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Title: Spallation in metallic systems: Effects of microstructure and loading

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Form 836 (7/06)

Spallation in metallic systems: Effects of microstructure and loading

Sheng-Nian Luo

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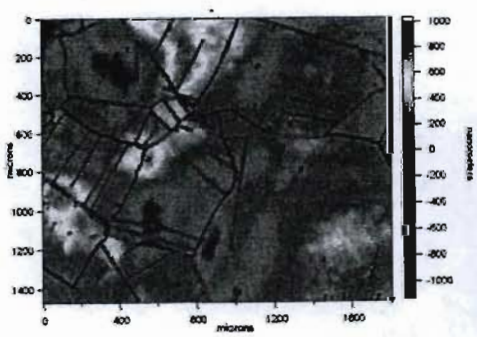
- Sponsors:
  - Laboratory Directed Research and Development (LDRD).
  - Advanced Simulation and Computing (ASC; C. Bronkhorst, M. Schraad).

Abstract

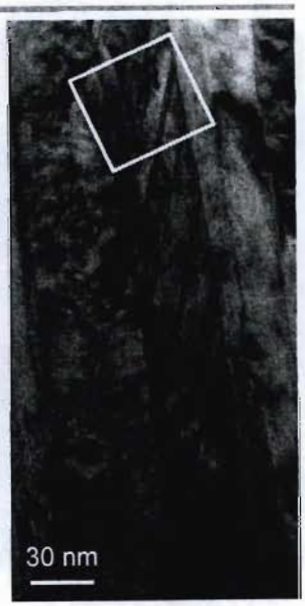
We present molecular dynamics simulations of shock-induced plasticity and spall damage (including void growth) in representative metallic systems, Cu and Cu-Nb, with emphasis on microstructure and loading effects. Microstructure includes atomic level heterogeneity, nanovoids, grain boundaries and triple junctions. For the loading dependence, we examine anisotropy, Taylor wave vs. square wave loading, and the growth dynamics of a nanovoid at different tension. The simulation results may help us define the "rules" for higher level modeling that has to incorporate both effects. LANL is operated by Los Alamos National Security, LLC for the U.S. Department of Energy under contract No. DE-AC52-06NA25396.

Motivation: microstructure



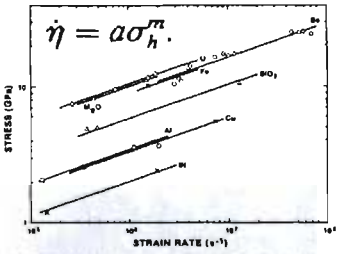
Unpublished data, the LDRD-DR-20060021 team, Los Alamos National Laboratory.

(P. Rae et al.)

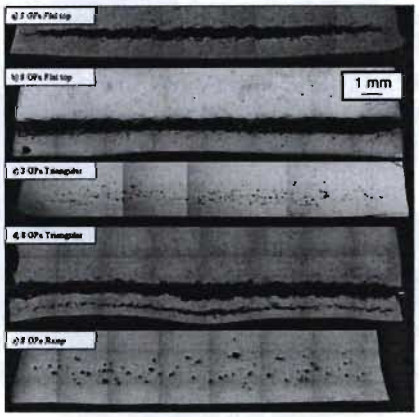


ARB Cu/Nb, Beyerlein LDRD-DR team

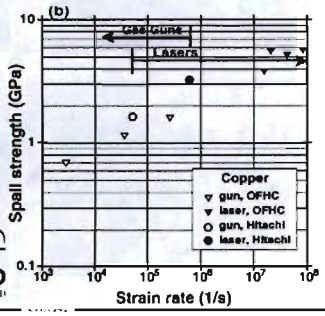
Background: loading effect



J. W. Swegle and D. E. Grady J. Appl. Phys. 58 (2), 15 July 1985

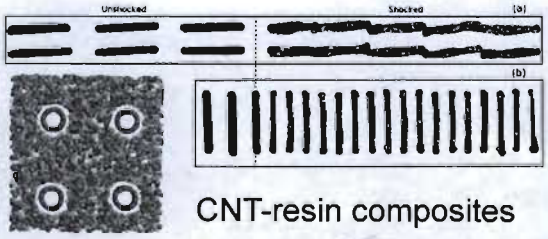


D. D. Koller, R. S. Hixson, G. T. Gray III, P. A. Rigg, L. B. Addessio, E. Cerreta, J. D. Maestas, and C. A. Yablinsky, J. Appl. Phys. 98, 103518 (2005).



Molecular dynamics: microstructure and loading effects on dynamic response

- Microstructure: defects (0-3D), inherent heterogeneity, impurity, phase boundaries, ...
- Loading: anisotropy; rate; pulse shape and width.
- MD: gain insights into fundamental mechanisms and help define the "rules" for higher-level modeling.
- Focus: metallic systems.

