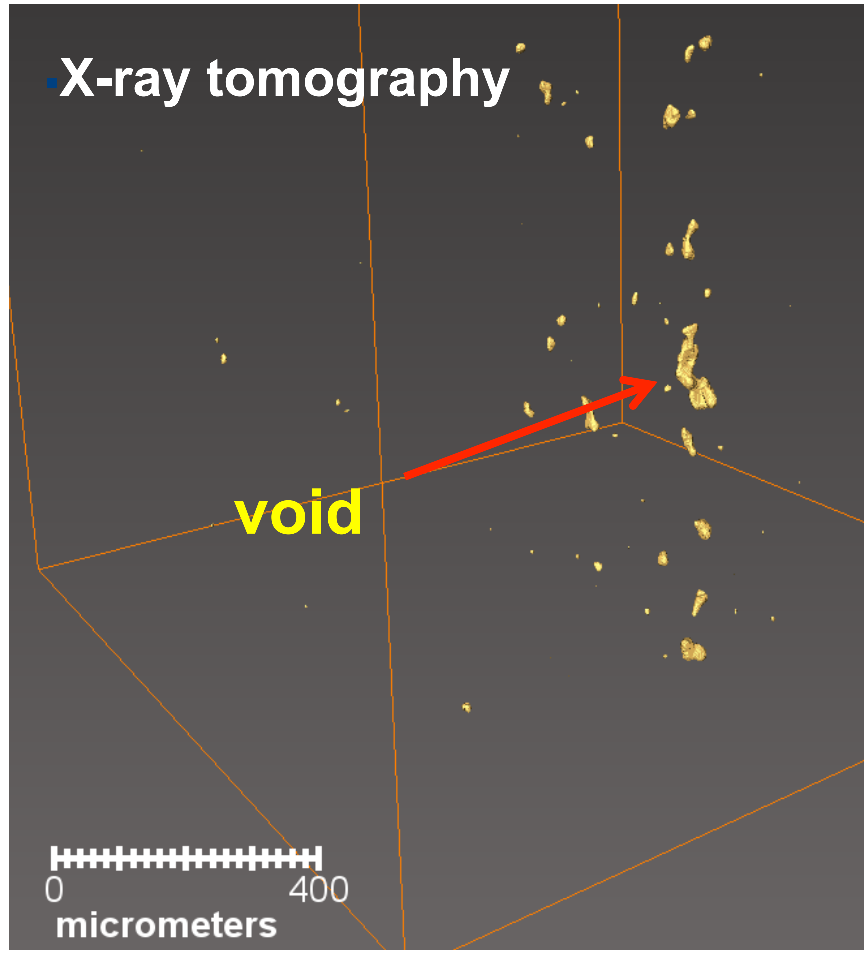




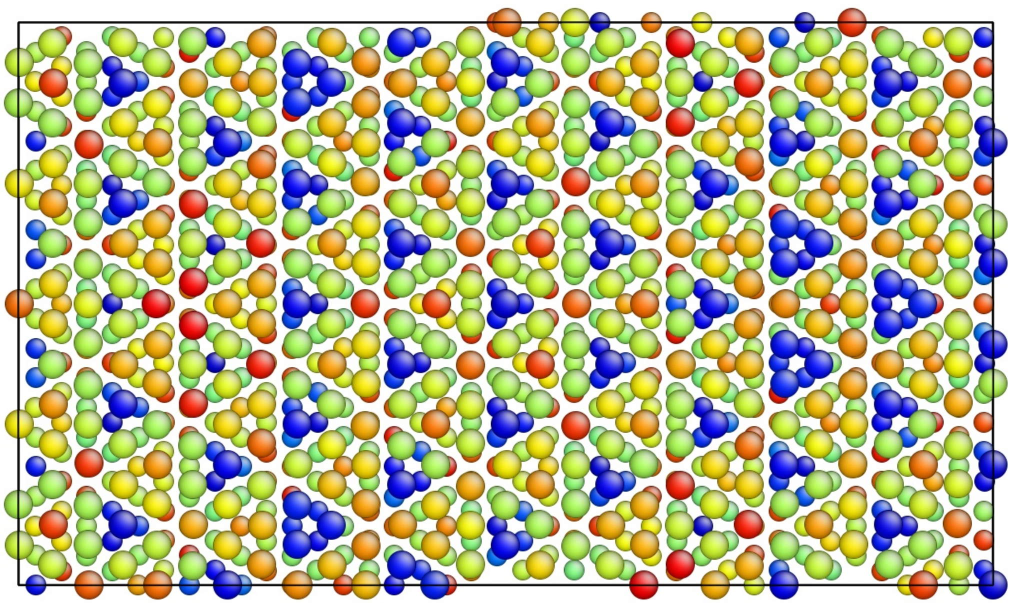
- **Non-Homogeneous distribution of Pb:**
  - **Mostly at grain boundaries and triple points**
- **Mesoscopic stringers in some regions, but not other**

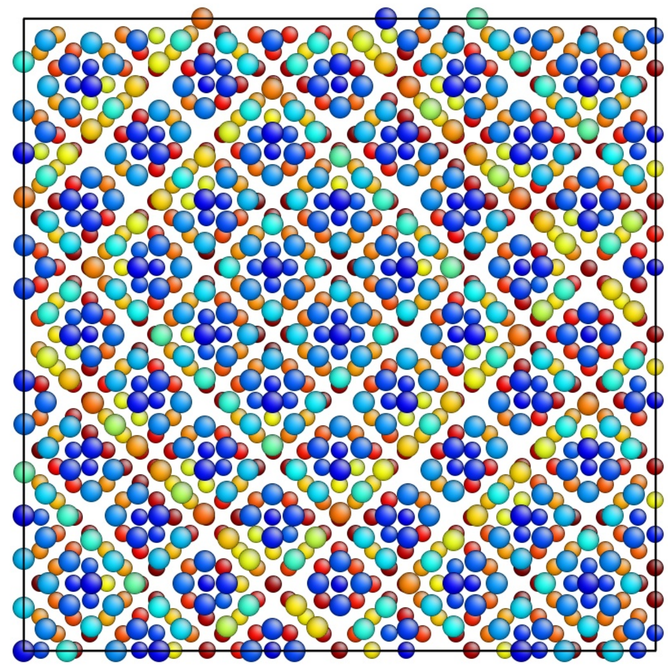
Lead “stringers” and voids/cavities: Micron scale





