LA-UR- 11-01299

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Title: Structure and Shock Response of a Sigma 11 Asymmetric Tilt Grain Boundary in Copper at Finite Temperature

Author(s): Saryu J. Fensin, Mark Asta, Richard Hoagland, Ellen Cerreta and Steven Valone

Intended for: TMS 2011, San Diego

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Structure and Shock Response of a Σ11 Asymmetric Tilt Grain Boundary in Copper at Finite Temperature

Saryu Fensin[1], *Mark Asta*[2,3], *Richard Hoagland*[1], *Ellen Cerreta*[1] *and Steve Valone*[1]

1. *Material Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM*
2. *Department of Chemical Engineering and Materials Science, University of California, Davis, CA*
3. *Department of Materials Science, University of California, Berkeley, CA*

Grain boundaries play an important role in governing the microstructure and deformation evolution in a material. Hence, it is important to understand the structure of grain boundaries that are subjected to high homologous temperatures. Boundaries that are susceptible to extreme structural disorder as the temperature is increased might drastically change the dynamic damage in a material under shock loading conditions. In this talk we will present the results of molecular dynamics simulations studying the temperature dependence of the structure of an asymmetric tilt grain boundary in copper. At high homologous temperatures a grain boundary can either form a disordered structure or can completely premelt. The change in grain boundary structure can be drastic enough to alter its response to an applied external force. The nature of the structural disorder in the grain boundary will be investigated by using the grain boundary width and its resistance to an applied shear strain.

NOTE: Slides 11 and 12 have movies showing shock simulations of pure copper

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Saryu Fensin[1], Mark Asta[2], Richard Hoagland[1], Ellen Cerreta[1] and Steven Valone[1]

Collaborators: Juan Escobedo-Diaz[1] and Alex Perez-Bergquist[1]

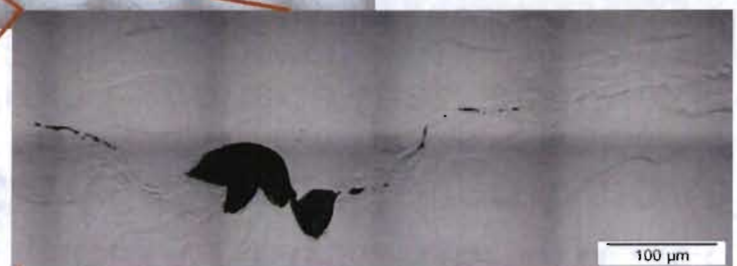
1. MST-8, Los Alamos National Laboratory, Los Alamos, NM
2. Department of Materials Science and Engineering, University of California, Berkeley

This Research was supported by the Office of Basic Energy Sciences and Advanced Simulations and Computing Program, US Department of Energy

Joint Munitions, Advanced Simulation and Computing

Motivation

- During shock release, voids nucleate, grow and coalesce



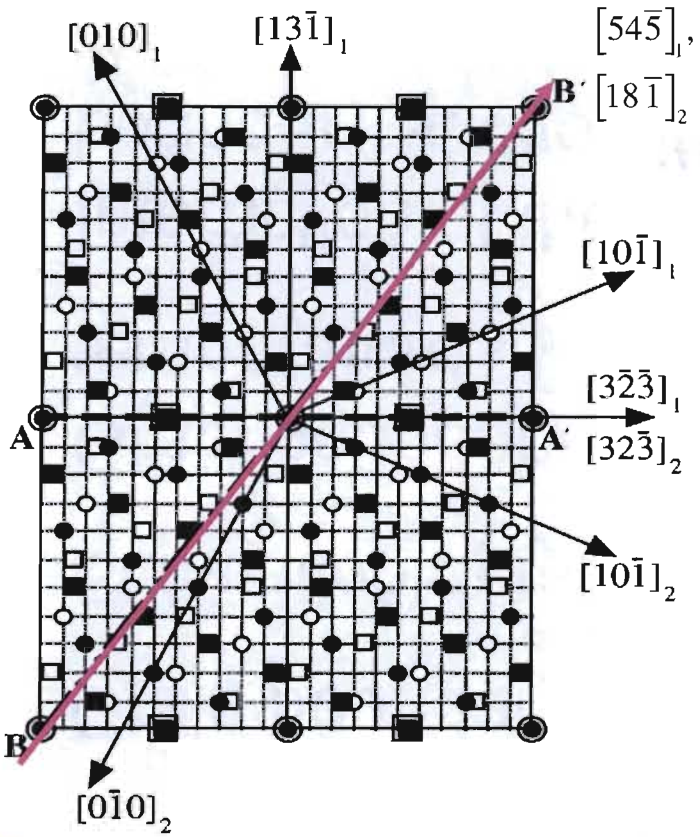
- Grain boundaries possible sites of nucleation