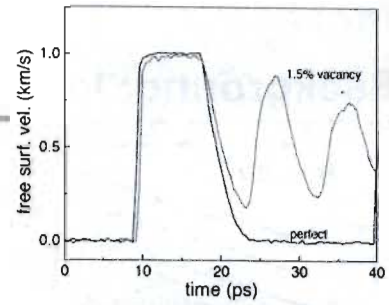


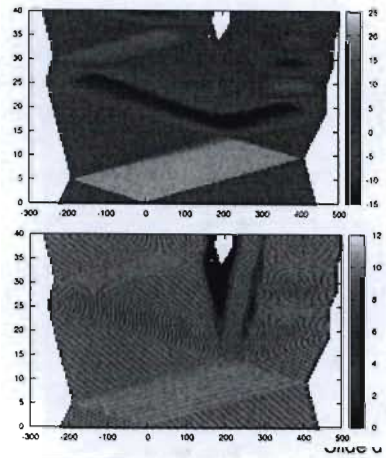
CNT-resin composites

Nanocrystalline Cu

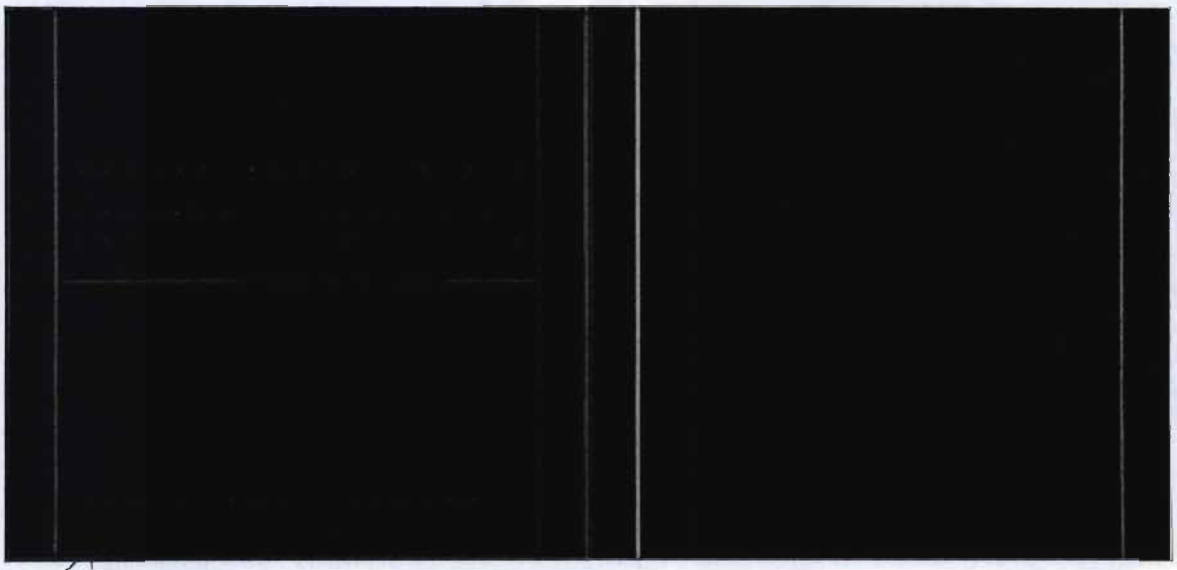
Methodology

- Cu: embedded-atom-method (EAM) potential (Mishin et al. PRB 2001).
- Cu-Zr: Finnis-Sinclair type (Mendelev et al. JAP 2007; Cheng et al., PRL).
- Radial distribution function (RDF), and coordination number.
- Static-structure-factor-type order parameter with 12 *k*-vectors and neighbor average (Luo et al., JCP 2007).
- Centrosymmetry (Kelchner et al., PRB 1998).
- Honeycutt-Andersen analysis (JPC 1987).
- von Mises shear strain (Shimizu et al. Mater. Trans. 2007).
- Void analysis (Luo et al. IJMPC 2006).
- Voronoi tessellation (Finney, Nature 1977).
- Shock simulations (Holian, Shock Waves,1995): *flyer plate impact on target.*

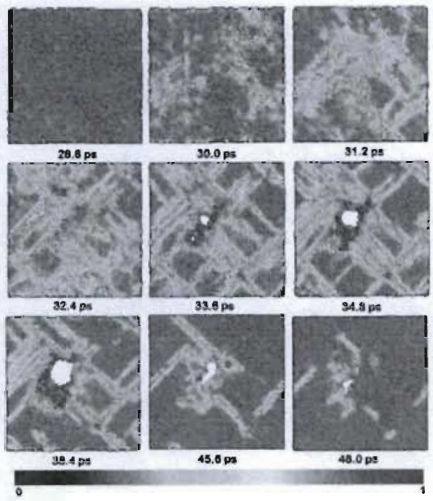




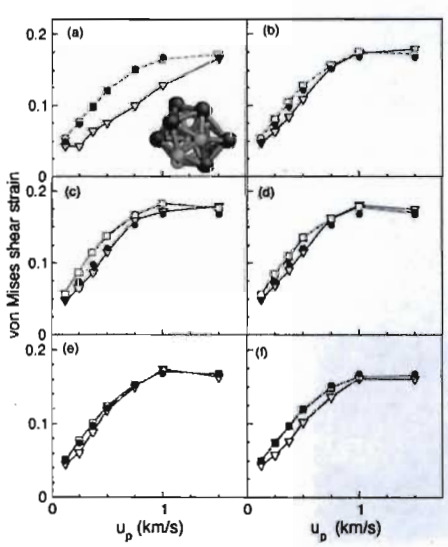
Methodology: an example of shock induced spallation

