LA-UR-16-25601
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Intended for: PRICM9, 2016-08-02/2016-08-05 (Kyoto, Japan)

Issued: 2016-07-27

NUCLEATION AND EVOLUTION OF DYNAMIC DAMAGE AT BIMETAL INTERFACES USING MOLECULAR DYNAMICS

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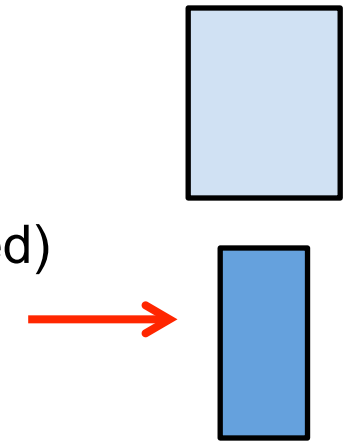
NNSA

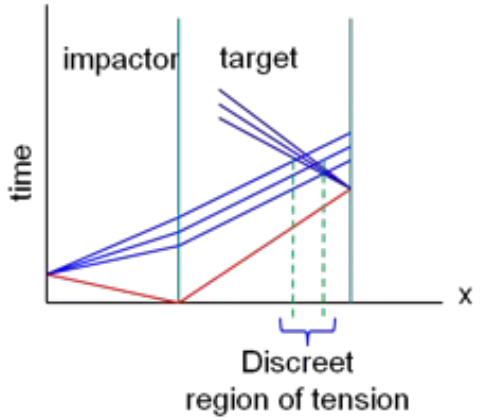
Materials Response in a Dynamic Tensile Experiment (Spall)

t_0: initial state

t_1: Compressed (shocked)

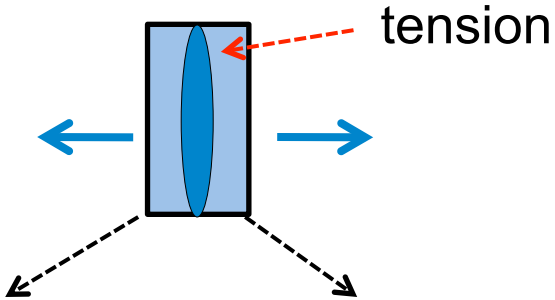
* Δt: Pulse duration (< 1μs)
* $\Delta V \leftrightarrow \sigma_c$(GPa): Peak state





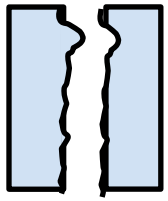
t_2: De-compression

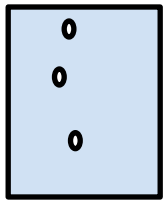
* Release rate

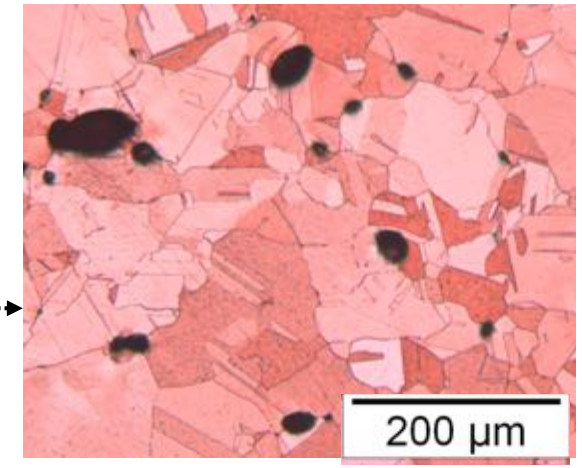


Full **spall**

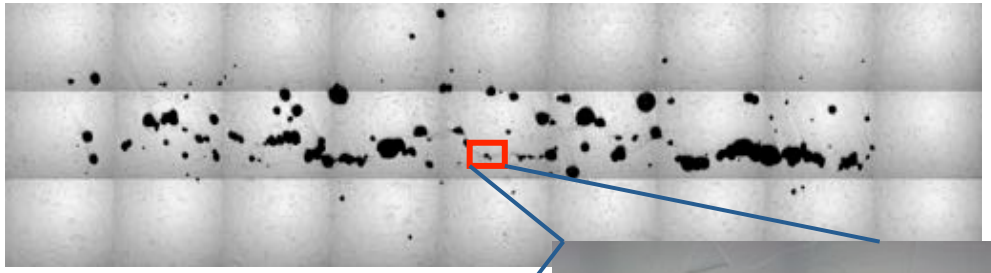
Incipient **spall**



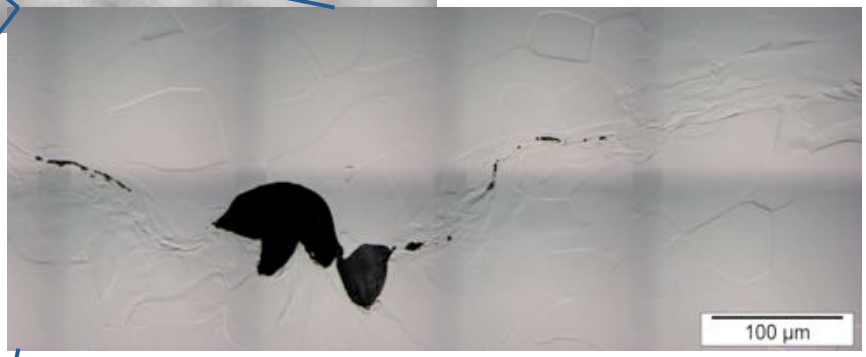




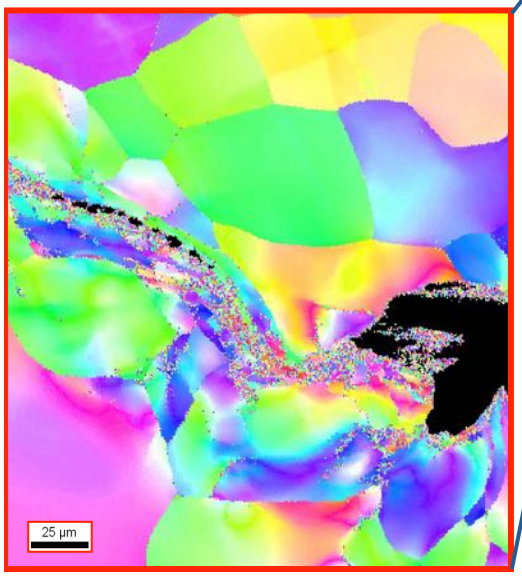
Motivation: Do Not Understand the Role of a Second Phase on Damage Evolution