Cu/Pb interface, relaxed structures



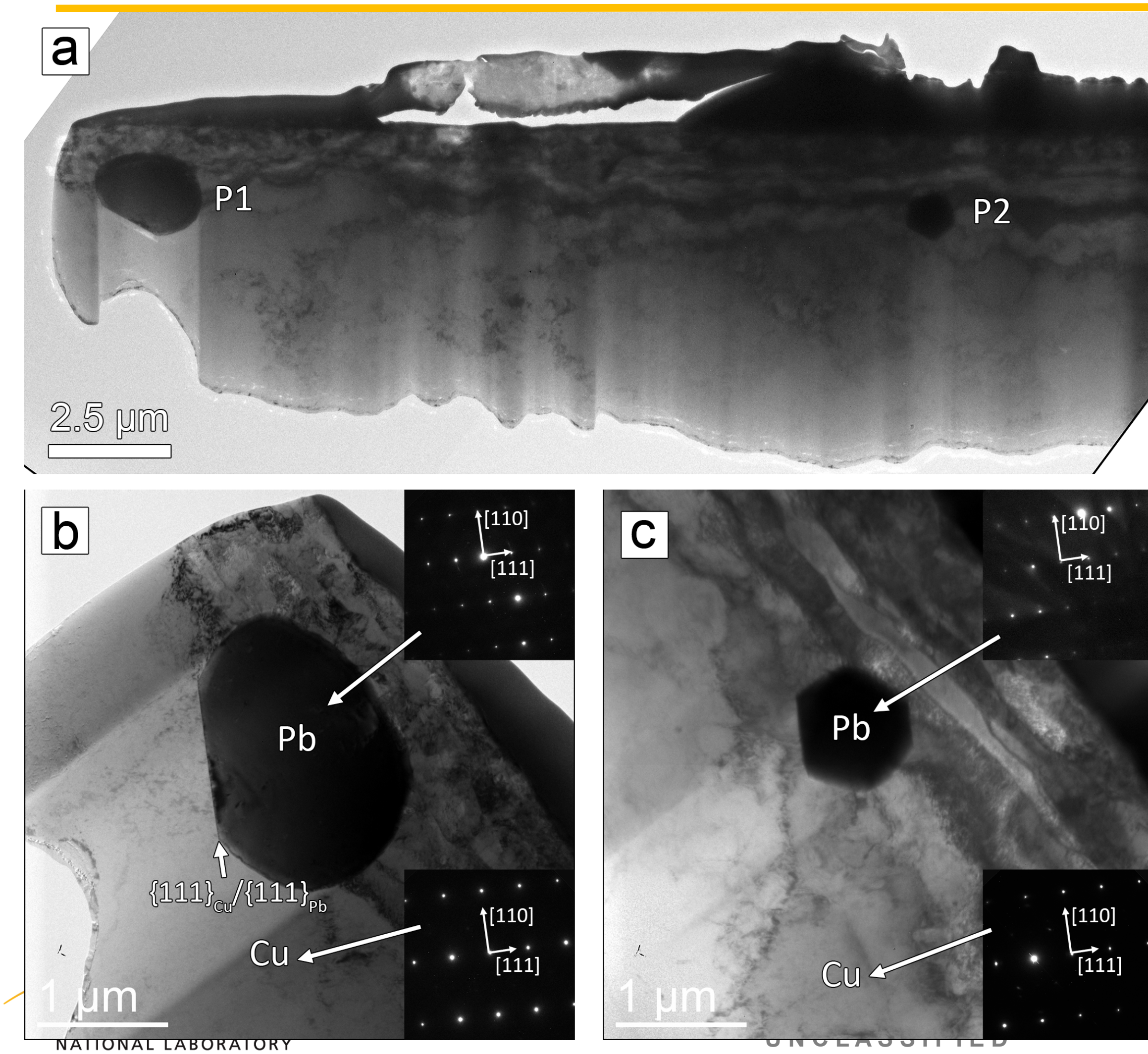


$\gamma^{111/111} = 0.58\ J/m^2$

$\gamma^{100/100} = 0.80\ J/m^2$

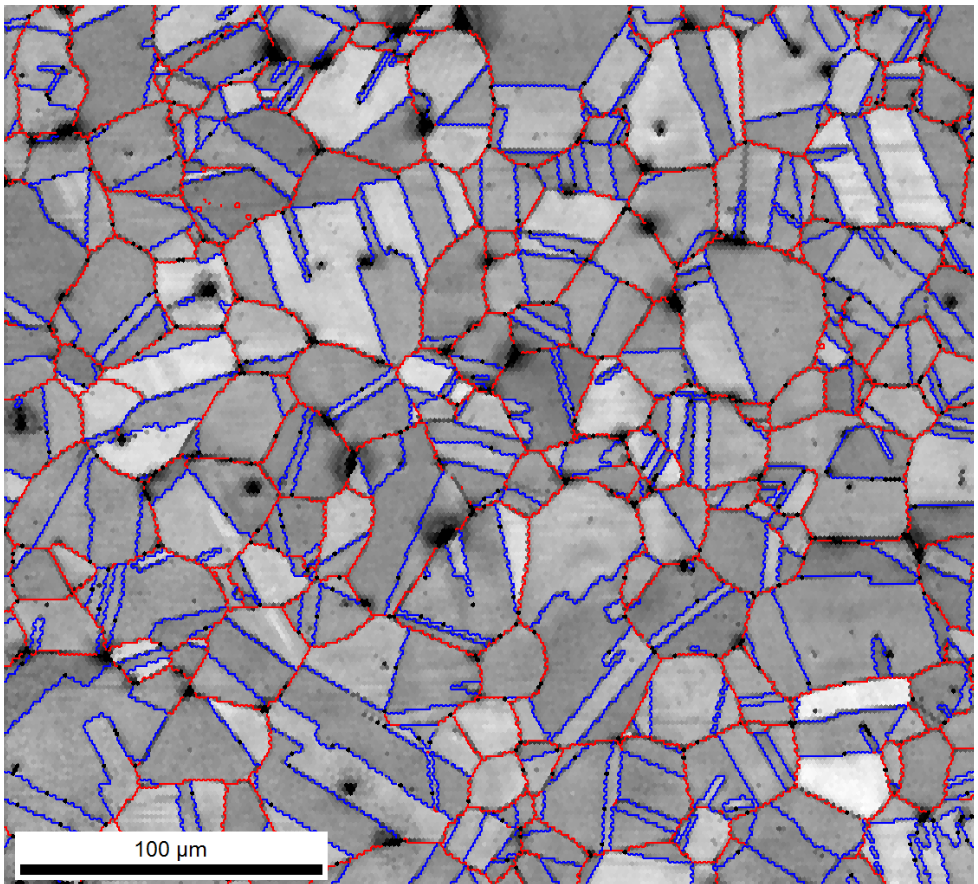
Colored by centrosymmetry parameter

Orientation Relationship Between Cu and Pb



TEM gives [111]/[111]

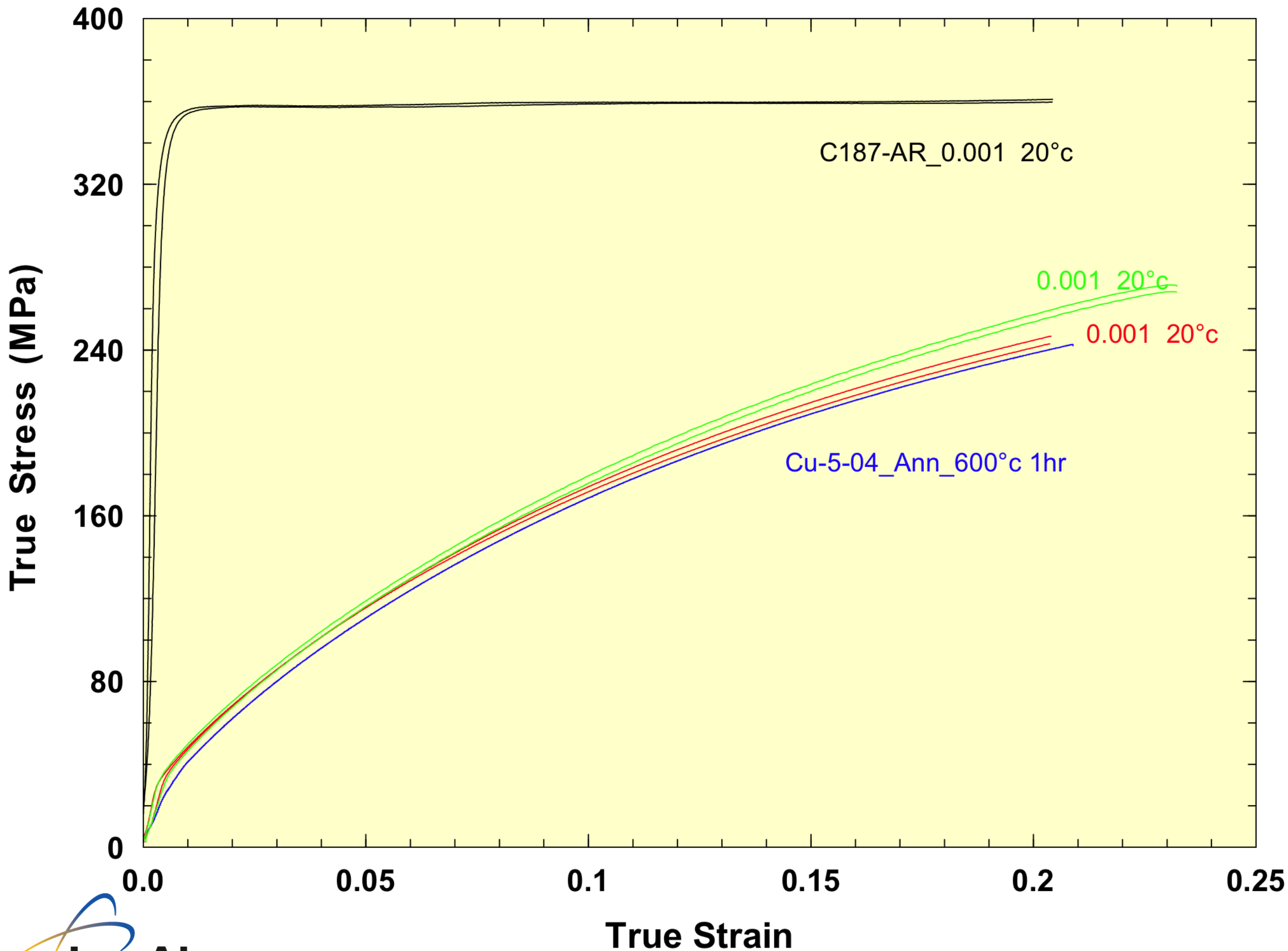
Distribution of Pb
Tracked by Grain Boundary Type



	Min	Max	Fraction
red line	5 °	58 °	0.421
blue line	59 °	61 °	0.564

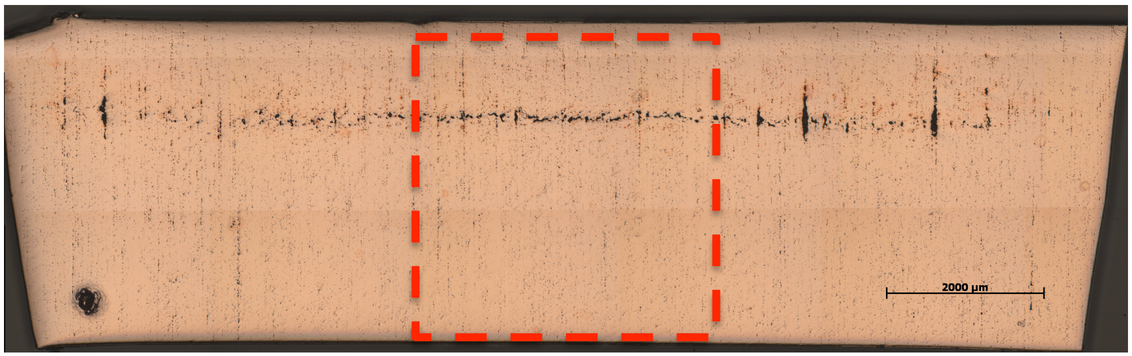
Pb predominantly at non-Σ3 boundaries

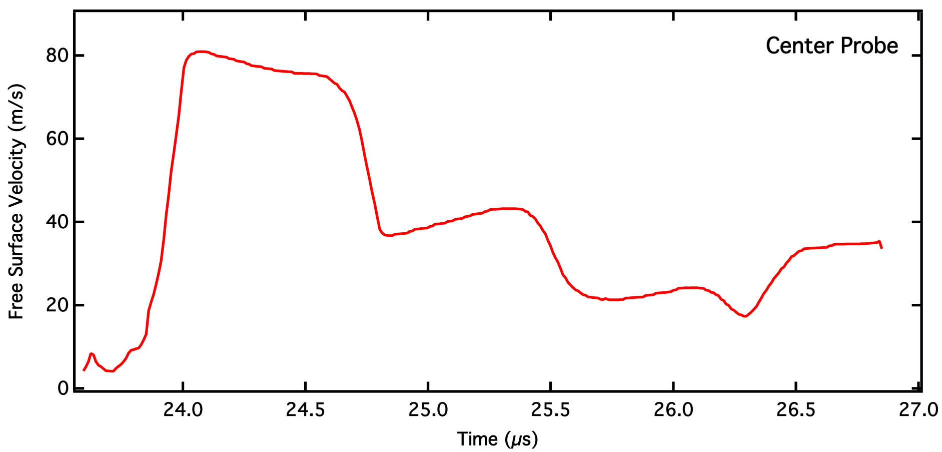
Role of Pb under Relatively Low, Uniaxial Stress