- In order to predict shock and shock release responses, it is important to understand the interaction of shock waves with grain boundaries

Outline

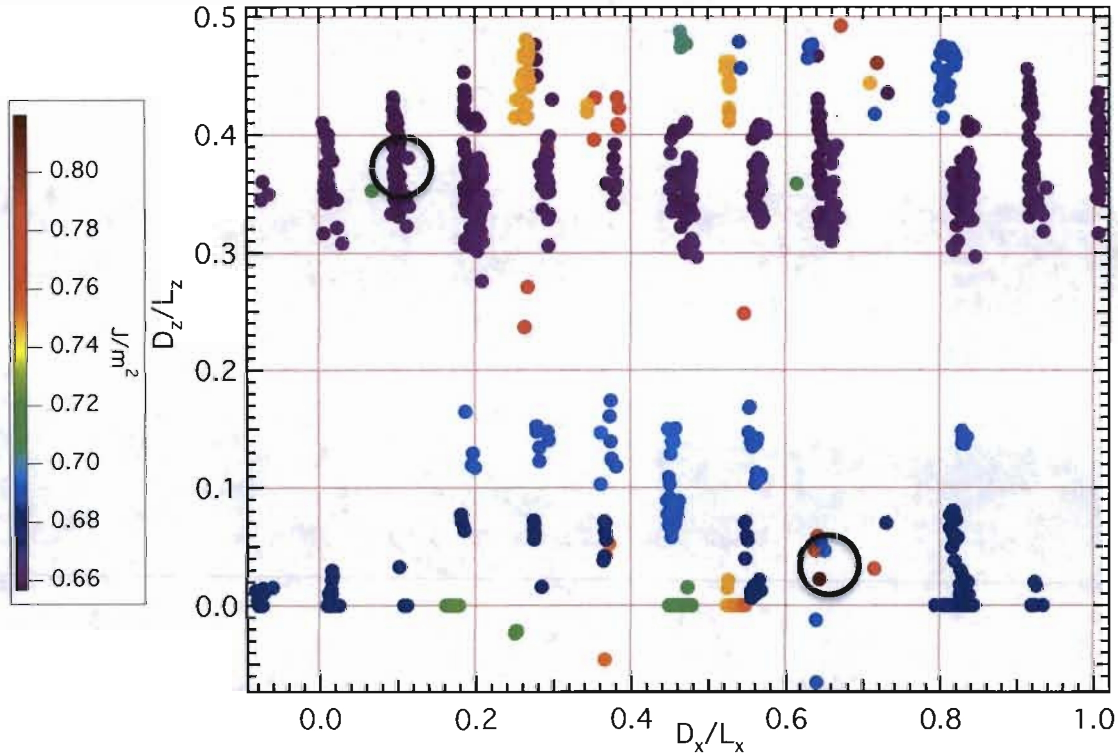
- Grain boundary crystallography
- Simulation details
- Grain boundary structure as a function of temperature
- Interaction of the shock wave with a grain boundary at two different temperatures