During shock release, voids nucleate grow and coalesce

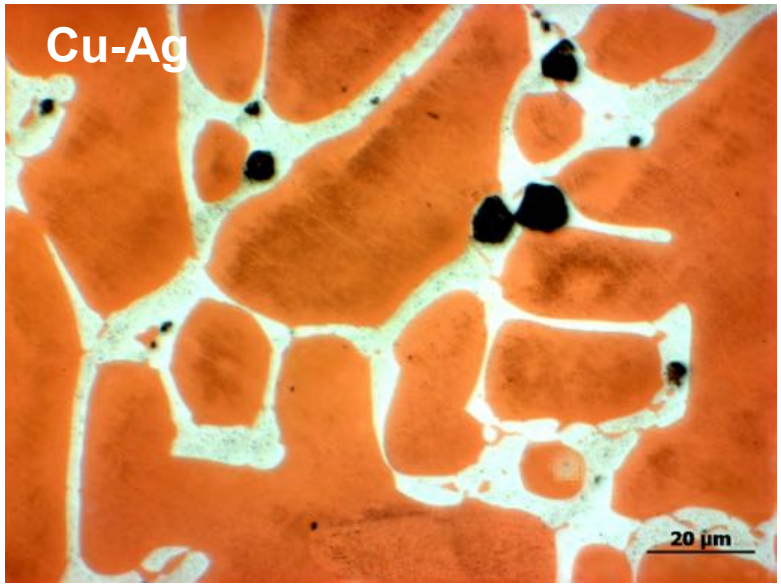


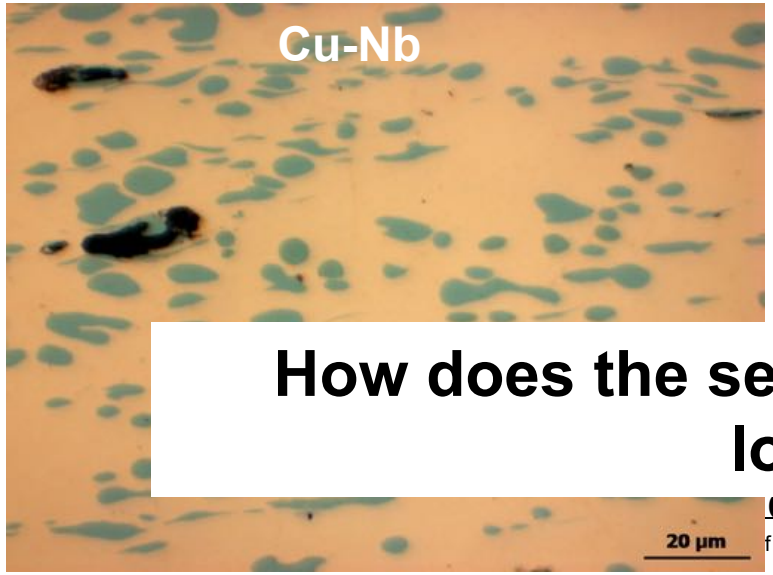
Grain boundaries are possible sites of nucleation

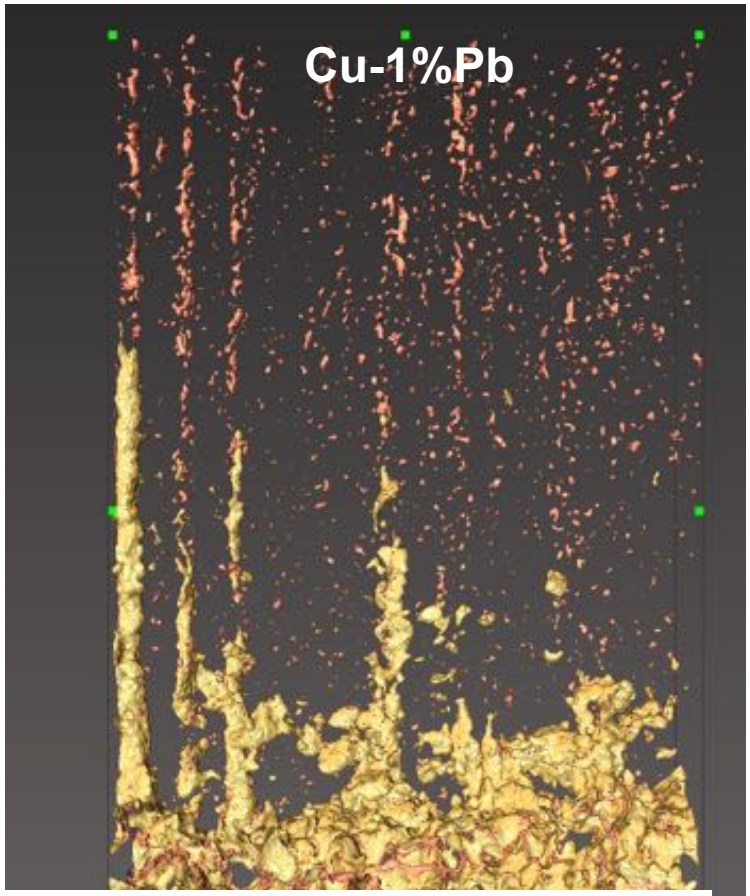


Role of second phase particles, inclusions in comparison to the grain boundaries during defect nucleation

Second Phase can alter the Location of Void Nucleation

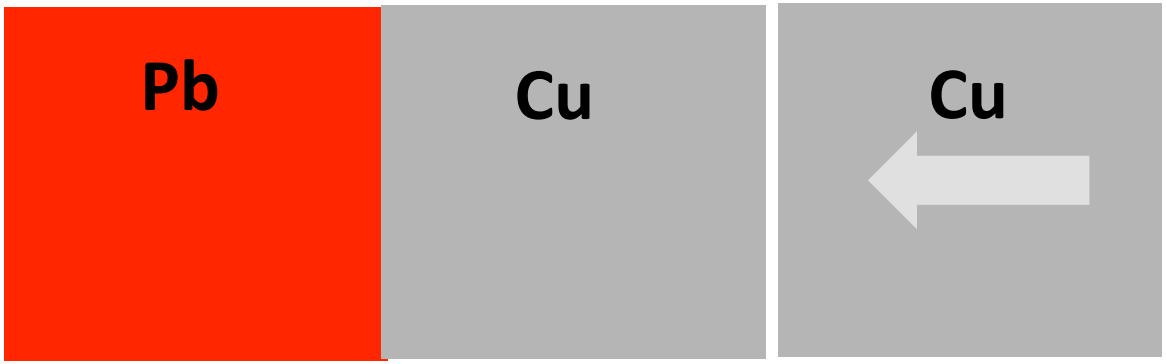






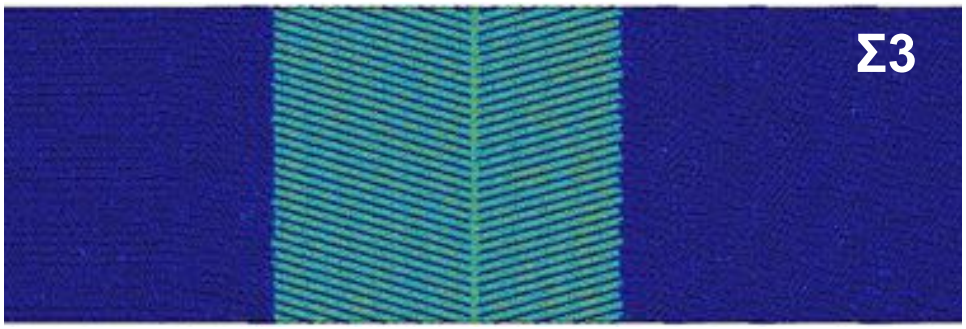
How does the second phase dictate the location?