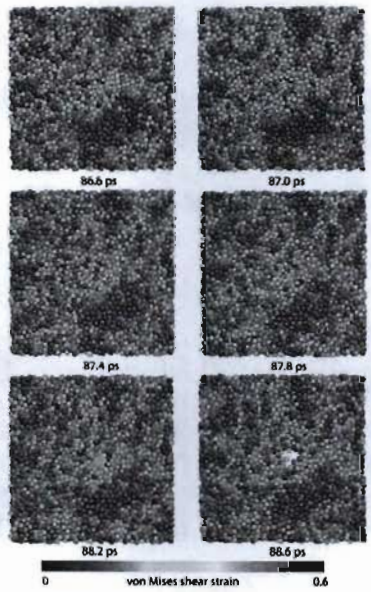


Atomic level structure: fluctuations in Cu single crystals

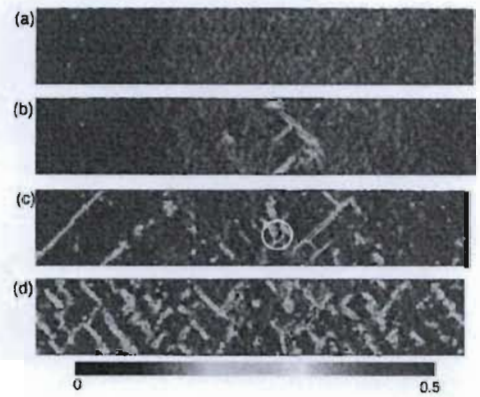


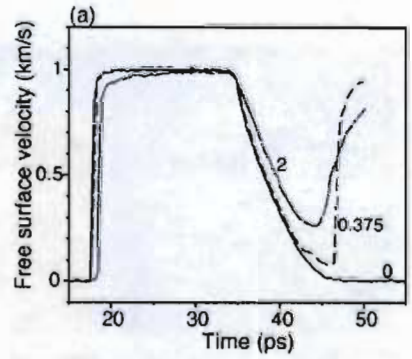
Atomic level structure: $Cu_{46}Zr_{54}$ metallic glass



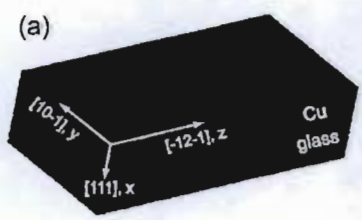


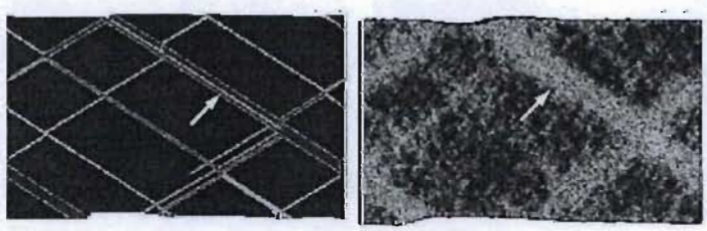
Atomic level structure: vacancies in Cu single crystals