Grain Boundary Crystallography



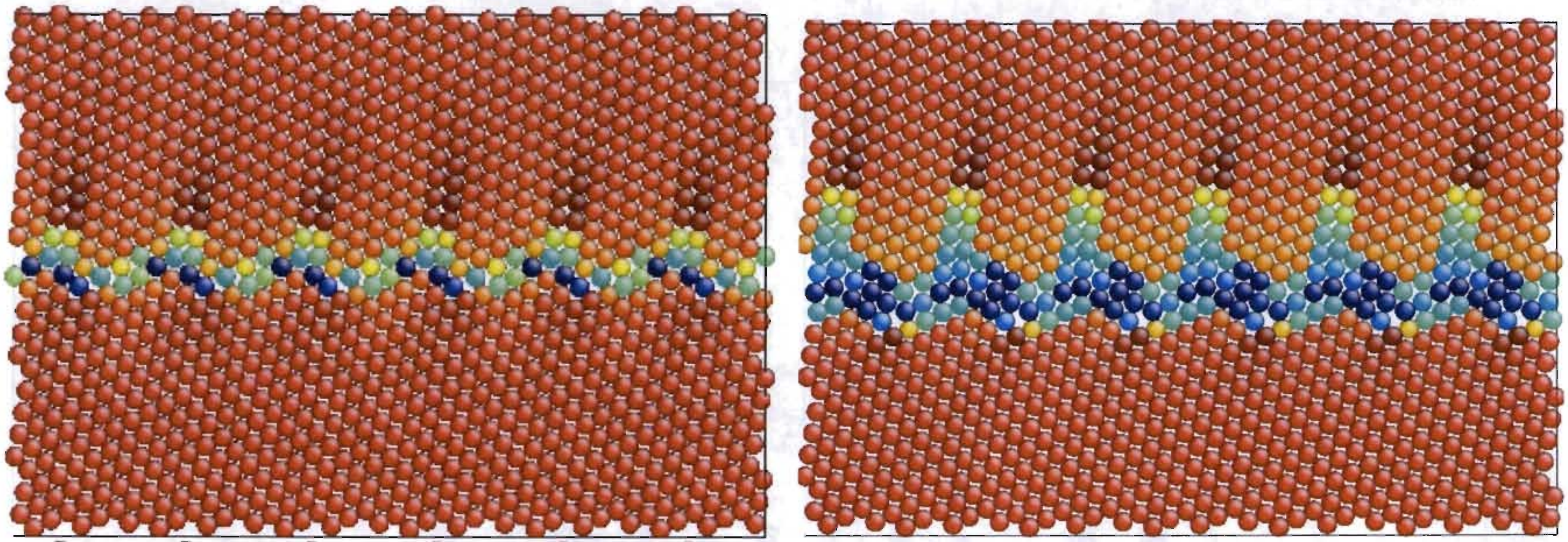
- Σ11 asymmetric tilt grain boundary
- Grain boundary plane parallel to {252} plane in one grain and {414} in the other
- Boundaries parallel to AA' are symmetric while those parallel to BB' are asymmetric
- Grain-boundary plane will be denoted as the x-z plane
- Dimensions of boundary unit cells: L_x =14.7 Å and L_z= 2.6 Å

Local Energy Minima Versus Relative Displacement of Grains



- Multiplicity of states & energies available to boundary at zero temperature
  - Purple points represent energy minima
  - Separated by a distance of 1.32 Å = |b|

Zero Temperature Structure



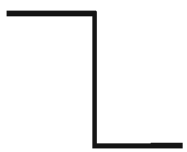
The atoms are colored by the order parameter where red color represent atoms in either of the two grains and blue color shows atoms that are disordered.