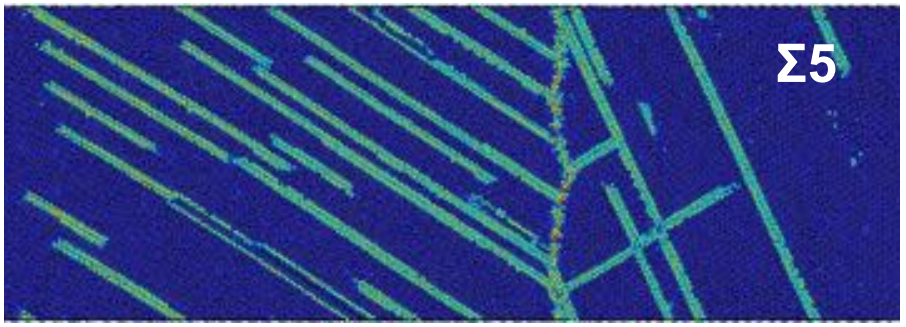
Simulation Details

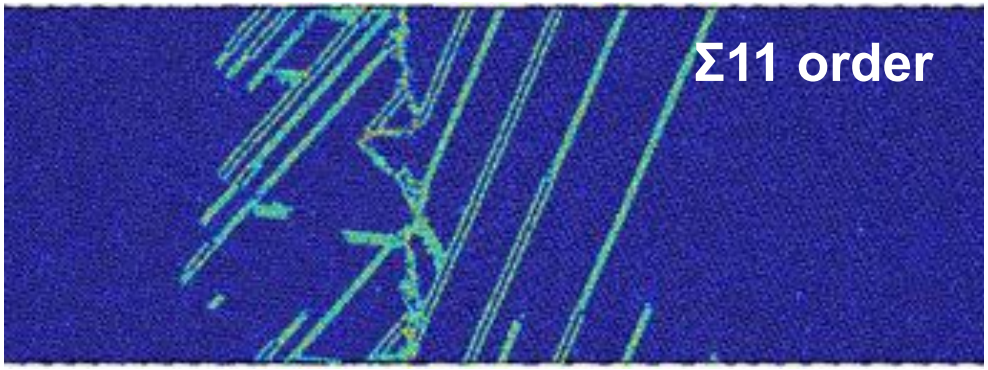


- Molecular-dynamics simulations using LAMMPS
- 6-8 million atoms with free surfaces/vacuum at the edges parallel to the interfaces
- EAM model for CuPb and CuAg
  - CuPb: Mishin Cu, Zhou Pb, Cross-term fit by B. Liu
  - CuAg: Developed by Yuri Mishin
- Plate type impact similar to experiments
- Particle velocities, $u_{p,}$ of 500 m/s
- Shock perpendicular to the interface, spall plane at interface
- Simulations performed at 100 K

Plastic Deformation Affected by Grain Boundary Structure



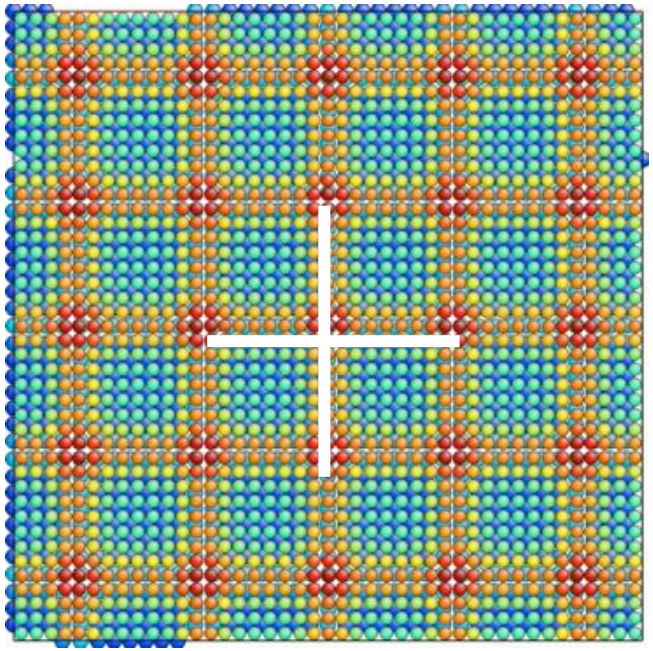




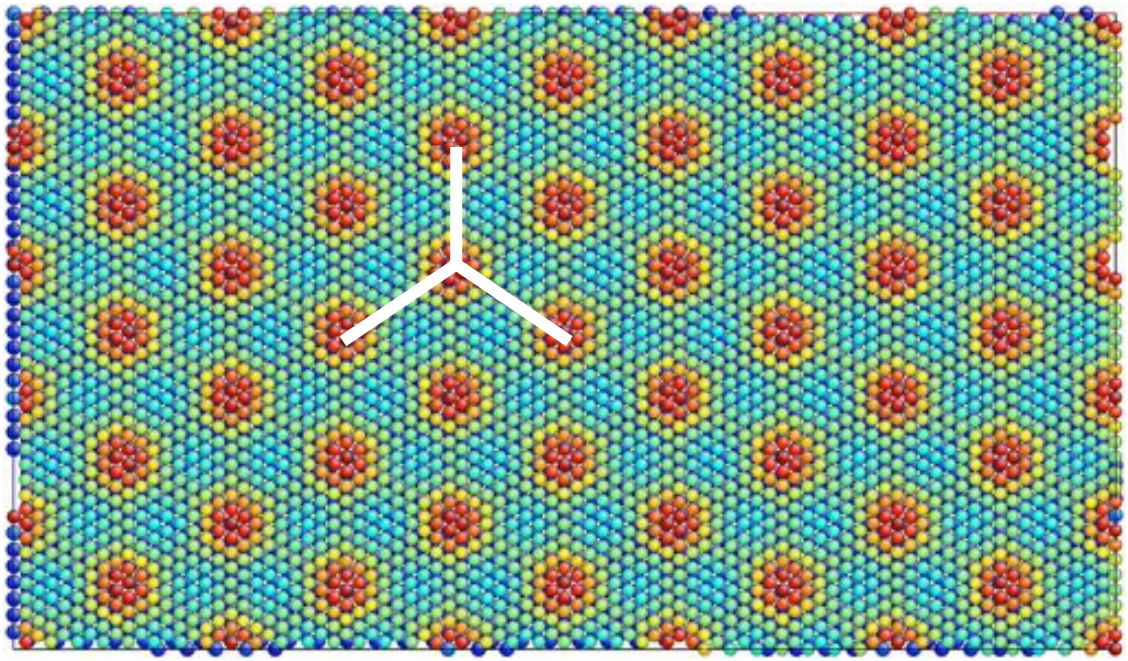
Interfacial Structures and Free Energies for Cu/Ag at 0 K