Phase boundary: Cu-$Cu_{46}Zr_{54}$ glass composites





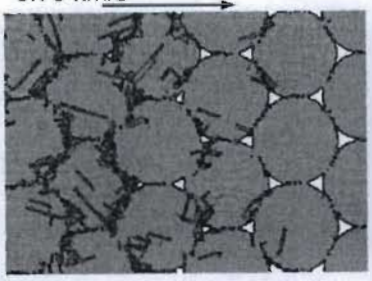
Nanoporous Cu

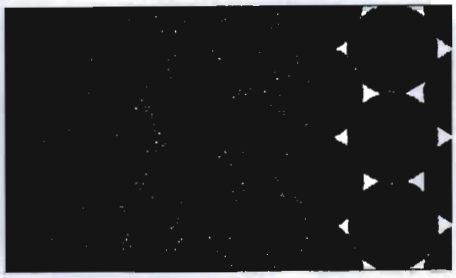
0.75 km/s

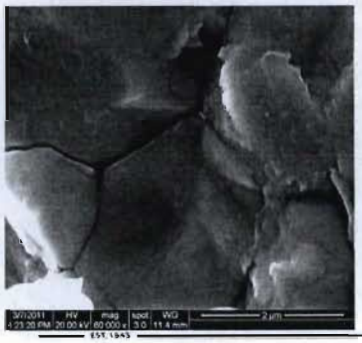
1 km/s

MD, 11 nm; Different

consolidation dynamics

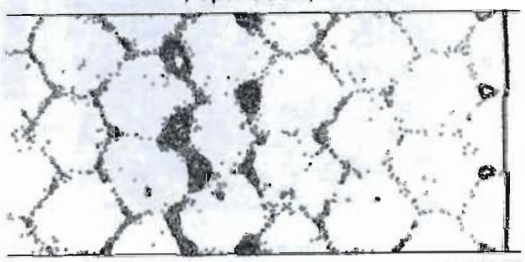






Shock experiments, 2-3 μm Cu, 0.3 km/s

MD, spallation, 1 km/s



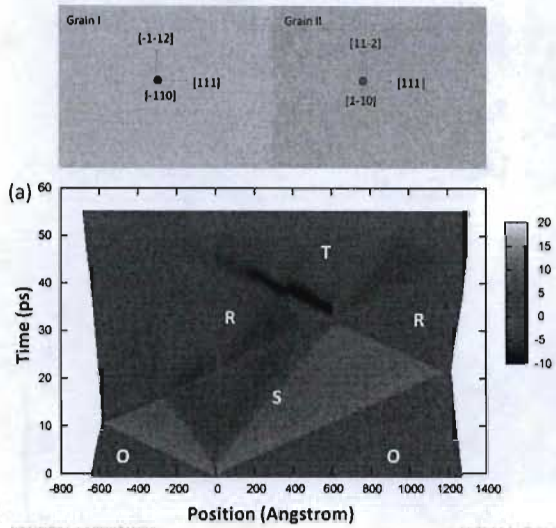
UNCLASSIFIED

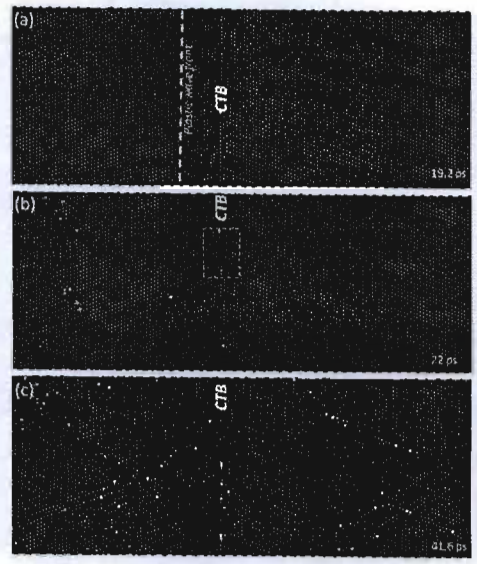
GB: Cu bicrystals, columnar nanocrystals

- Σ3 (110): coherent and incoherent twins; normal shock.
- Σ3 <110>(110)/(114): parallel shock.
- Σ11 <110>: parallel shock.
- Columnar <100>: GB triple junctions, anisotropy.

Cu bicrystals: coherent twin boundary

CTB is relatively rigid.





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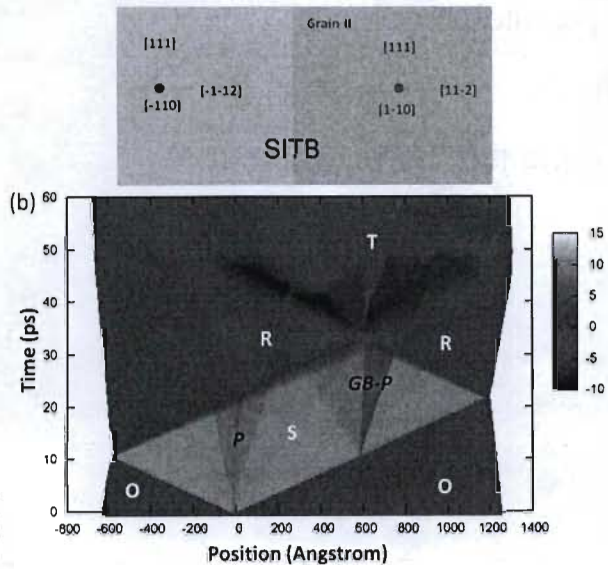
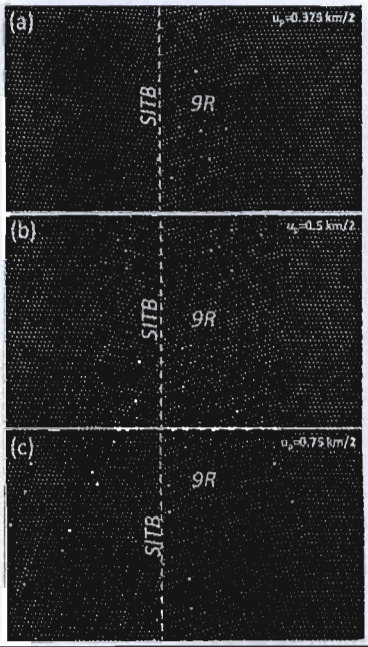
Cu bicrystals: incoherent twin boundary

