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Molecular Dynamics Simulation of Elastic-Plastic and Spall Mechanisms in Cu when Dynamic Loading

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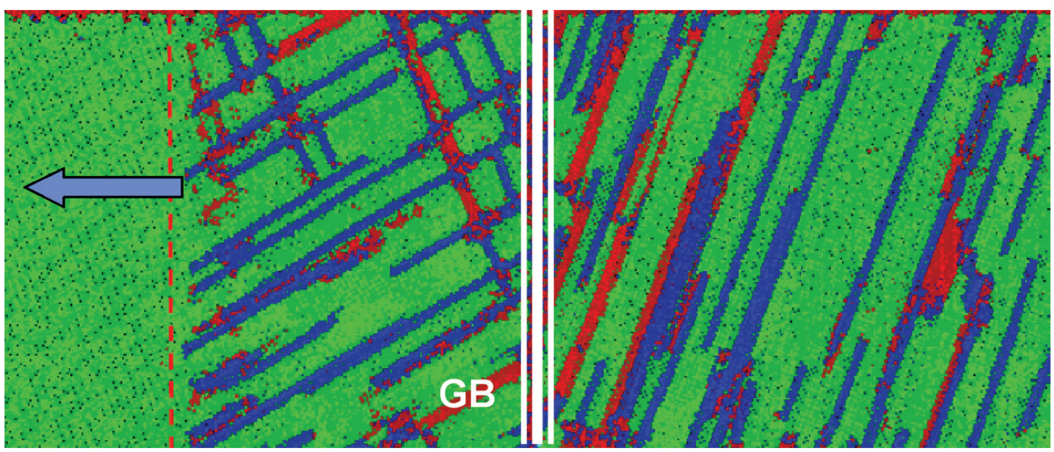
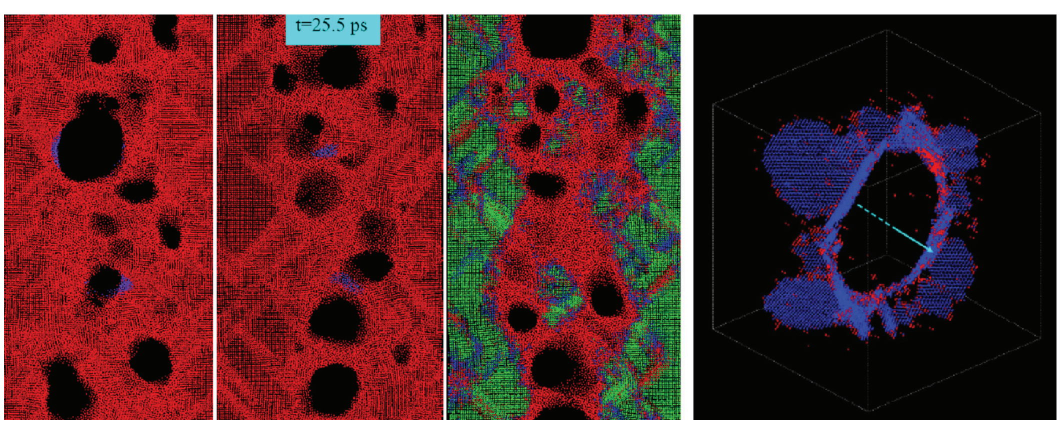
Project Description

The objective of this project is to perform molecular dynamics simulations of the interaction of shocks with crystal grain boundaries, dislocations, and inclusions to investigate elastic/plastic deformation of shock-loaded copper and to elucidate the influence of nano-inclusions in spall.

Typical simulations involve 10^7 atoms modeling a copper bicrystal. The EAM potential of Mishin was used. A set of simulations was performed with the grain boundary at five different angles with respect to the shock front (0, 30, 45, 65, and 90 degrees) and two different pressures. The simulations with loading involved four types of short pulses: square, triangular, Gaussian, and linear rise plus flat top. The spall simulations used randomly distributed nanoparticles (at least one near the spall plane) with a radius of 1 and 2 nm. The nanoparticles were simulated with the same potential, but changing the mass of the atoms. Two masses were considered: carbon-like and lead-like atoms.





Top: Molecular dynamics simulation showing a shock-grain boundary (GB) interaction. The blue arrow shows the shock propagation direction.

Bottom: The first, second, and third images are Cu+C, Cu+Pb, and Cu, respectively. Shock-induced spall is modified by nano-inclusions (blue). The fourth image shows a shock-dislocation loop interaction.

Technical Purpose and Benefits

The simulation of the interaction of shocks with highly symmetric grain boundaries will yield better understanding of experiments and simulations in polycrystals. The investigation into the elastic/plastic deformation of monocrystalline copper when shock loaded with short pulses of different shape yields improved understanding of the final microstructure in the shocked targets. Recent experiments have found nanoparticles at every void at the spall plane of copper targets: the investigation into the influence of nanoparticles in spall may clarify whether nanoparticles act as stress concentrators, significantly decreasing the spall strength. All these contribute to the development and validation of improved constitutive models for shock-loaded polycrystalline materials.

Collaboration between Lawrence Livermore National Laboratory (LLNL), Livermore, CA, USA, and the Russian Federal Nuclear Center - All Russian Research Institute of Technical Physics (RFNC-VNIITF), Snezhinsk, Russia

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