111: x[11-2]; y[111]; z[1-10]
110: x[1-10]; y[010]; z[-101]

110: 430 mJ/m^2



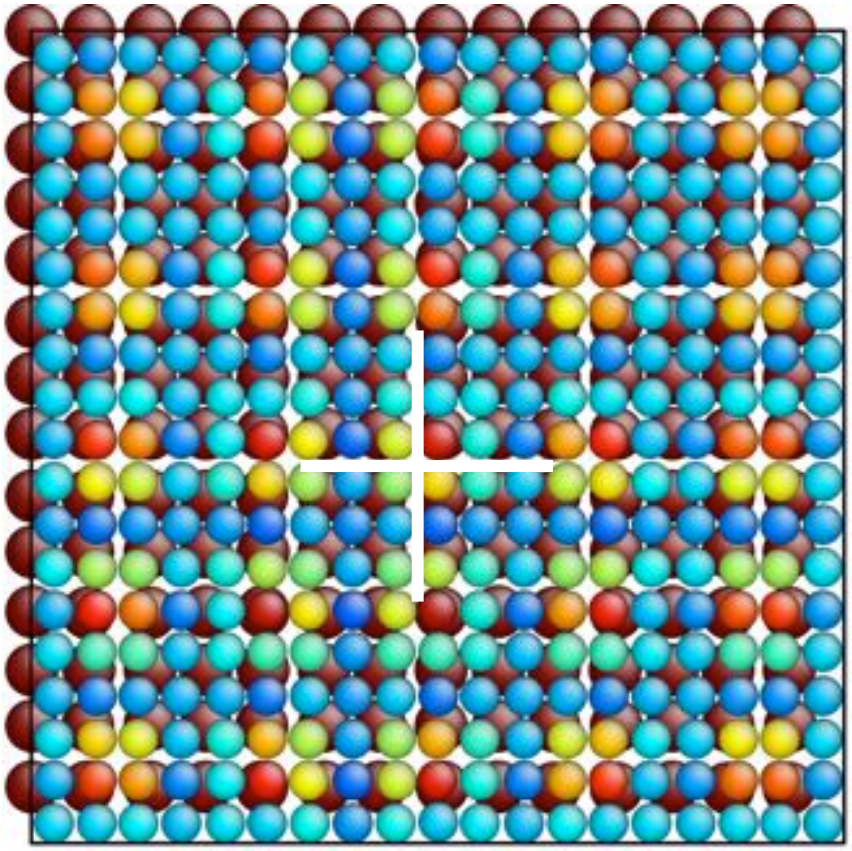
111: 141 mJ/m^2



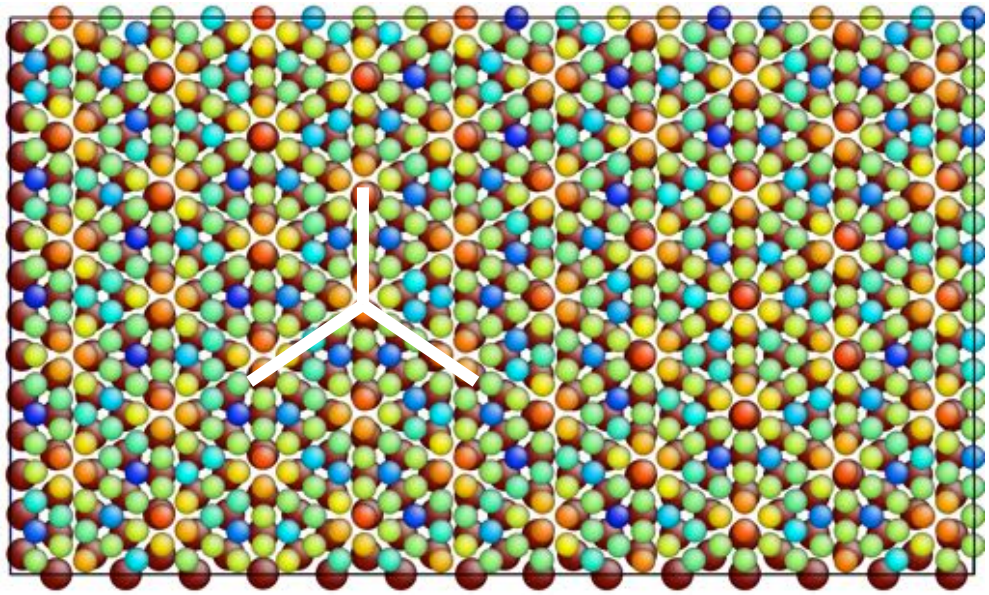
Atoms colored by excess potential energy