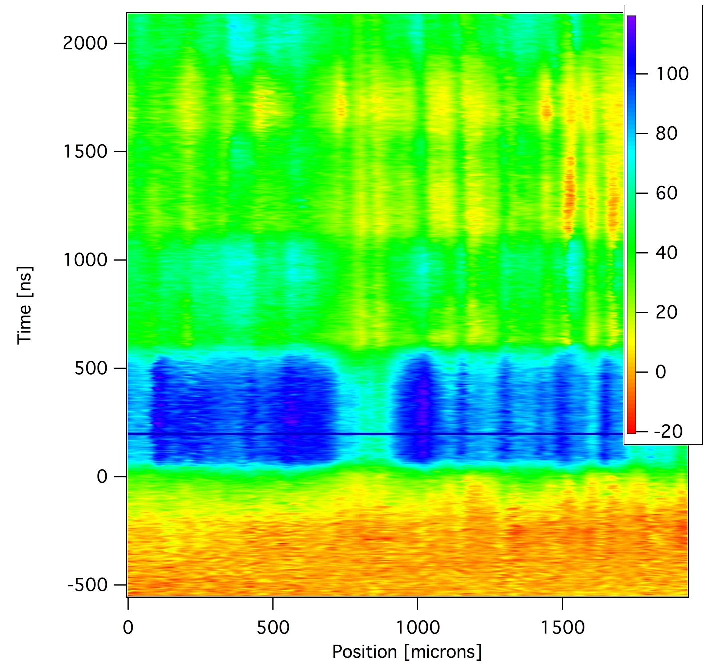


- Quasi-static response of the Cu-Pb alloy is similar to as-annealed Cu: No effect?

Spalled CuPb with Line Visar Probe shows a decrease in peak velocity

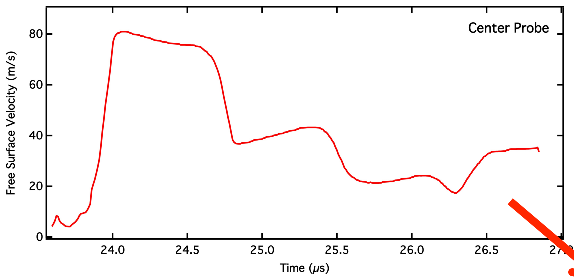






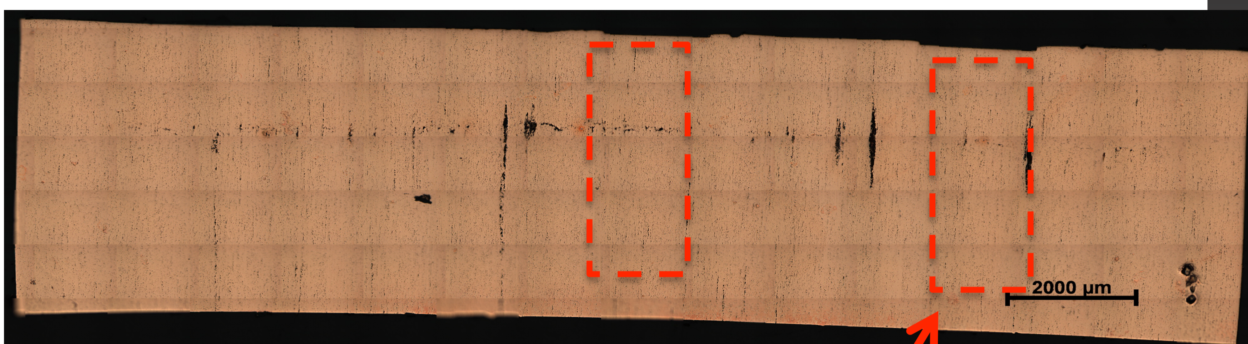
- **Change in the velocimetry data in middle of probe**
- **Correlate change to microstructural features**

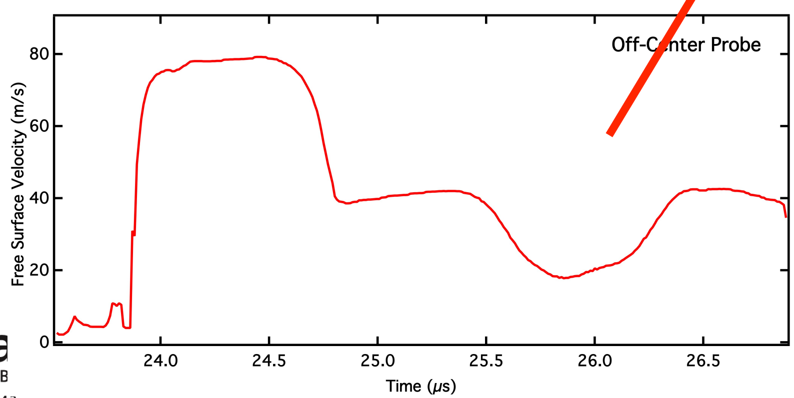
Effects Possibly Associated with Pb Distribution

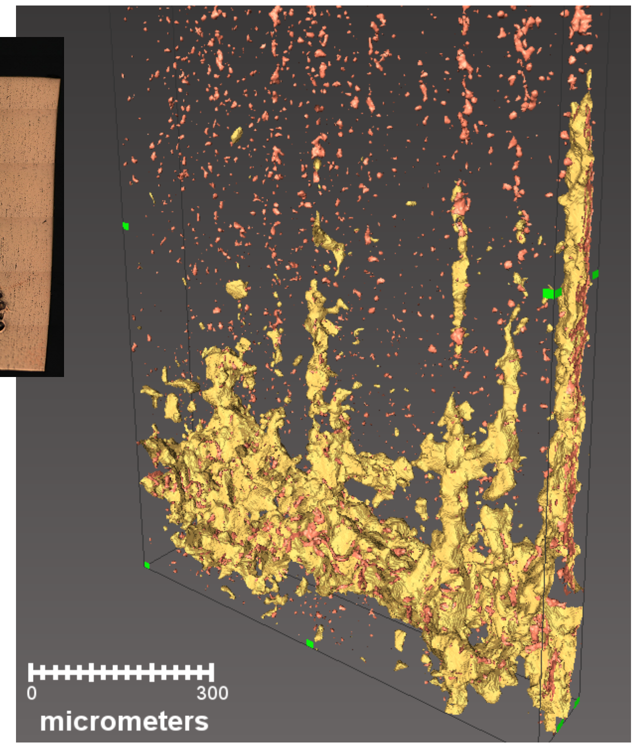


3 mm zQ on 4mm Cu/Pb
@ 122 m/s

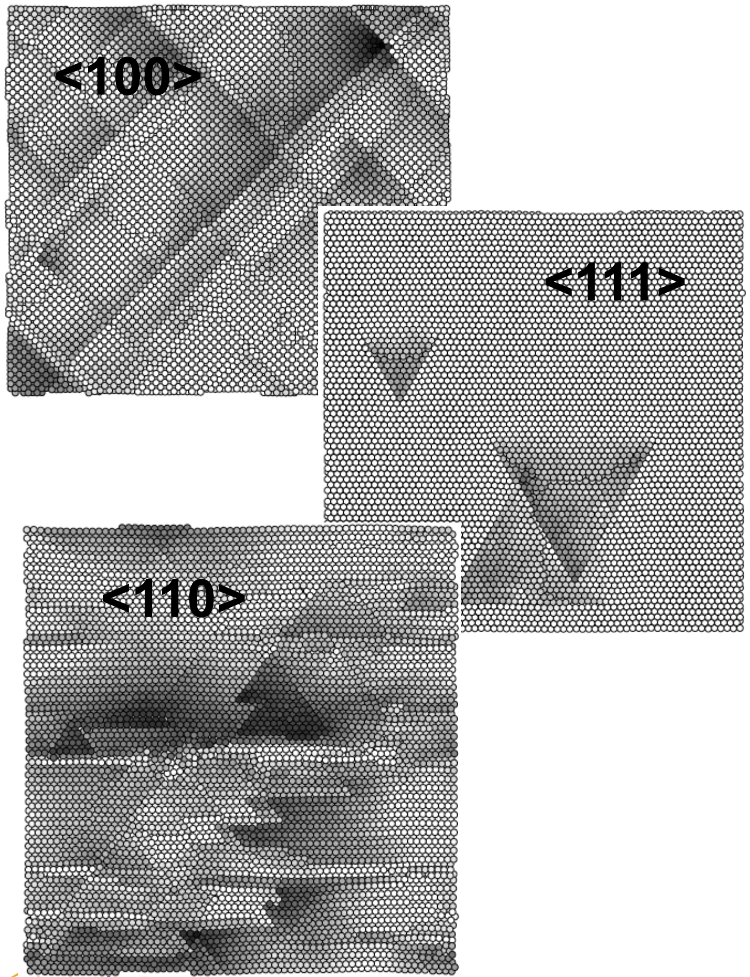
X-ray Tomography shows voids nucleating along Pb stringers