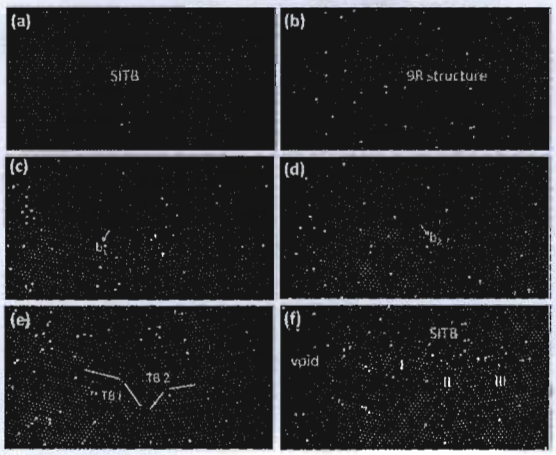
Elastic precursor induces GB plasticity, due to preexisting partial dislocations.

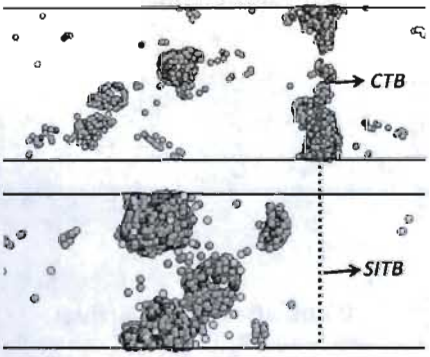




Cu bicrystals: coherent vs. incoherent twins

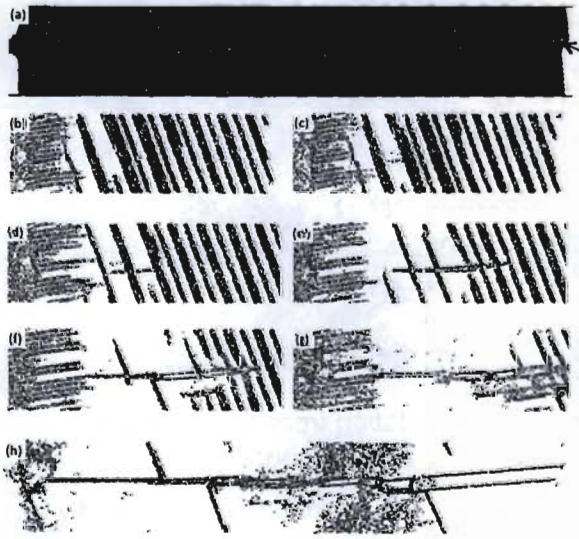
SITB



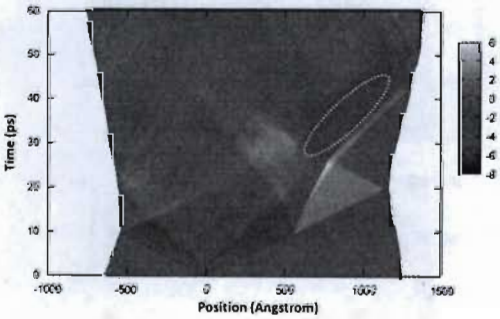


- SITB: formation of three-fold twin upon tension.
- Mobility: mobile SITB vs. "rigid" CTB, thus different void nucleation.

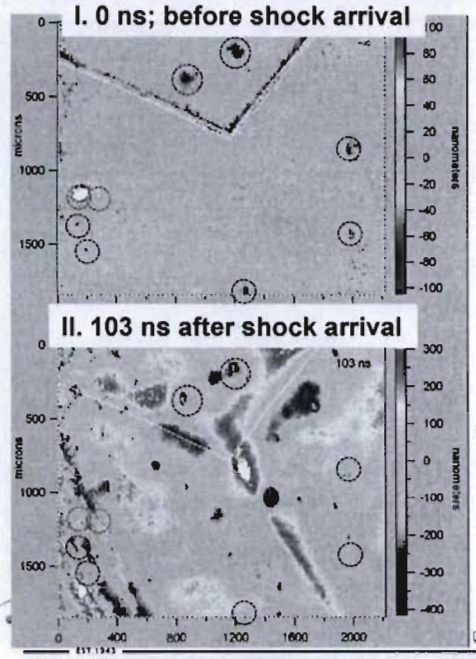
Cu bicrystals: incoherent twins



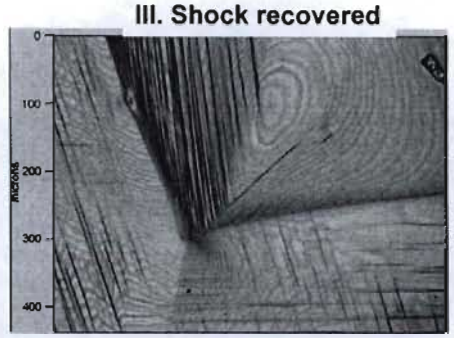
Surface ledge/step formation via twinning due to shearing at later stages.