Interfacial Structures and Free Energies for Cu/Pb at 0 K

110: 989 mJ/m^2



111:773 mJ/m^2

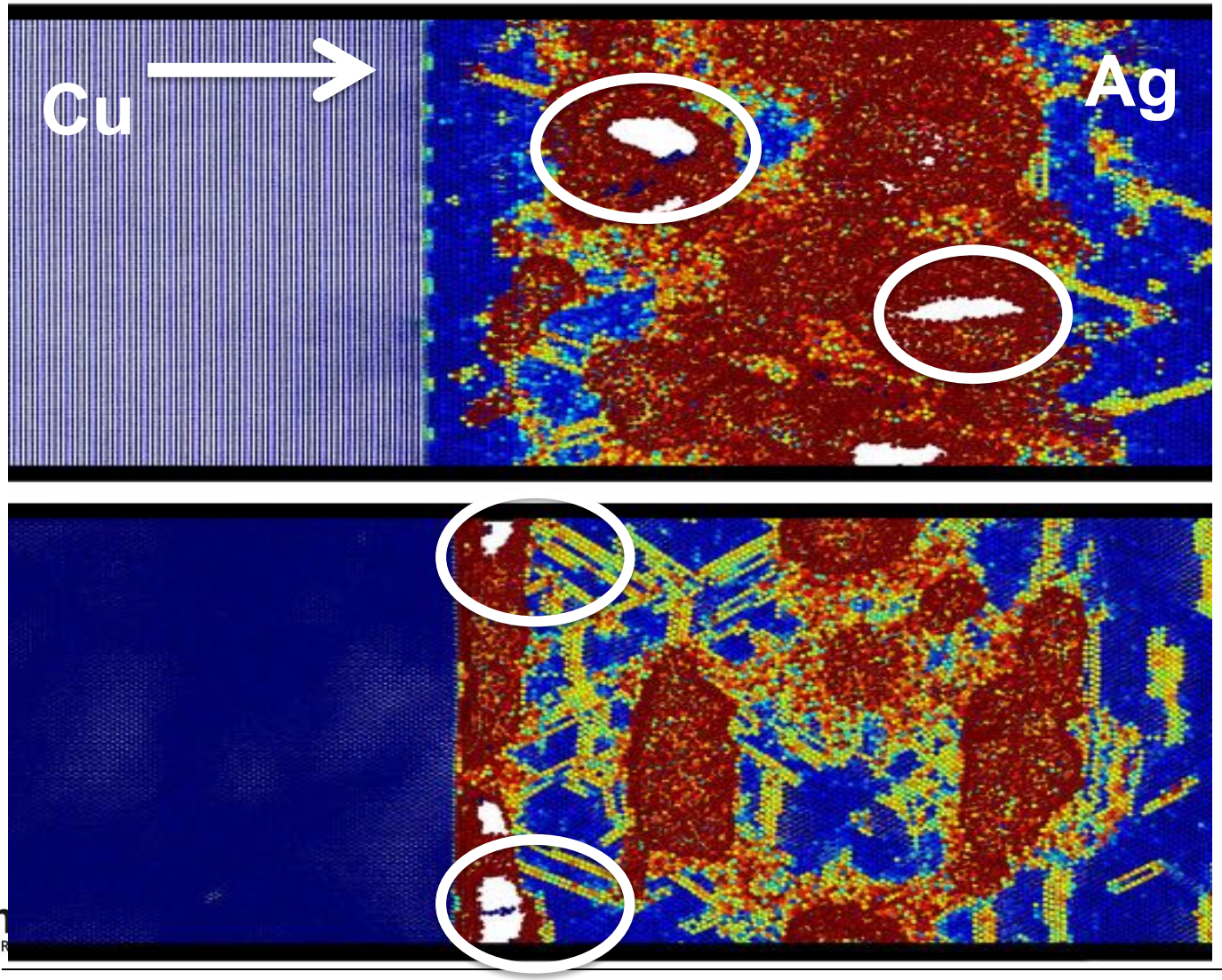


Atoms colored by excess potential energy

Voids Located within Ag in Cu/Ag Independent of Orientation

{111}

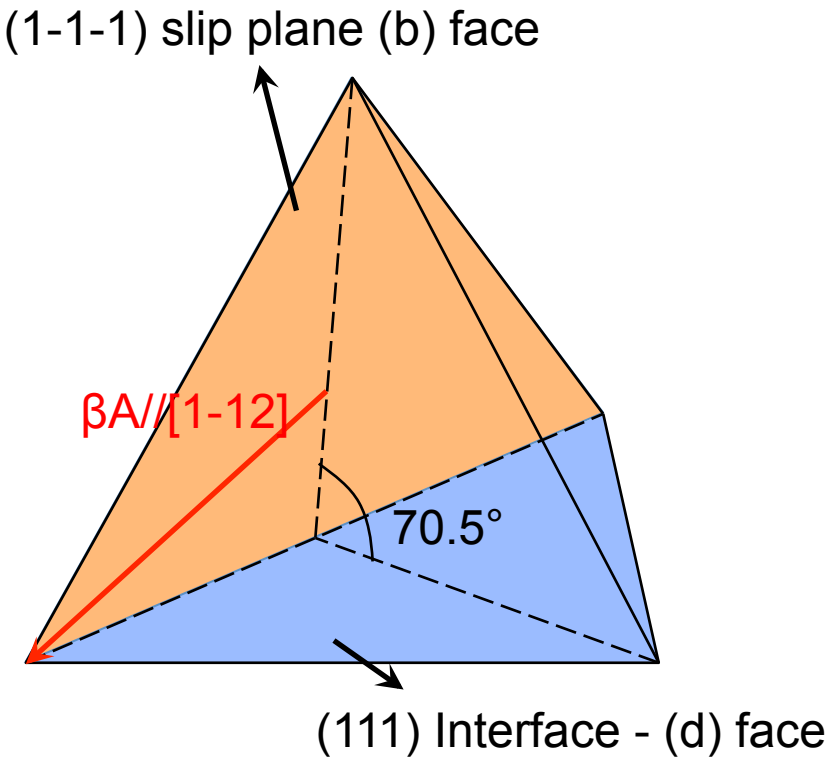
{110}

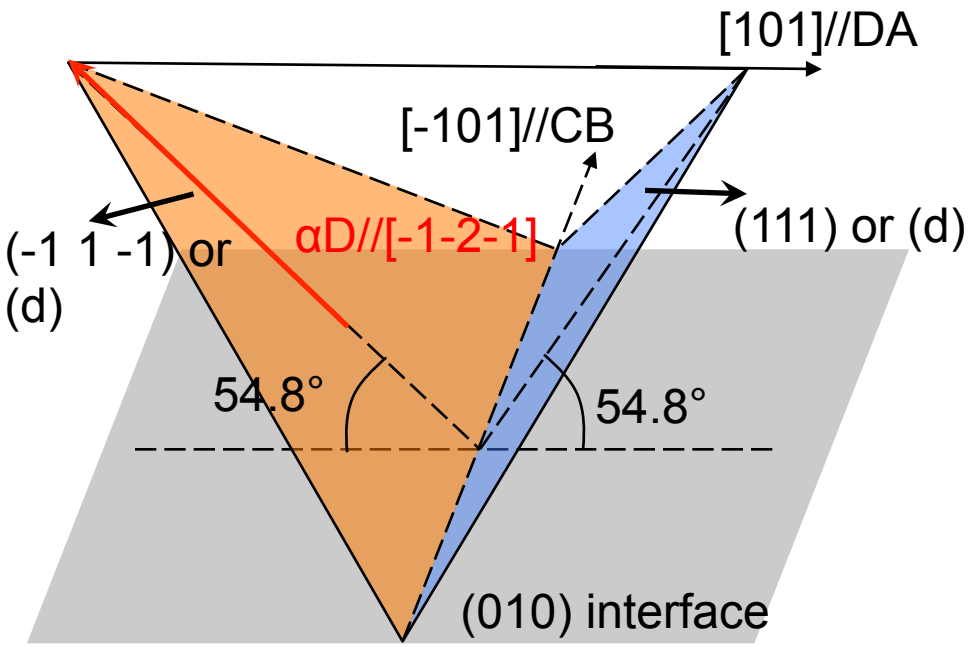


No Plastic Deformation in the {111} Interface under Shock Compression

Plastic Deformation in the {100} Interface under Shock Compression

