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Title: The Role of the Structure of Grain Boundary Interfaces during Shock Loading

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The Role of the Structure of Grain Boundary Interfaces During Shock Loading

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In order to understand the role of interfaces in the shock tolerance of metals, three specific copper bi-crystal boundaries have been studied under shock loading and incipient spall conditions. These boundaries, two 001/111 boundaries and a 001/001 tilt boundary and their structures have been characterized prior to deformation using both electron back scattered diffraction (EBSD) and transmission electron microscopy (TEM) to obtain their axis/angle pair relationship and the structure at the boundary. This characterization has been utilized as input for MD simulations to examine in-situ dislocation/grain boundary interactions. These boundaries were then shocked at 2.5 and 10GPa in an 80mm gas gun and soft recovered. Post-mortem characterization, EBSD and TEM, has revealed that typical grain boundaries readily form damage during shock loading but the special boundaries ($\Sigma 3$) are resistant to failure. This is linked to differences in slip transmissibility across these types of boundaries.

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Overview

- Background and Goals
- Experimental Procedures
 - Shock loading and Spall Experiments
 - Analysis Techniques
- Analysis of Shock Loaded Cu Grain Boundaries
 - Substructure Damage
 - Grain Boundary Structure
- Analysis of Damaged Cu Grain Boundaries
- Conclusions



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Background and Goals

■ Hypotheses:

1. The atomic structure of an interface controls the absorption, emission, storage and annihilation of defects at that interface.
2. The cohesive strength/mechanical damage evolution behavior of a given interface structure may change at high strain rates

■ Our Goal:

- To show that the response of grain boundaries during shock loading is dependent on structure and not merely upon grain orientation

■ Our Method:

- Shock Cu multicrystals at different peak shock pressures and under different shock conditions
- Investigate the structure of the grain boundaries and substructure of the grains via electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM)



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Background and Goals

■ Why Study the Role of Interface Structure in Copper?

- Copper is a relatively simple, well characterized system
- A controlled sample allowed for a tight study of the role of grain orientation versus boundary structures to be probed
- One of the boundaries easily produced in copper is a $\Sigma 3$ boundary – a boundary that has also been investigated in irradiation environments and has proved to be resistant to irradiation damage
- Such a controlled specimen also allowed for a tight study of generalized and special boundaries

■ Why Pick the Mechanical Extreme of Shock?

- Long history of shock physics research performed at LANL
- Produces large amounts of damage that can induce boundary failure
- Examines a strain rate that is directly relevant to MD



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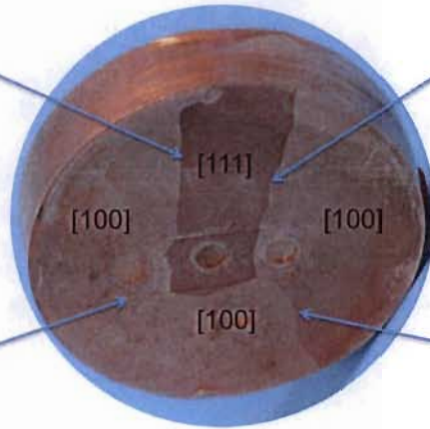
Experimental Procedures

001/111 $\Sigma 3$ Twin
Boundary (60°)

001/111 High Angle
Boundary ($\sim 50^\circ$)

001/001 Tilt
Boundary ($\sim 28^\circ$)

001/001 Low Angle
Boundary ($\sim 2^\circ$)



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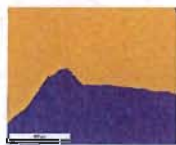
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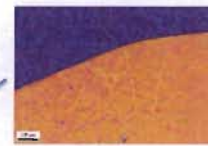
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Experimental Procedures

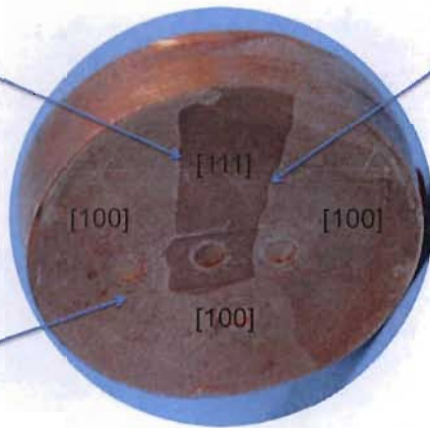
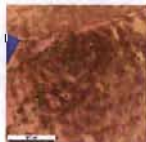