Grain Boundary Width

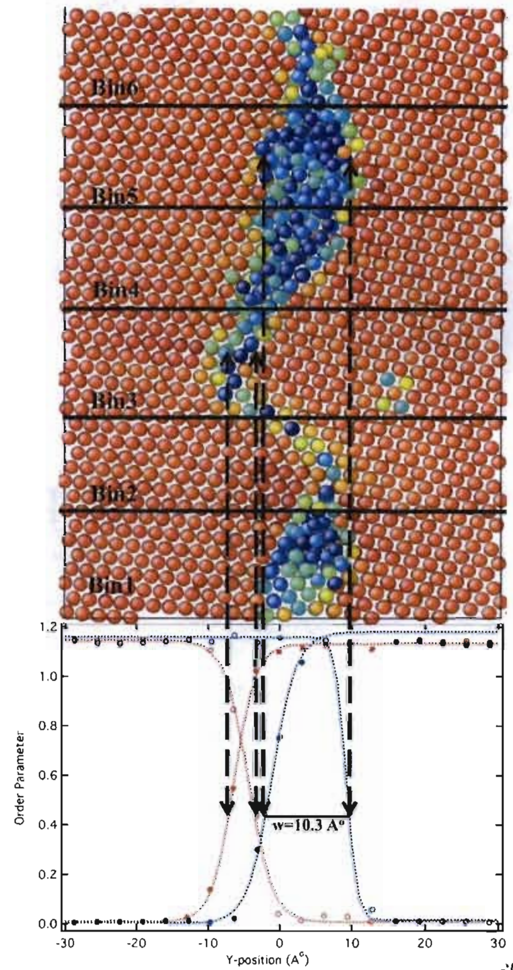
Shear Effect

Position of BUCs

Impedance mismatch

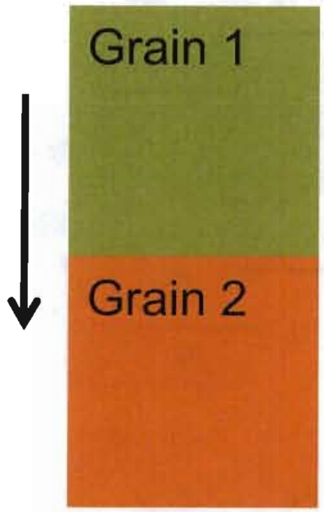


Temperature jump

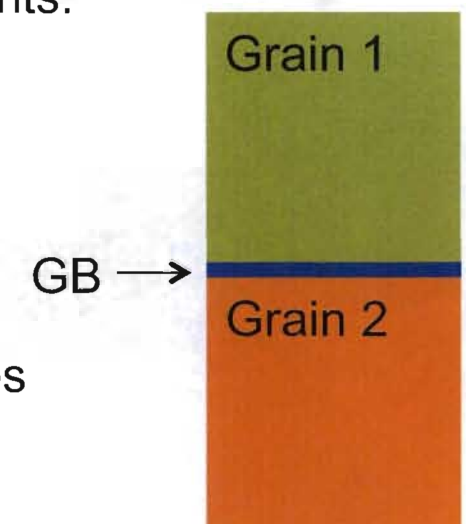


Impedance mismatch

$z = \rho_0 u_s$ where z is impedance mismatch, ρ_o is density of the GB and u_s $\approx c_L$ (longitudinal sound speed) when u_p is small.