The Difference in Mechanisms can be Attributed Various Factors

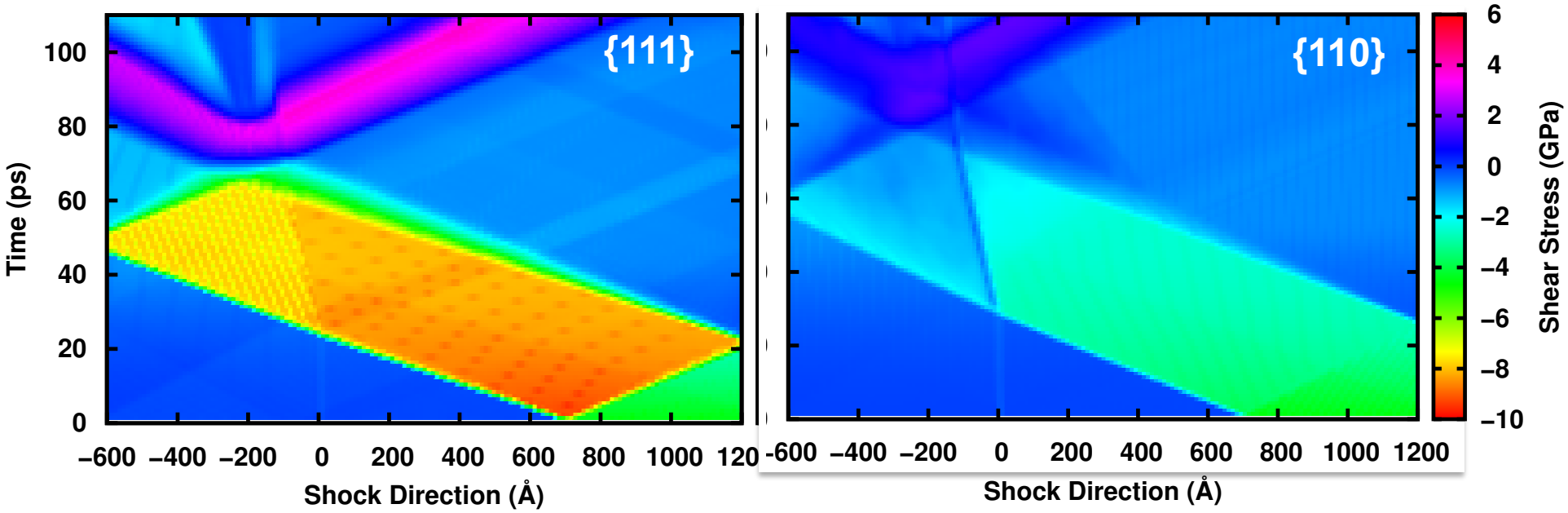




The Schmid factor for load normal to interface plane: **0.157**

The Schmid factor for load normal to interface plane: **0.471**

Differences in Shear Stress as a Function of Orientation

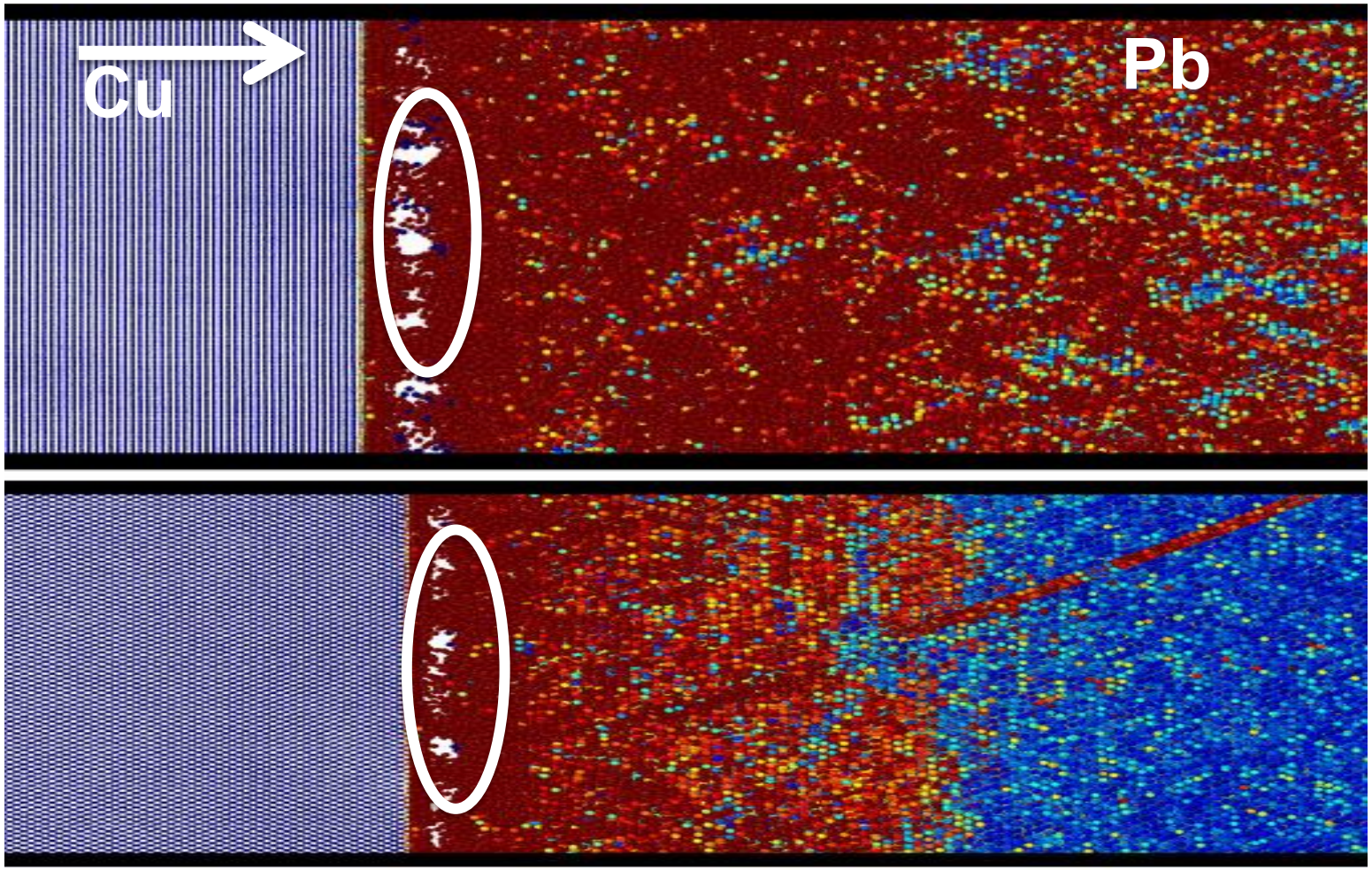


Stress required to nucleate voids in {111} and {110} interface is 11.3 and 10.4 GPa, respectively.