Axis Angle Pair: $60^\circ/[1-1-1]$

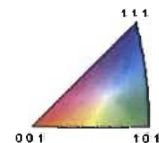


Axis Angle Pair:
 $50.8^\circ/[-24,13,-7]$

Axis Angle Pair: $28.3^\circ/[0-21-2]$



Copper



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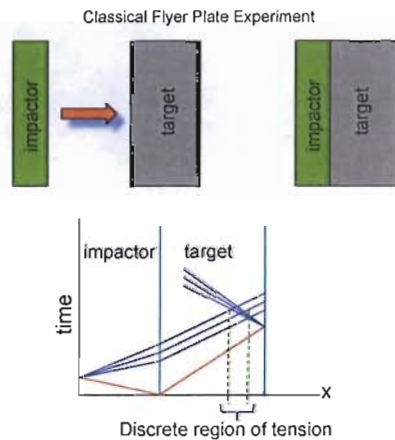
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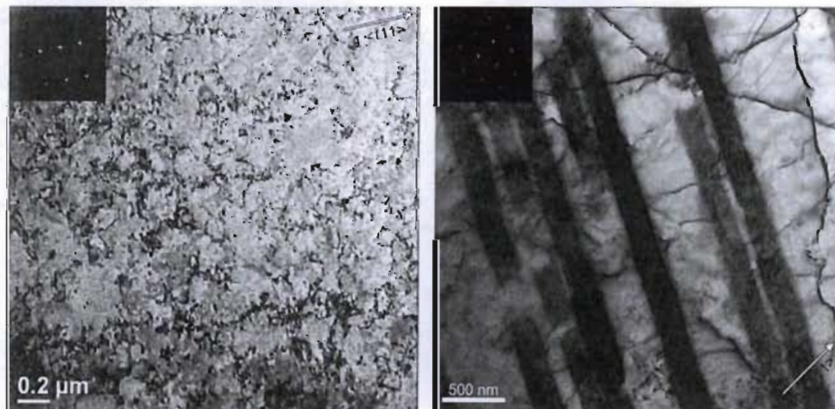
Experimental Procedures

- Shock experiments performed using an 80 mm single stage gas gun
- **Shock Loading Experiment**
 - Peak shock pressure of 10 GPa
 - Soft-recovered and sectioned for post-mortem TEM analysis
- **Damage Experiment**
 - Peak shock pressure of 2.1 GPa
 - Pressure release waves interact within the sample
 - In situ pressure rise measurements taken
 - Soft-recovered and sectioned for post-mortem EBSD analysis



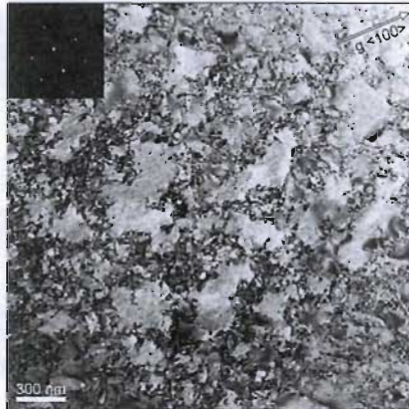
Substructure of Shock Loaded Cu Grains

- 100 Grains:



Substructure of Shock Loaded Cu Grains

- 111 Grains:



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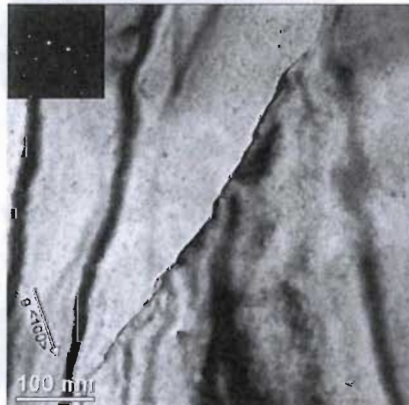
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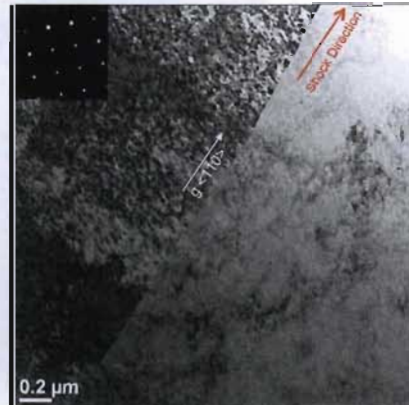
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Grain Boundary Structure of Shock Loaded Cu Grains