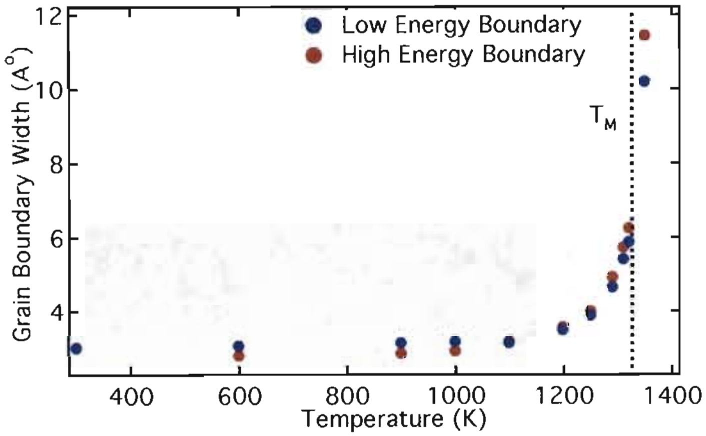


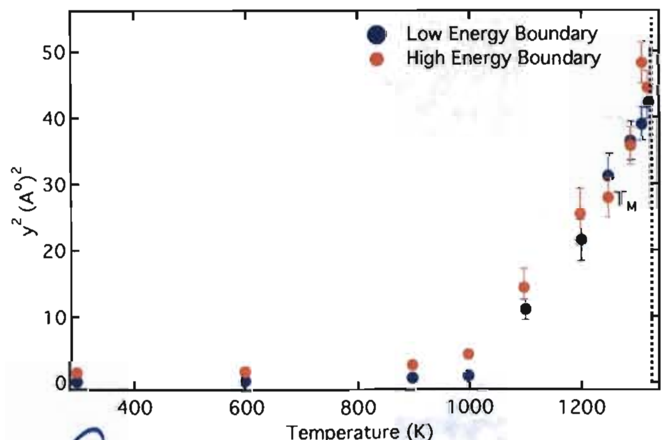
- Density similar in both grains.
- Particle velocity (u_p) in each grain depends on the elastic constants in the shock direction.
- Difference of 4% between elastic constants.

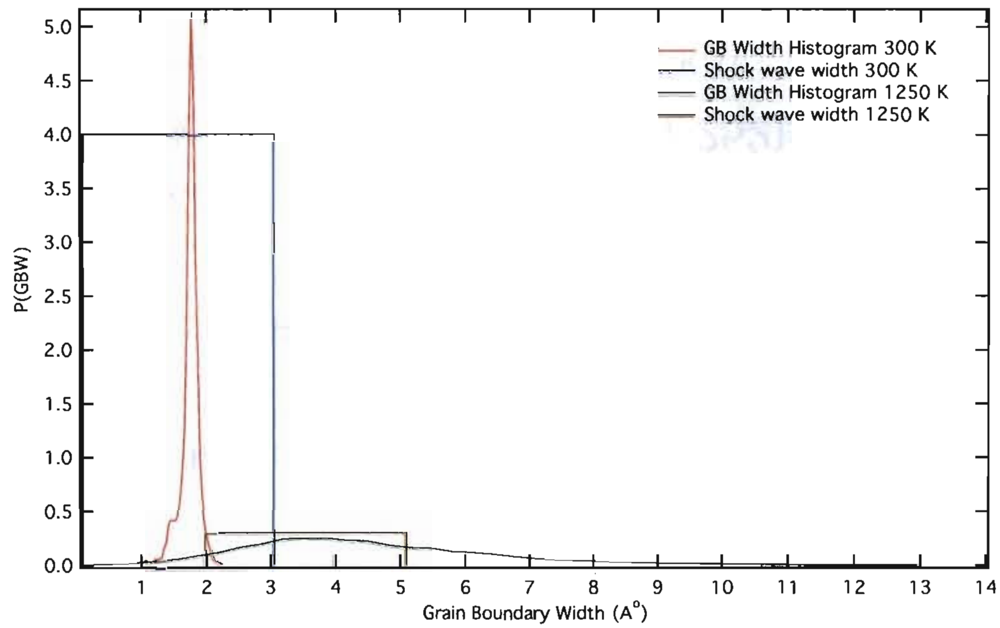


- ρ_o and c_L different at the GB as compared to bulk
- Interested in state of GB after the shock wave passes