Voids Located within Pb in Cu/Pb Independent of Orientation

{111}

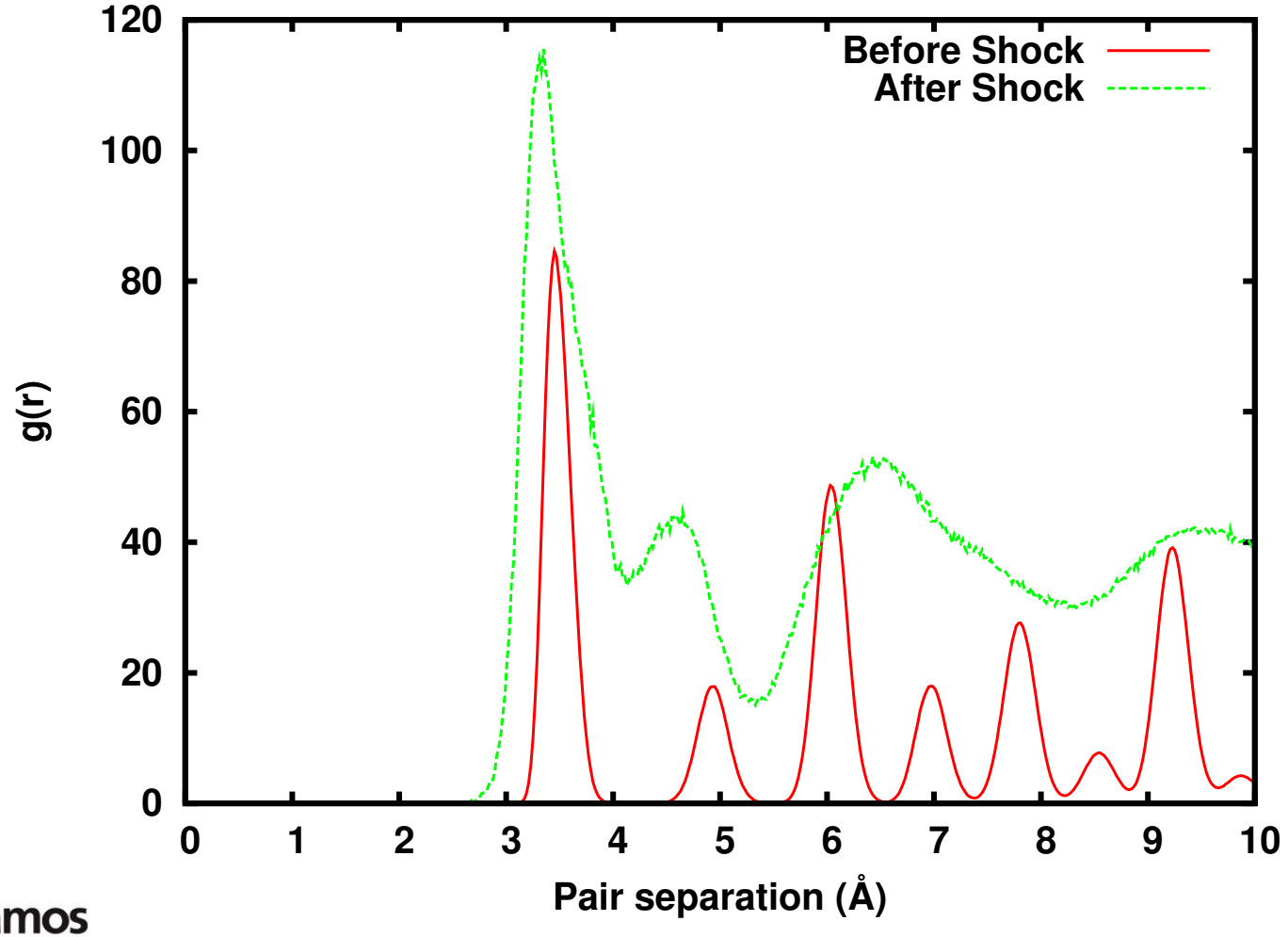
{110}



Low Plastic Deformation of in the {111} Interface under Shock Compression

Plastic Deformation in the {110} Interface under Shock Compression

Solid Pb becomes Disordered during Release Leading to Low Strength



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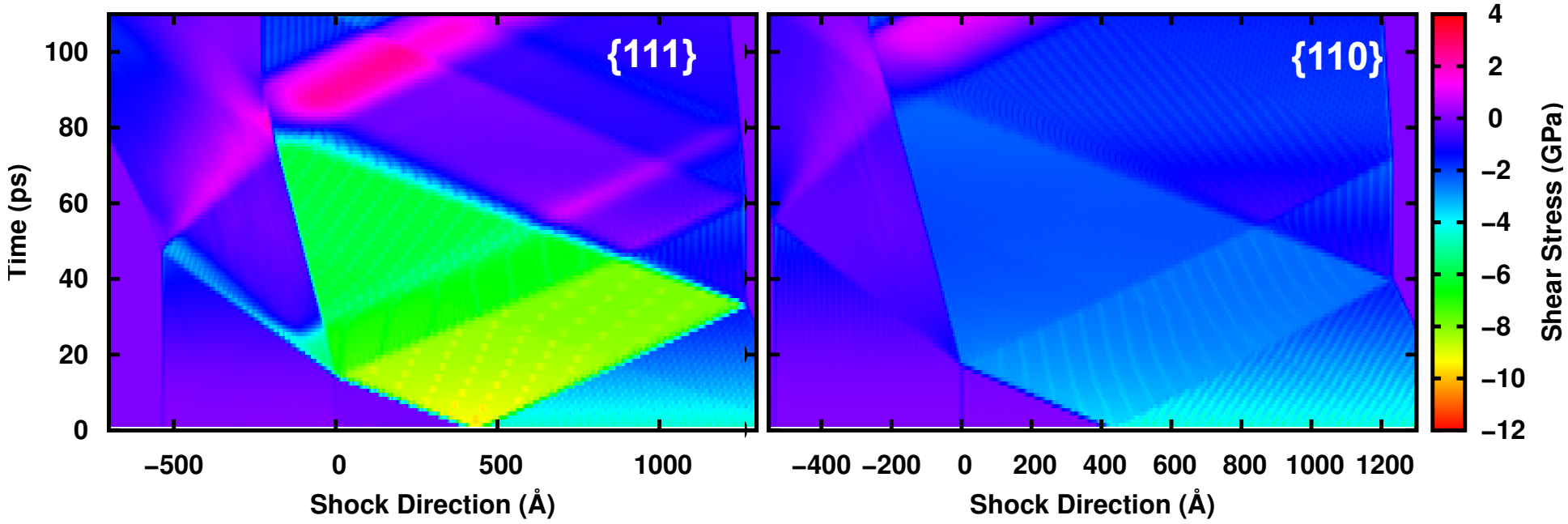
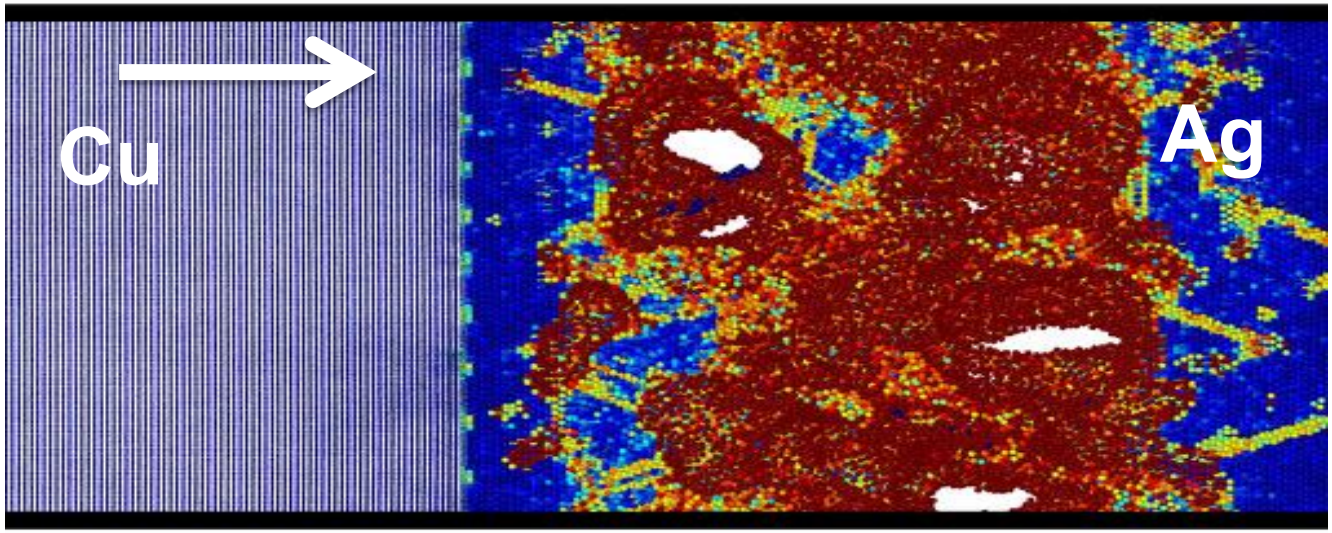
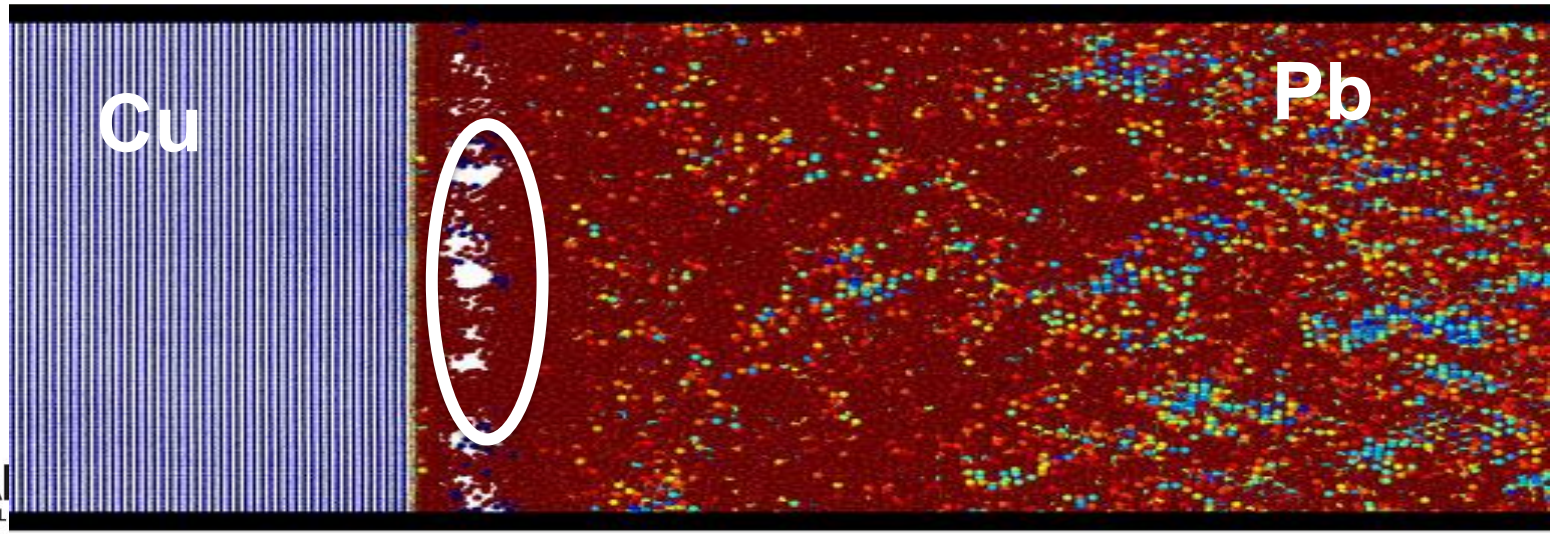
Differences in Shear Stress as a Function of Orientation



Stress required to nucleate voids in {111} and {110} interface is 8.8 and 8.5 GPa, respectively.

Affect of Second Phase Materials on Void nucleation





Conclusions

- The difference in properties between the phases can determine the location for void nucleation.
- The orientation of the interface itself can affect the specific mechanisms for plastic deformation and affect the spall strength of the material.
- The {111} interfaces do not undergo plastic deformation under compression in comparison to the {110} interfaces.
- This could be attributed to low Schmid factors associated with that orientation. In addition, the stacking fault energy also plays a role in determining nucleation of dislocations.
- In CuAg, voids nucleate at twin-twin and dislocation intersections within Ag.
- In CuPb, regardless of the orientation void nucleate in Pb because it becomes “superheated” under release.

Questions?