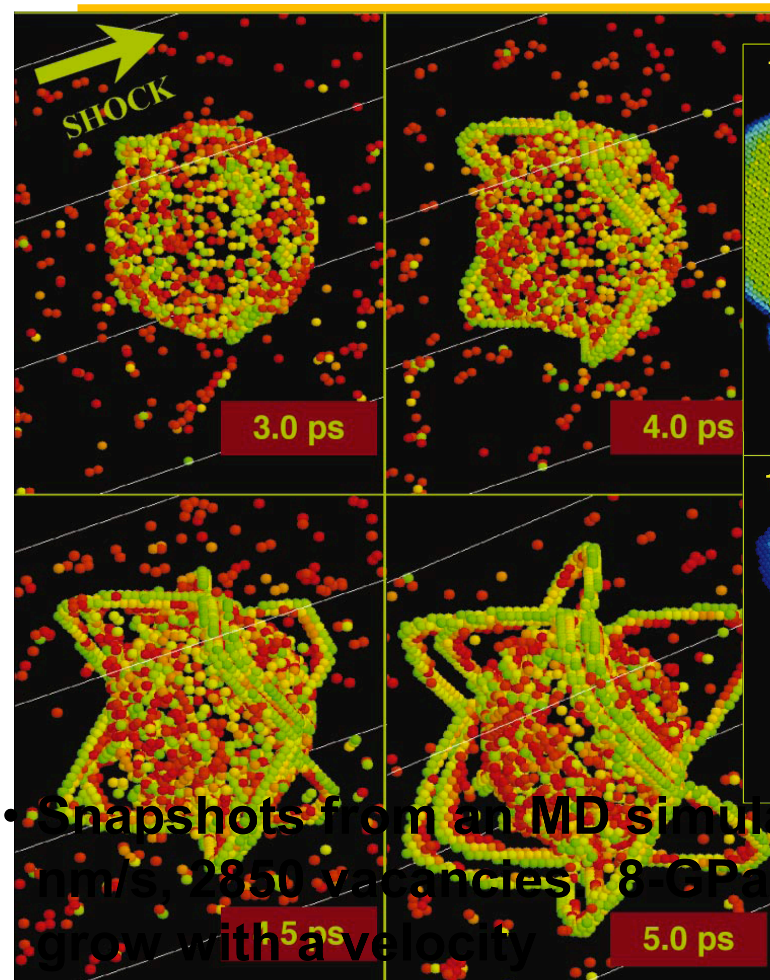
Shock & Microstructure: Shock MD Simulations of Cu GBs

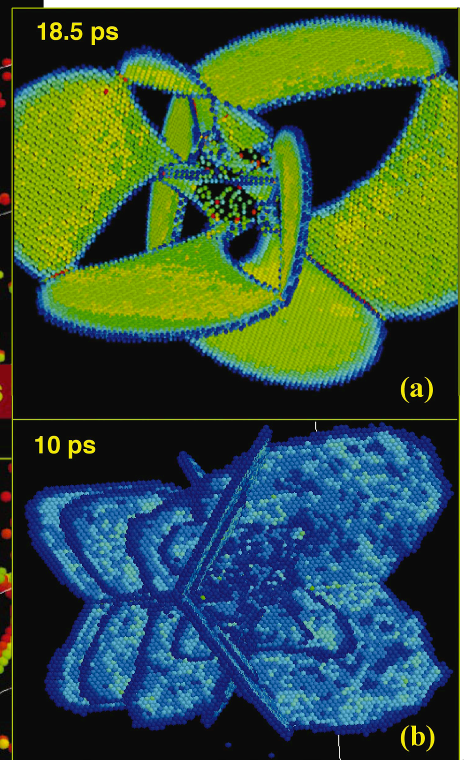


Germann, Holian, Lomdahl, Ravelo (2000)

- Sample shocks in <100>, <111>, and <110> crystallographic directions
- Atoms shaded in proportion to the transverse displacement from initial lattice positions
- Shrinking periodic boundary conditions, with a piston velocity u_p 0.2 c_L (longitudinal sound velocity)
- c_L per directions: $\sqrt{72}$, $\sqrt{96}$, and $\sqrt{90}$, respectively.

MD Simulations of Cu GBs





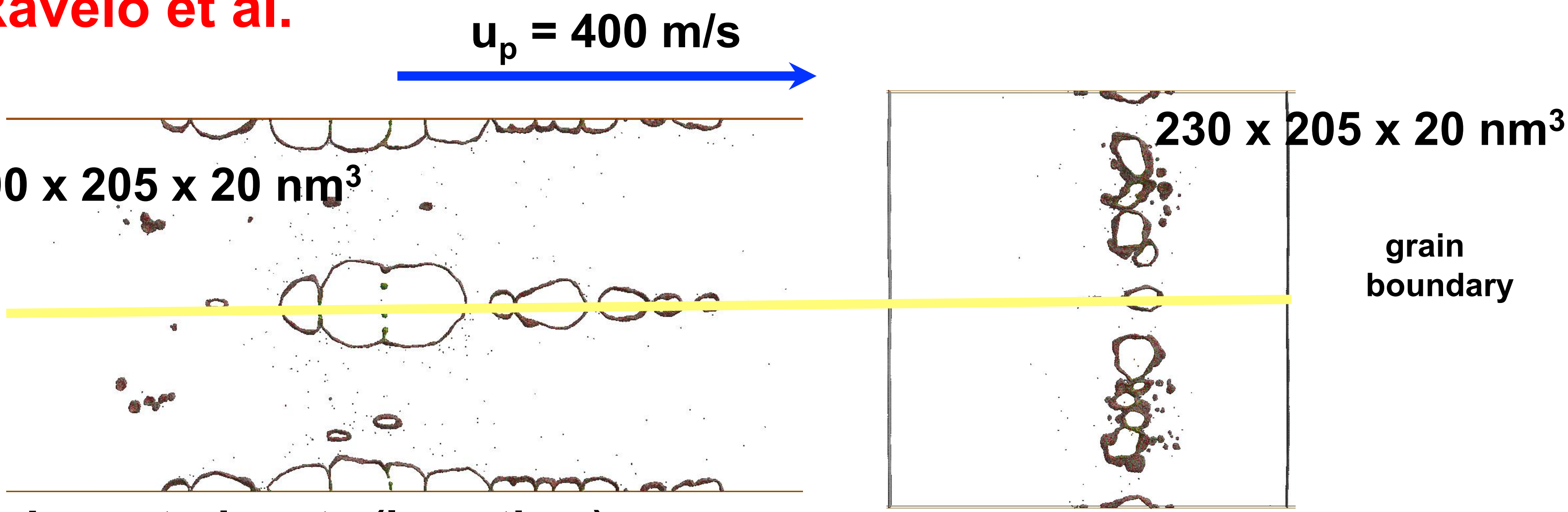
Davila et al. (2005): Evolution of void collapse

- **8 GPa shock
  Void radius R=1.5 nm
  up = m/s1200**
- **vacancies. Only defective atoms are shown. Numbers in boxes indicate**
- **time in ps after shock was applied; emission of loops starts at 3 ps**

- **Snapshots from an MD simulation with R_{void} =2 nm/s, 2850 vacancies, 8-GPa shock. Shear loops grow with a velocity**
- ***v/c_0, 0.15, where c_0 is the sound speed at normal conditions. Snapshot* from a similar MD simulation for sbd a 21-GPa shock. Loops grow at nearly the sound speed c_0.**

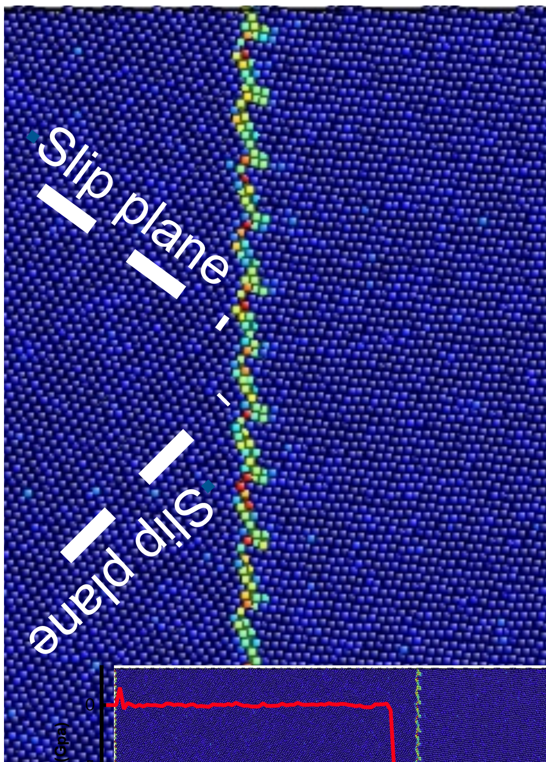
Interface strength and damage sensitive to strain-rate

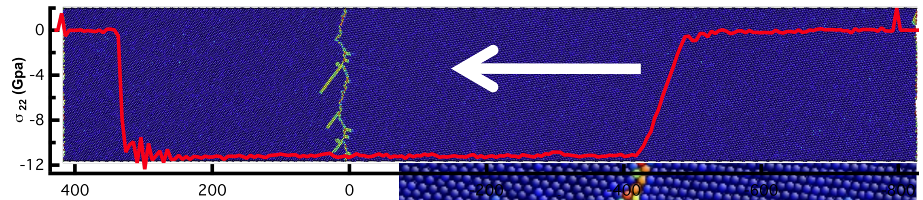
- **Simulations of dynamic ductile failure in Cu predict void nucleation, growth, and coalescence**
  Ravelo et al.



- **Low strain rate (long time): heterogeneous nucleation, failure reorients along GB**
- **High strain rate (short time): nucleation, failure away from GB**