- High Angle Boundary ($\sim 50^\circ$)



- Undeformed



- Shocked

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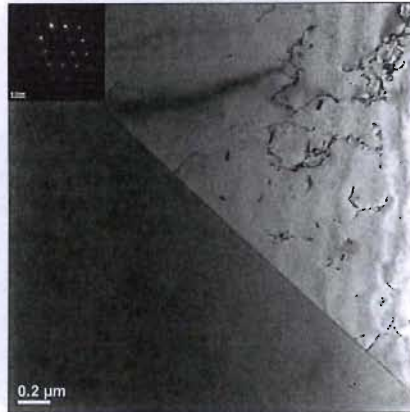
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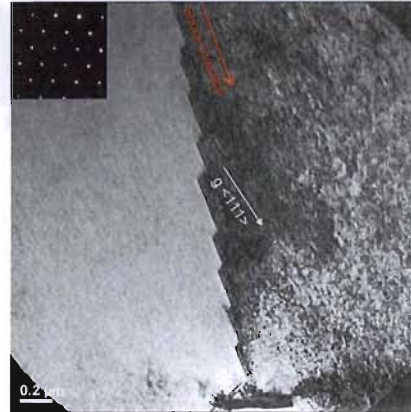
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Grain Boundary Structure of Shock Loaded Cu Grains

■ $\Sigma 3$ Twin Boundary (60°)



- Undeformed



- Shocked

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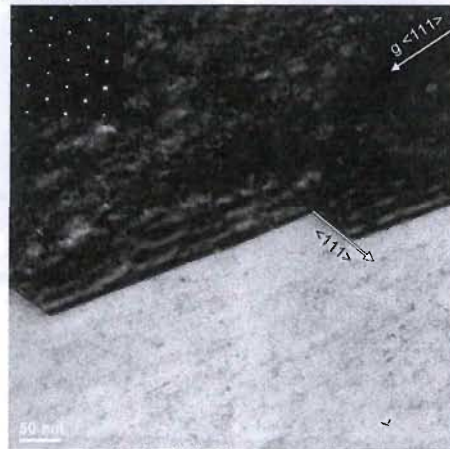
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Grain Boundary Structure of Shock Loaded Cu Grains

■ $\Sigma 3$ Twin Boundary (60°)



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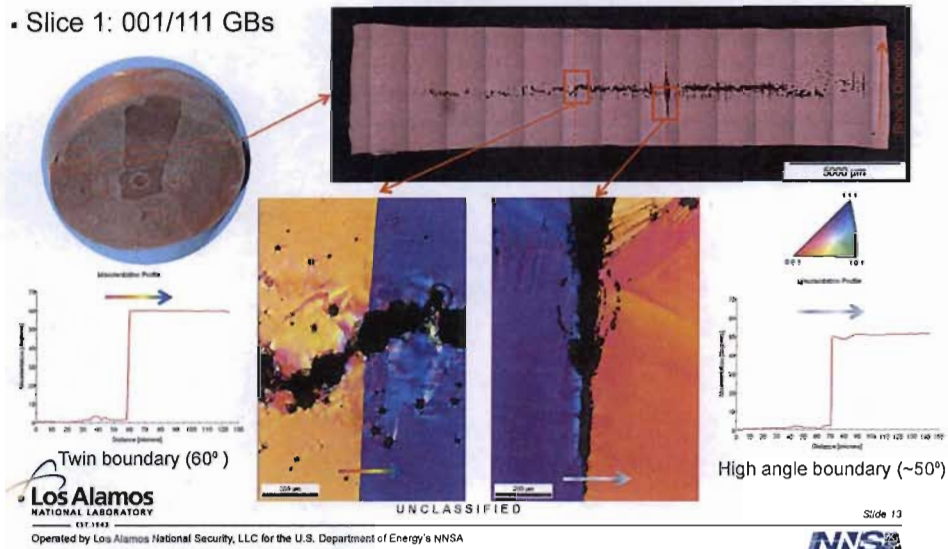
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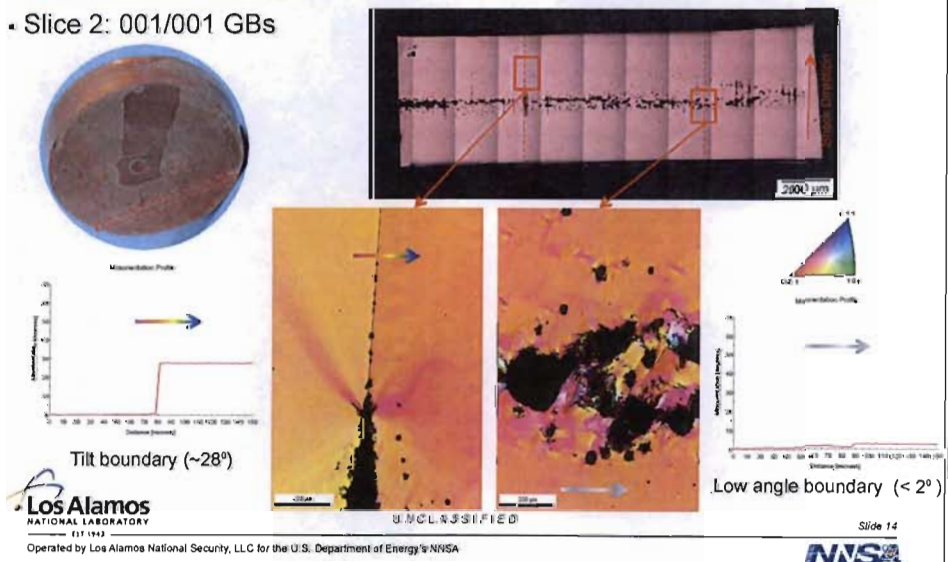
Structure of Damaged Cu Grains