Experimental observation of "slip bands"



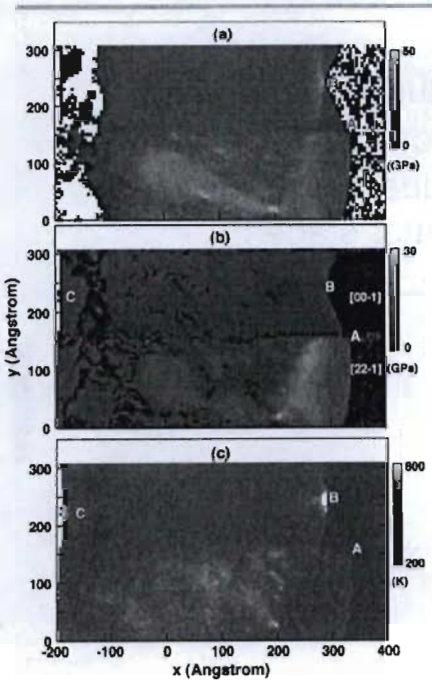
III. Shock recovered

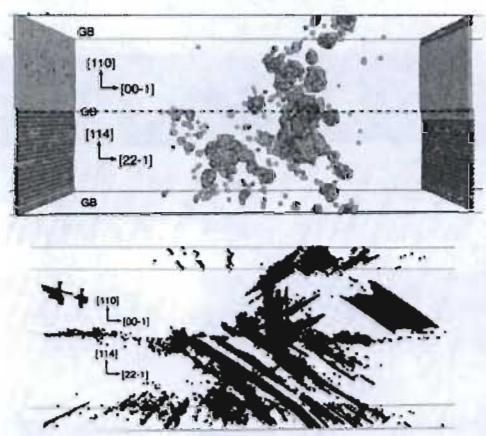


(Trident 19824; LDRD-DR-20060021 team)

- The sequence I-III suggests that "slip bands" do NOT form during shock but at later stages, consistent with MD.

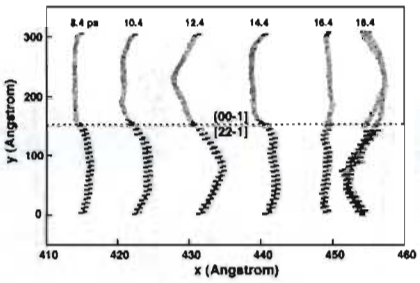
Cu bicrystal: Σ3 <110> asymmetric GB

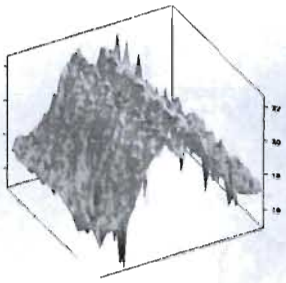


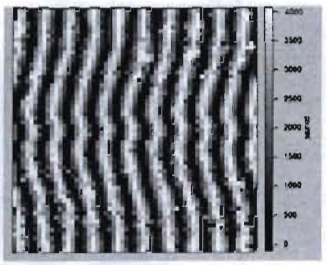


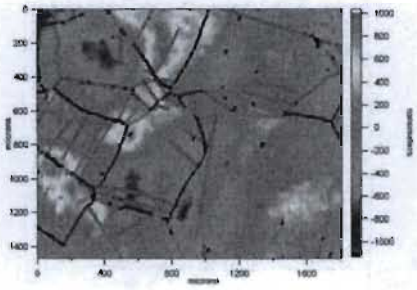
- Strong deviation from planar shock (wave front spreading).
- Void nucleation not necessary exactly at GB, but due to GB.