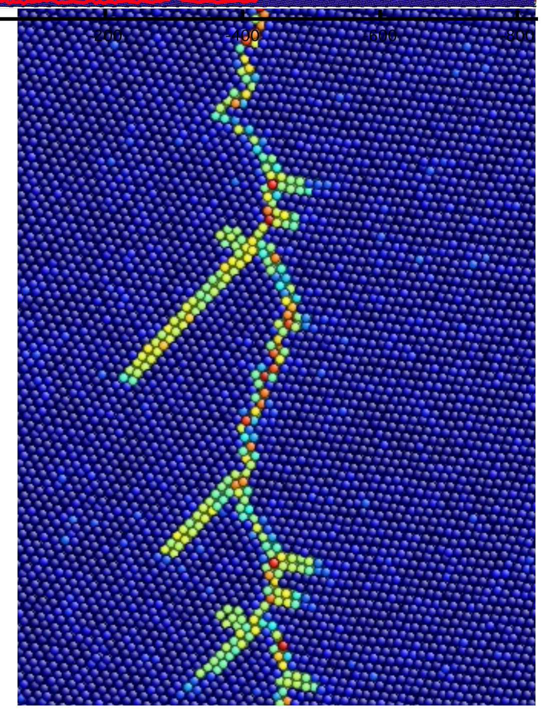
MD Simulations of Cu GBs

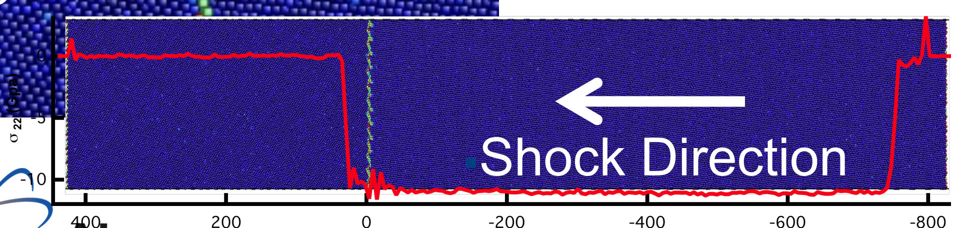




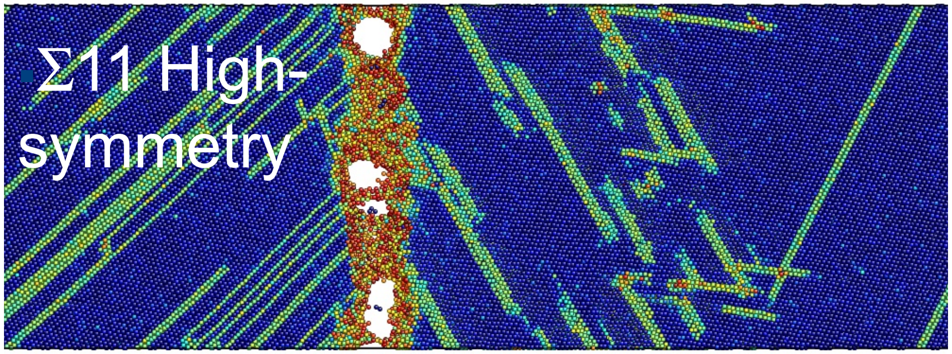
- **High & low symmetries versions of Σ11 asymmetric tilt Cu bdys**

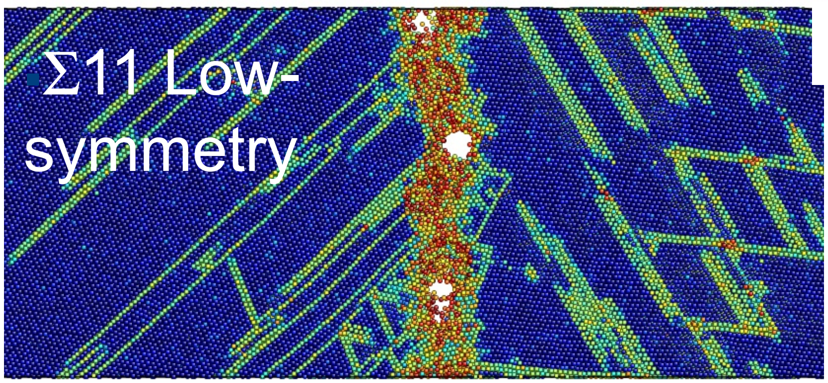
- **Emit different types of Shockley partials along varying slip planes**



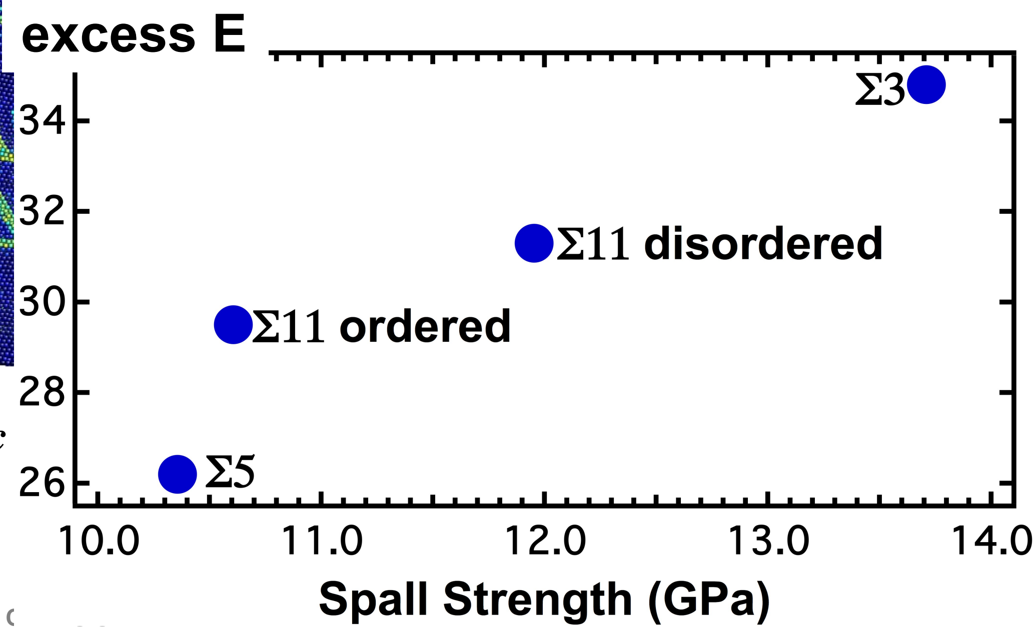


Shock Simulations of Cu GBs





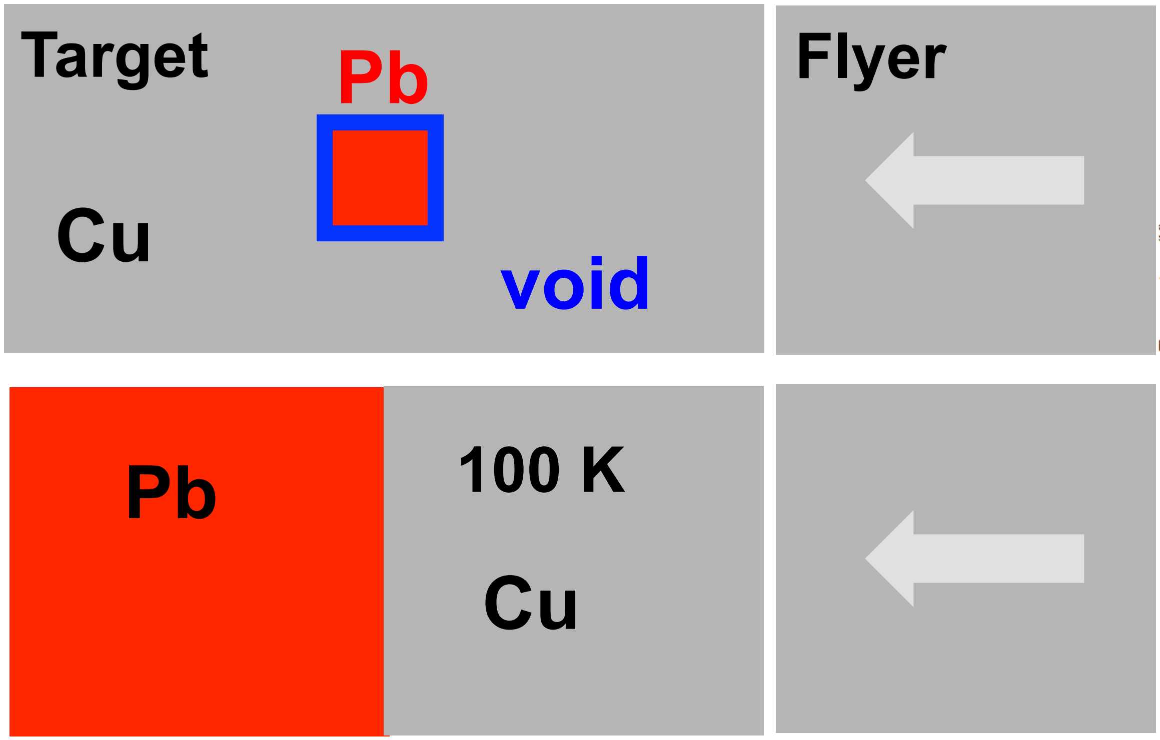
- **Correlation between spall strength and excess energy due to plastic deformation**