- Slice 1: 001/111 GBs



Structure of Damaged Cu Grains

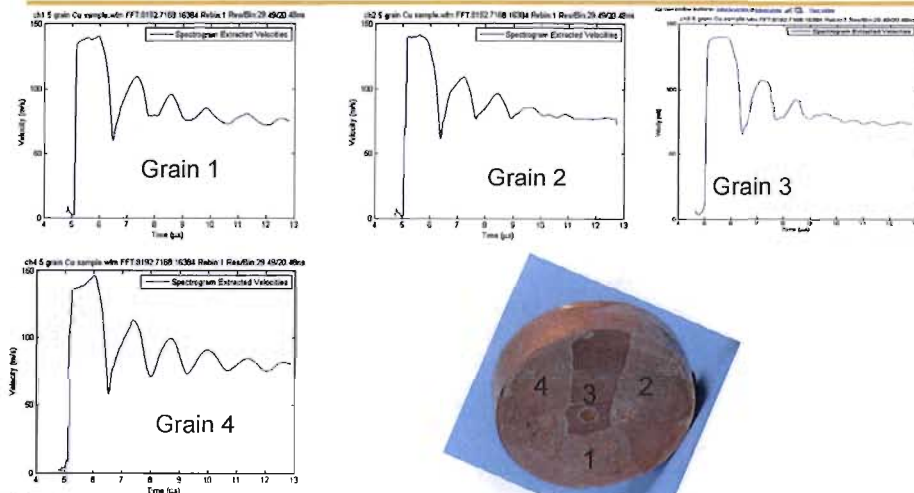
- Slice 2: 001/001 GBs



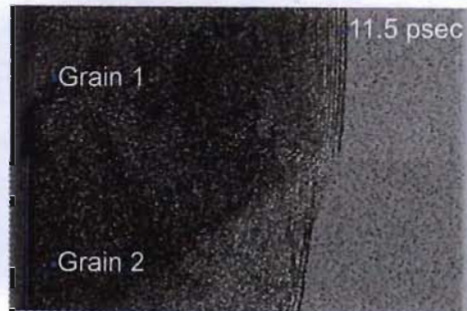
Conclusions

- EBSD analysis shows that certain grain boundaries are resistant to damage and failure
 - Low angle ($<5^\circ$) and special GBs resist void nucleation under spall conditions
- TEM of shock loaded Cu specimens shows distinct jogging of the $\Sigma 3$ grain boundary along slip planes
 - May be an alternate stress release method, possibly explaining resistance of the $\Sigma 3$ boundary to failure
- Overall, results show that grain boundary structure, and not just grain orientation, strongly affect strength and damage evolution at grain boundary interfaces

Damage Experiments Measure Shock Velocity in Each Grain



Simulation of the $\Sigma 3$ Boundary Reveals Details of the Propagating Shock Front and Boundary Motion



- Common neighbor analysis:
- Suggest partial dislocation mediated GB motion
- Particle velocity (shock direction):
- Two shock fronts have different propagation speeds
- Shock front in grain 1 is inclined to the piston velocity direction, whereas in grain 2 the shock front stays in the same direction



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