Cu bicrystal: Σ3 <110> asymmetric GB



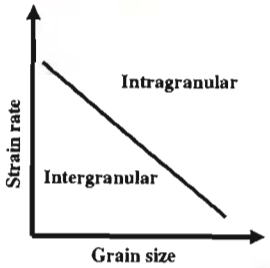


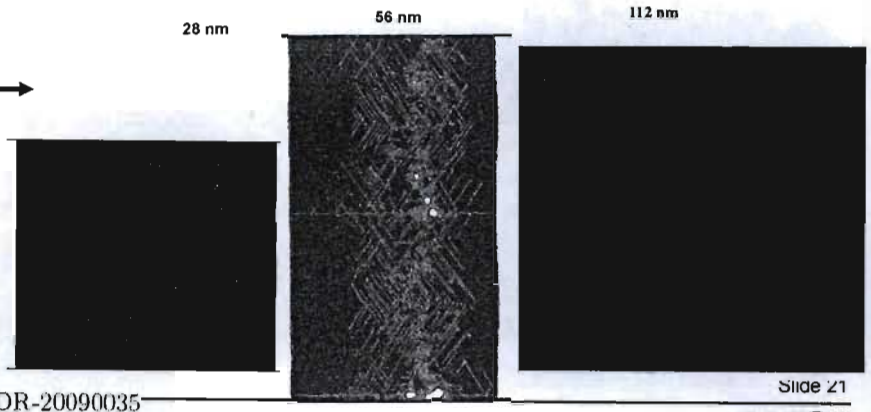




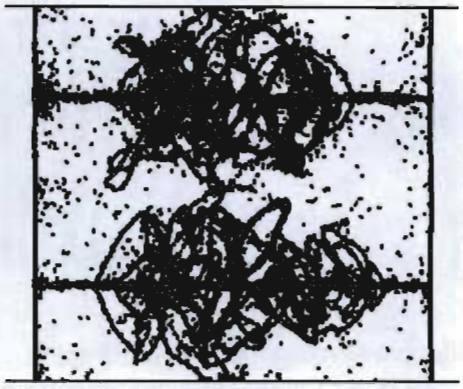
- Differential movement of different grains due to elastic/plastic anisotropy and their interactions.
- Such spatial variations can be modeled or measured with 2D dispalcement interferometry or proton radiography (pRad).

Cu bicrystal: Σ11 <110> symmetric GB





Cu bicrystal: Σ11 <110> symmetric GB



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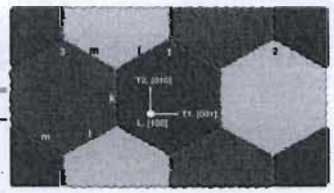
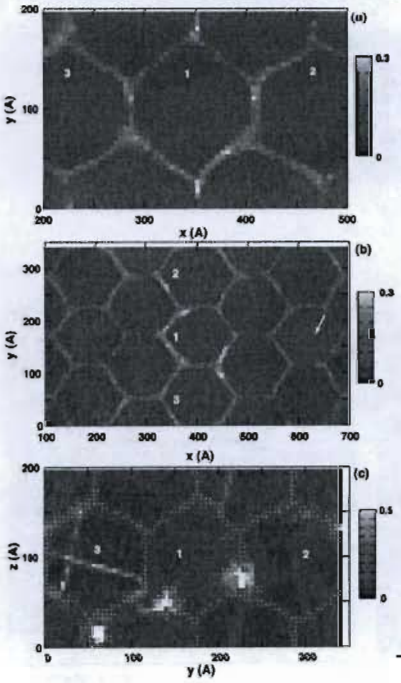
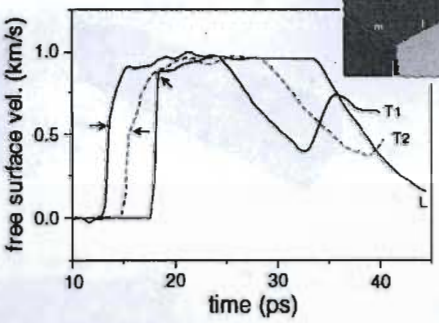
Columnar nanocrystalline Cu





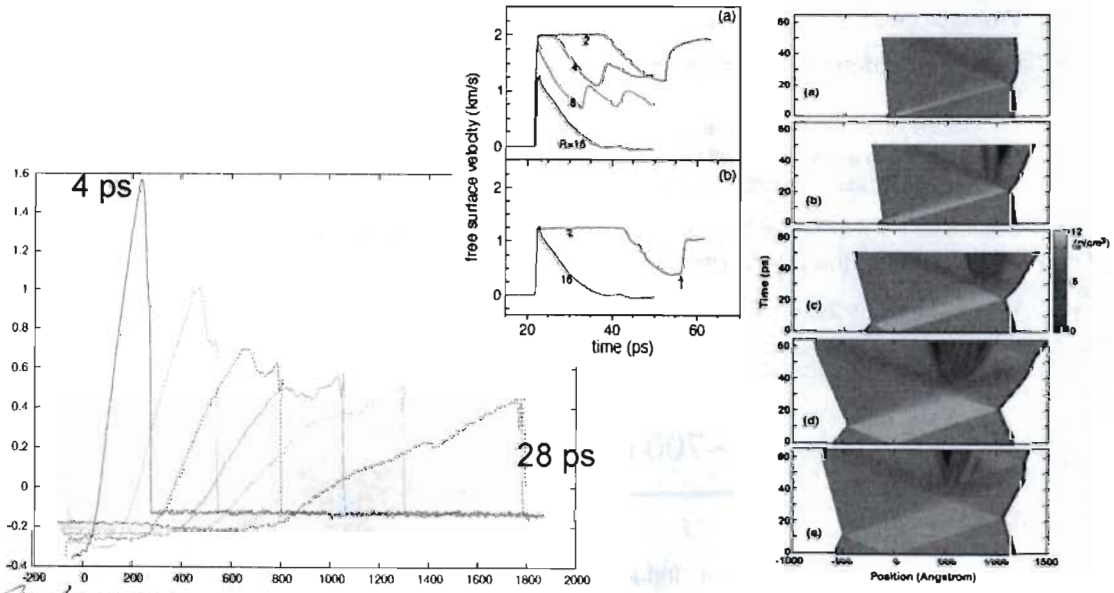


- Plasticity: GB "accommodation" and crystal plasticity.
- Void nucleation: GB and triple junctions.
- Strong anisotropy in plasticity and spall damage.