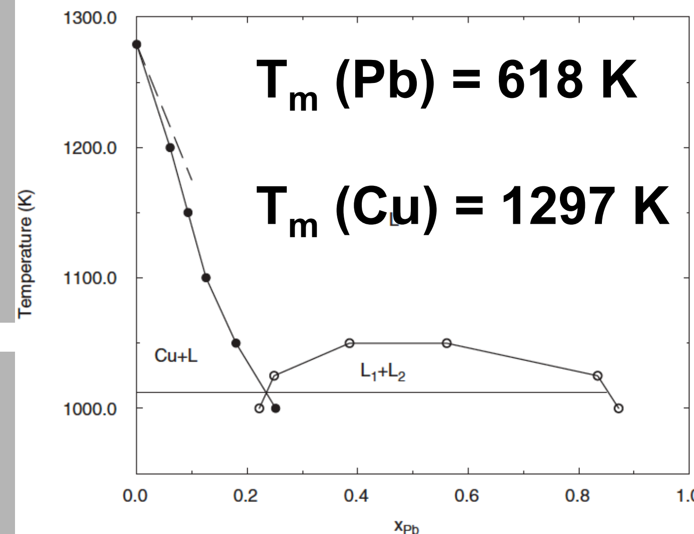


$$E_{Ex} = \gamma_{plastic} + \gamma_{elastic}$$

$$\sigma_f^2 \propto \gamma_f \propto E_{Ex}$$

MD Simulations of Cu-Pb Interfaces



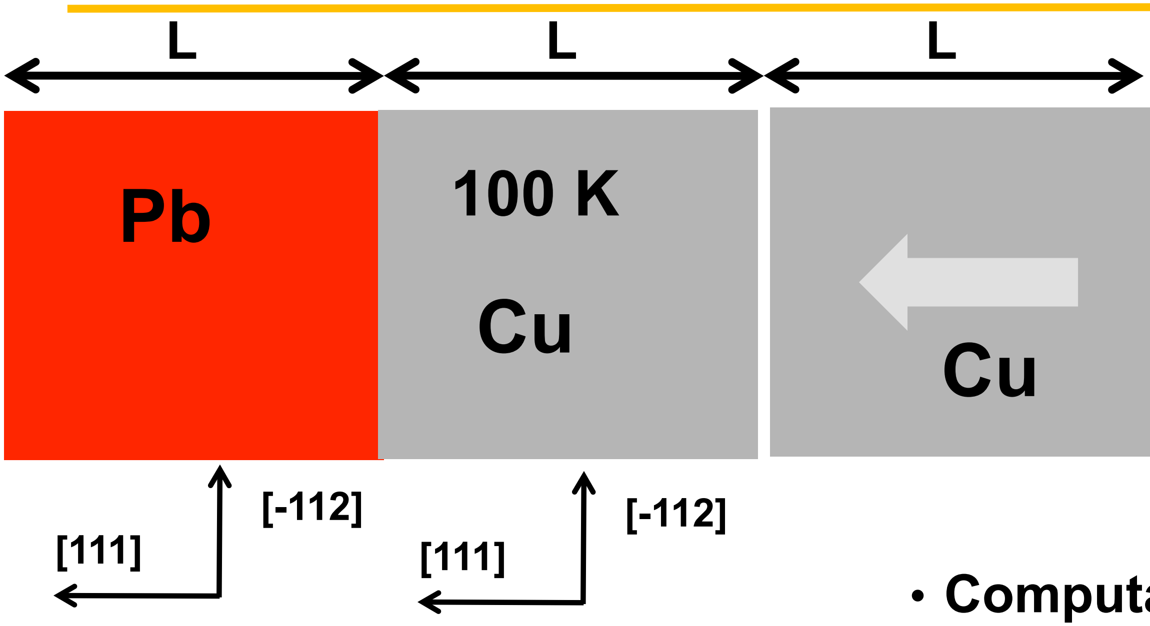


Hoyt-Garvin-Webb-Asta EAM Model (2003)

- u_p in Cu target 250 m/s
- Impedance mismatch w/ Pb = 2.12
  u_p(Pb) = 0.71 u_p(Cu)

- Lattice mismatch 37 %
- No phase transformations

Details for Molecular Dynamics Simulations: Interfaces

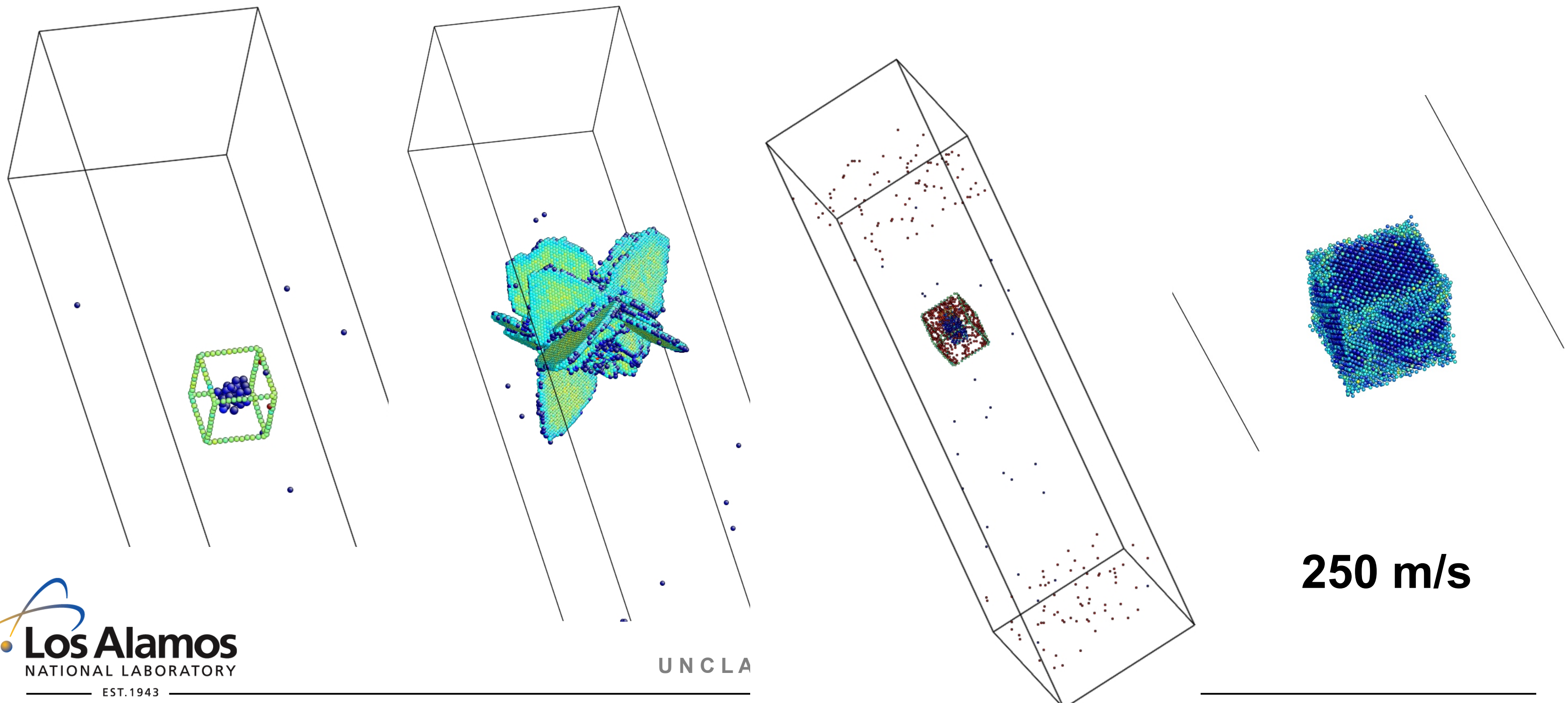


- Minimize misfit strain
- NVE molecular dynamics (MD) Sandia LAMMPS code

- Computational cell size:
  Cross-section: L: 19 Cu, 14 Pb
  Shock direction: L: 241 Cu, 47 Pb
- Periodic in 2 directions
  free in 3rd
  3.5 M atoms

Pb Inclusions Under Shock

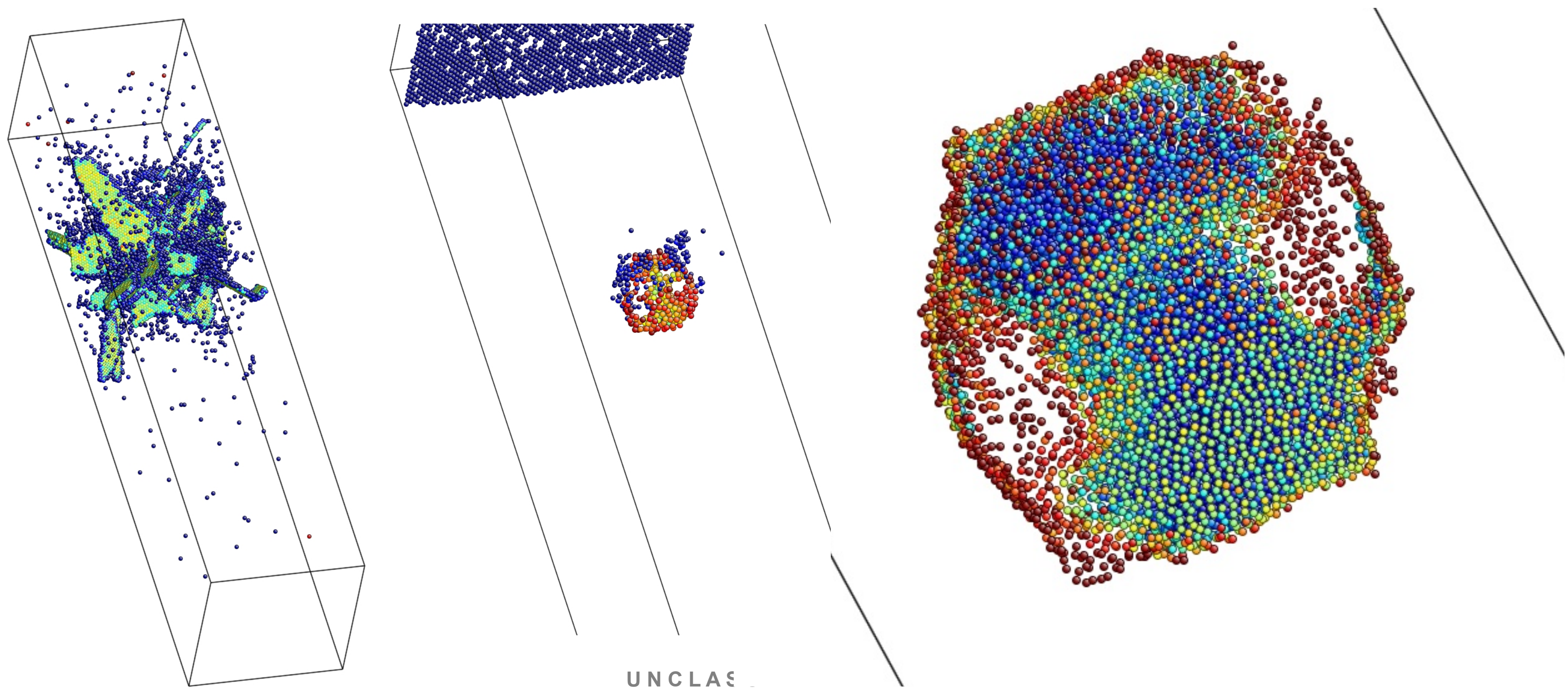
- **Matrix around voids and small inclusions show dislocation emission on compression**
- **Larger inclusions transmit shocks**