Quantitative Analysis of GB structure as a function of Temperature







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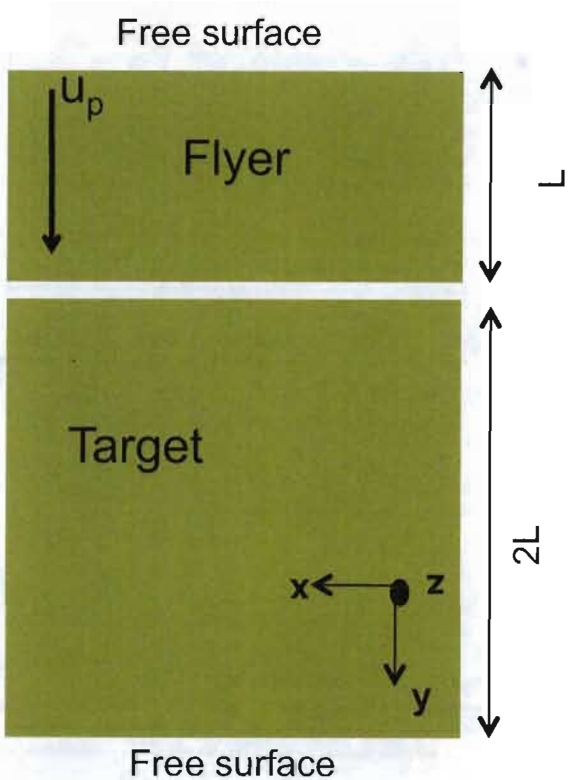
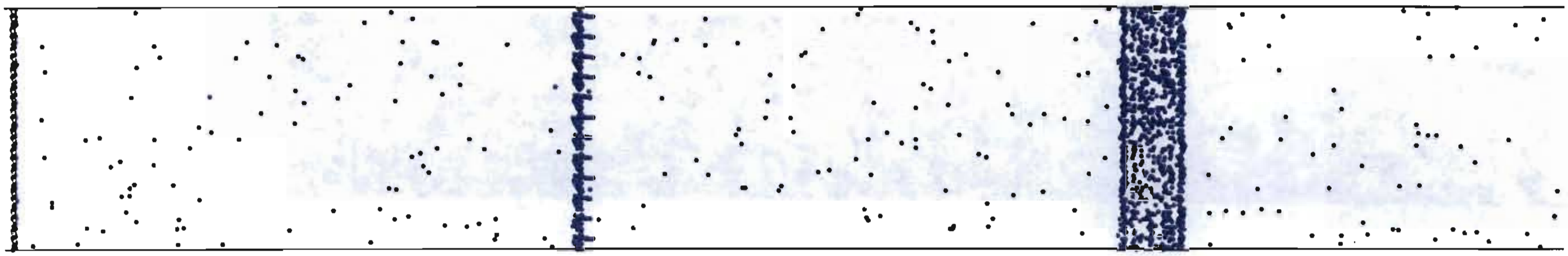
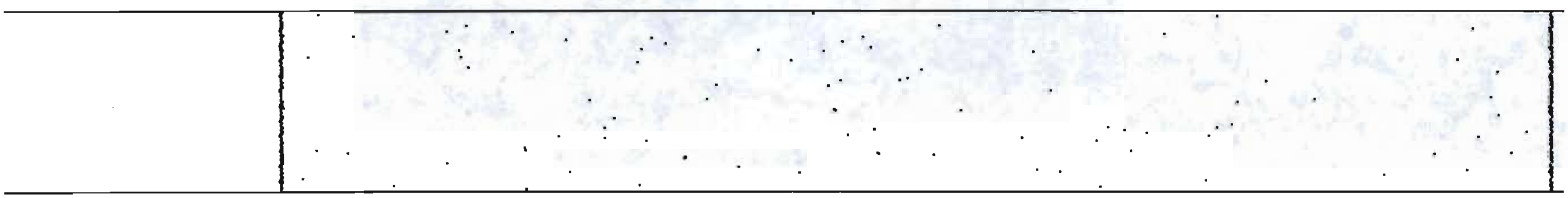
Simulations Details: Shock



- Computational cell size: 200, 28 and 18 lattice spacing's in y, x and z directions.
- Periodic in x, y and z directions with a total of 2M atoms.
- Equilibrated for 50-100 ps.
- Free surfaces/vacuum at both ends of the y-direction.
- Shock along y-direction [18-1/-252].
- Particle velocities (u_p) of 0.25 km/s.
- NVE molecular dynamics (MD) simulations performed using Sandia LAMMPS code.

Shock Wave at 300 K





Shock Simulations at 300 K

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Conclusions

- The grain boundary structure disorders as the temperature is increased.
- There are no defects that form in the bulk crystal after the shock wave passes through it.
- At the same shock speed, the GB forms various stacking faults as the shock wave passes through it.
- The initial structure of the GB changes after the rarefaction wave interacts with the GB structure formed after the shock wave has passed through the grain boundary

Talks by Collaborators

- Juan Escobedo-Diaz: Dynamic Behavior of Materials V: Dynamic Effects in Materials, Wednesday at 5:40 pm
- Alex Perez-Bergquist: Dynamic Behavior of Materials V: Shock Compression, Tuesday at 5:40 pm