Loading dependent

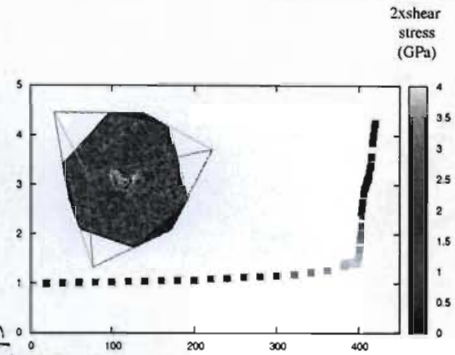
- Loading geometry: bicrystals, columnar crystals.
- Load pulse width: Taylor vs. square
- Rate
  - Change length of flyer plate and target (limited).
  - Void growth rate @ a given load.
    - Conventional MD (ns regime).
    - Accelerated MD (us regime).

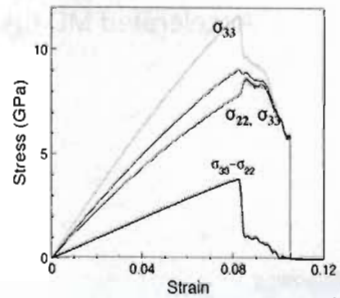
Taylor wave vs. square wave loading



Void growth: rate dependence

- 30x30x30 repeating unit cells (108,000 atoms).
- Void diameter = 2 nm; 336 atoms.
- 150 K, strain rate $2x10^8$ s^{-1}.
- ``spall" strength ($\sigma_{33,max}$), and yield strength at critical strain.



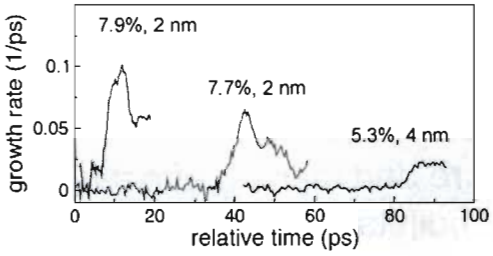


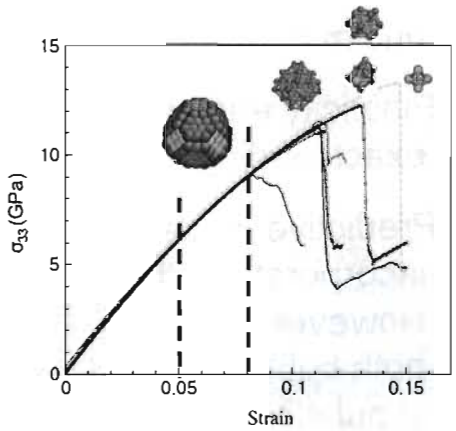
AMD results for void growth

- We explore $2x10^5$ – $2x10^7$ s^{-1}.
- The transition-state dynamics shows back-and-forth crossing around the saddle point.
  - Interesting from theoretical point of view, e.g., reaction rate. We are still in the process of achieving a full understanding.
  - Useful for the embedding technique.
- Similar to conventional MD, we can determine the critical strain (stresses) at the onset of the plastic growth.
- We are in μs-regime.

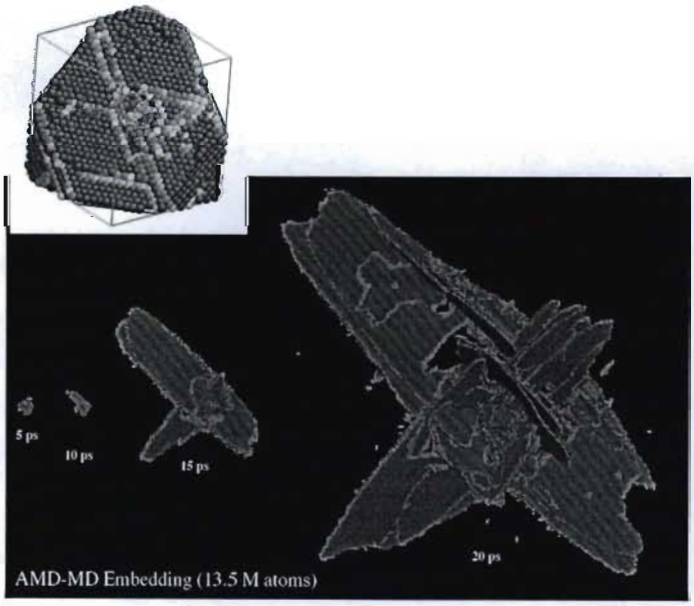
13-vacancy void, 300 K, $2x10^5$ s^{-1}.

Early void growth at constant load (strain)





Later dynamics of void growth embedding



Conclusion

- Microstructure plays a vital role in plasticity and void nucleation.
- Plasticity and spall damage may strongly depend on exact loading.
- Predictive models for deformation and damage should incorporate both microstructure and loading effects. However, there are no silver bullets: we need to exploit both bottom-up and top-down experimental and simulation approaches to bridge gaps in spatial and temporal scales. MD has its critical share.