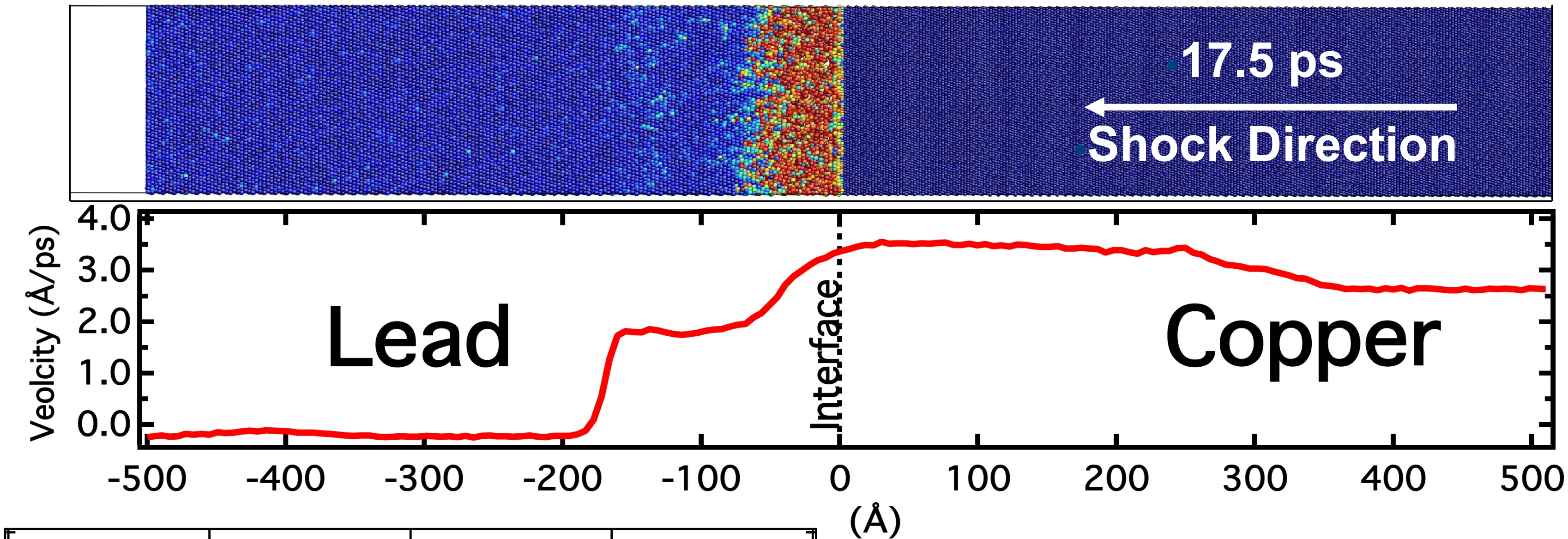
250 m/s

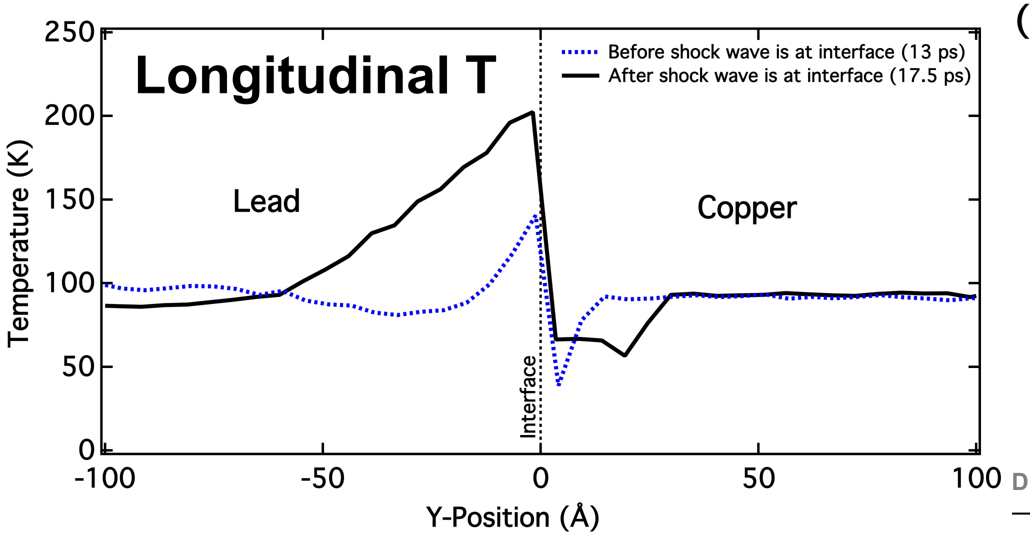
Pb Inclusions Under Tension

- Cu matrix continues to emit partials
- Pb distorts into jet on tension
- Independent of size
- Likely T dependent



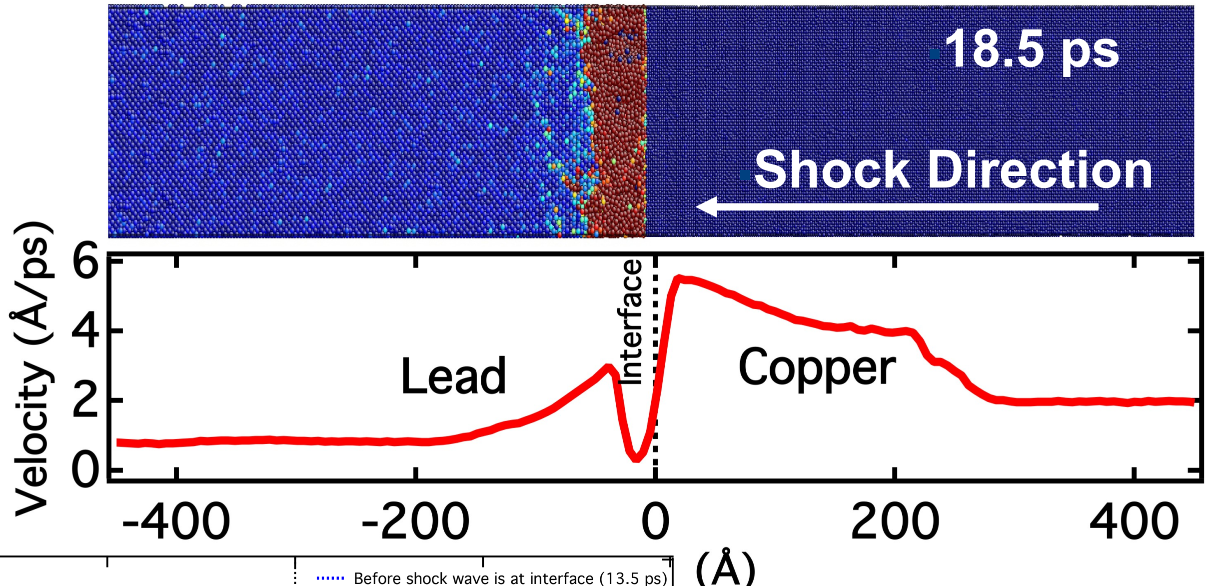
Shock MD Simulations: Cu(111)/Pb(111) Interfaces

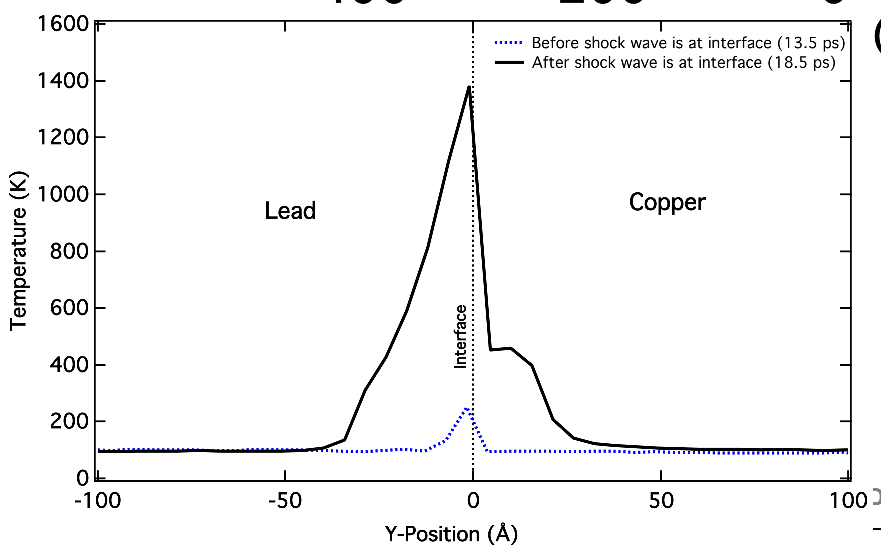




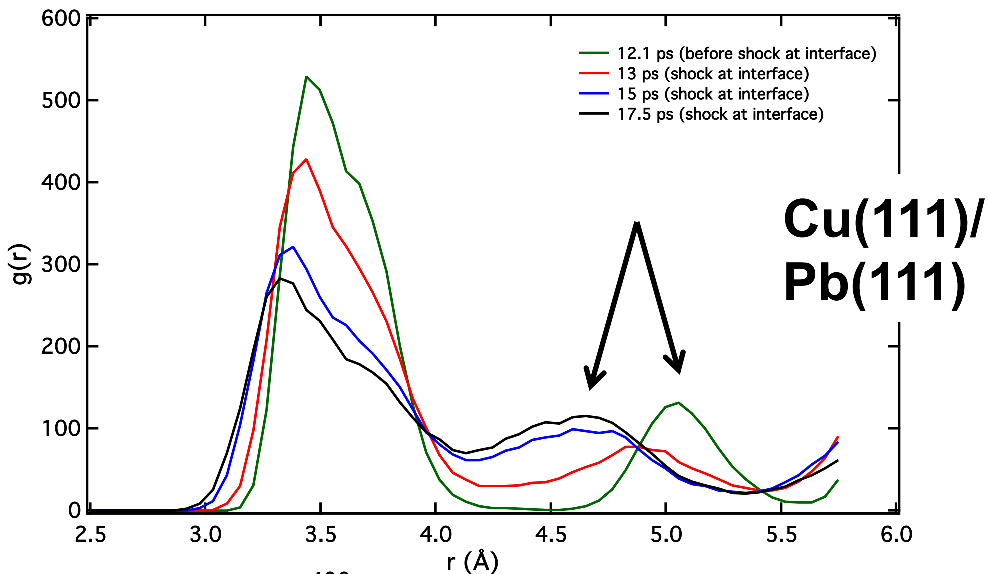
- **100 K, 250 m/s**
- **After shock, <T> in Cu ~100 K and Pb ~150 K near bdy**

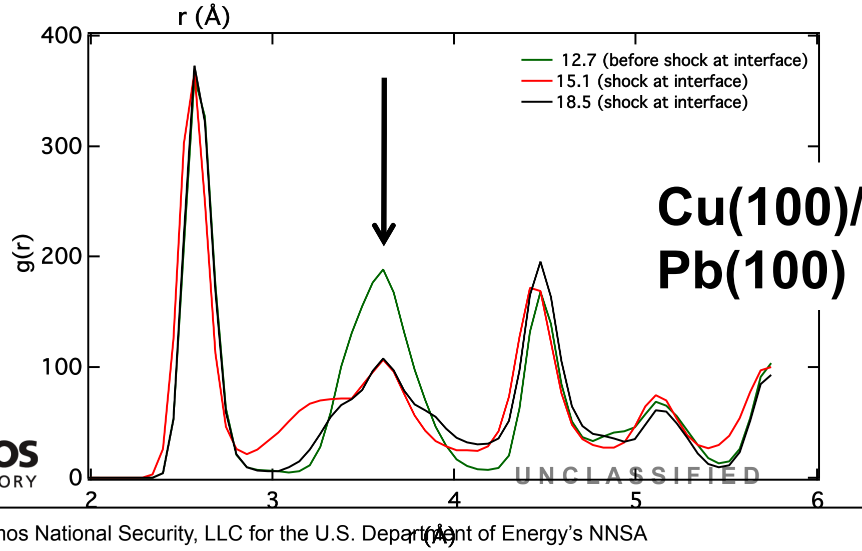
Cu(100)/Pb(100) at 100 K





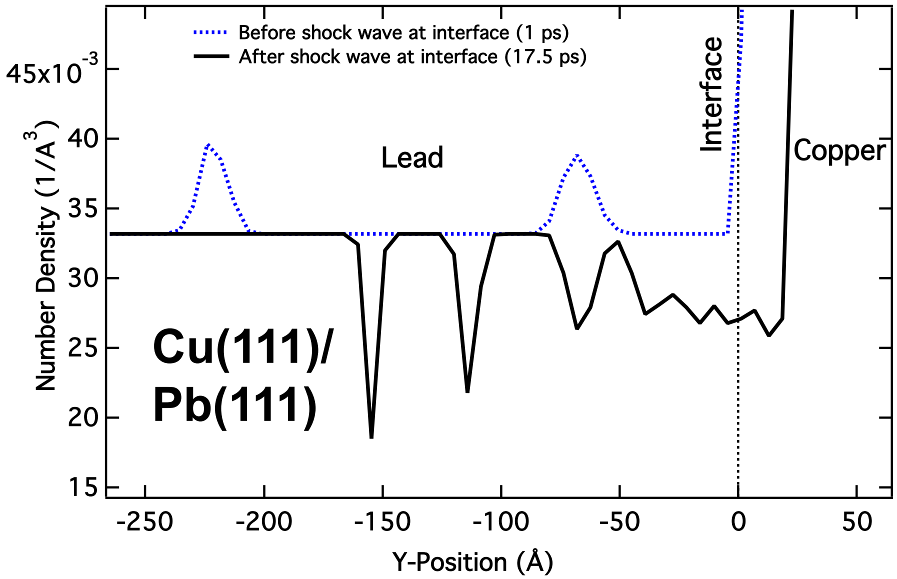
Radial Distribution Functions

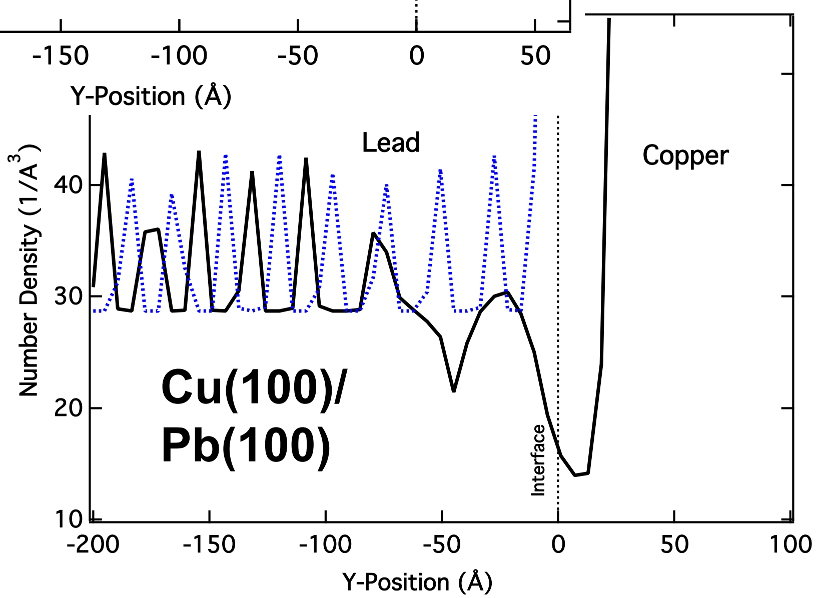




- Pb atoms close to interface
- Smearing of 2nd neighbor peak after shock
- Consistent with disordered or amorphous structure immediately after shock

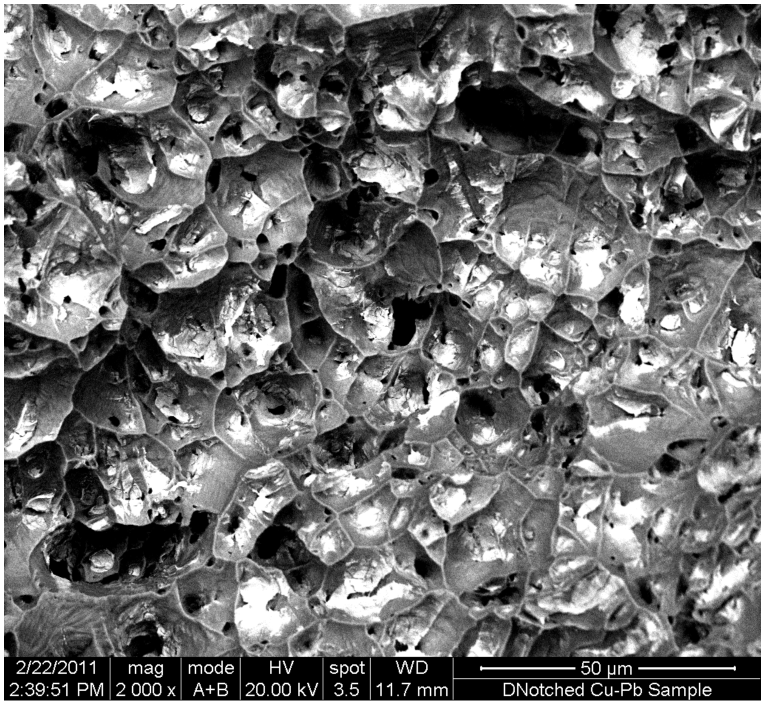
Number Density Drops at Cu-Pb Interfaces

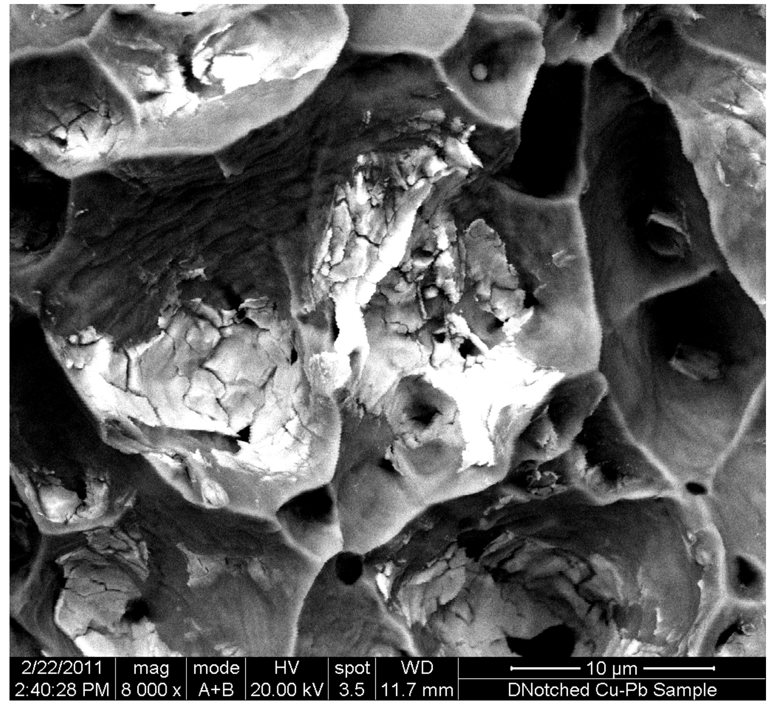


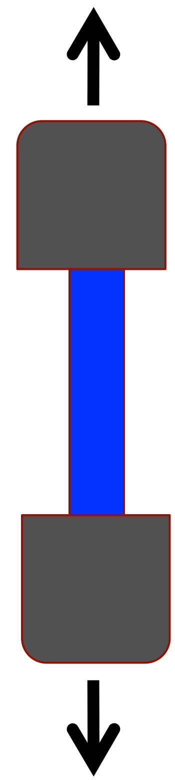


- Impedance mismatch sets up reflected and transmitted waves
- Drops interfacial density initially
- Drives plastic response?
- Suggests certain level of independence of response to interface type

Quasi-Static Tension Tests







SEM micrographs with back scatter electron

White regions – Lead and Other – Copper

Strain-rate
10^{-3} /s

Conclusion

- Equation of state not predictive of spall response
  Spall strength varies by ~10 % with boundary type & structure
- Grain boundaries with dissimilar structures emit observably different Shockleys under shock loading
- High T rise at bdy with & w/o void space
- Pb carries load with little plastic response in Cu in bicrystals

Statistics From the 2D and 3D Characterizations

	2D		3D	
Grain Size	**# of voids**	**Area (%)**	**# of voids**	**Area (%)**
30	236	.50	904	.49
60	343	.25	2495	.16
100	267	.45		.42
200	111	.51	1262	.71

Remarkable agreement between the measurements