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Abstract

The MagLab and many facilities around the world make extensive use of copper for conductors and other purposes. In some applications, such as conductors for high field magnets, Ag is added to hinder dislocation motion and enhance mechanical strength. Molecular Dynamics (MD) simulations were performed to investigate and visualize the nucleation and motion of dislocations in high strain rate tension and compression experiments. The simulation were undertaken on pure copper, pure silver and a roughly 20 at.% Ag - 80 at.% Cu lamella system (80-20 lamella).

Introduction

Sandia National Lab developed a software package called Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)^[1]. Guides from Tschopp^[2] and some trial and error provided sufficient knowledge of the program for executing the tensile and compression tests. An updated guide was written and can be obtained from Ke Han.

MD Simulations use experimentally-found interatomic potentials with Newtonian equations of motion in order to calculate the interactions and movements of individual atoms in a predefined lattice. Over many time steps, certain processes can be achieved, such as equilibration, tension, and compression. Due to the large volume and intense nature of the calculations, the time steps are best left very short (1 fs = 10⁻¹⁵ s).

Results obtained from a MD simulation in this way should be taken with a grain of salt, due to both the unrealistic speed of the test and the ideal layout of atoms in a perfect single crystal. One of the stronger functions of MD is to study the nucleation and motion of dislocations during various processes, as animating a computer-generated image is typically much cheaper and easier to visually examine than a real-world specimen.

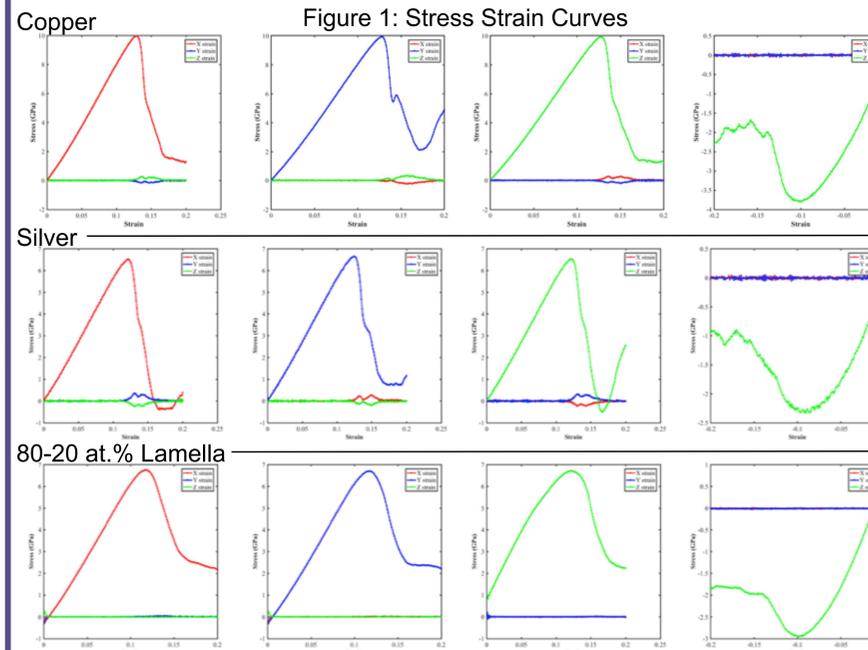
The results of various calculations can be stored in different files so that plots can be generated using other software. For example, Matlab can be used to generate a stress strain plot or AtomEye^[3] can generate animations of the simulation with various "views" applied to show only desired or relevant information, such as dislocated atoms (centrosymmetry/csyz).

Procedure

LAMMPS input scripts were prepared and executed using Matlab for uniaxial tension in all three orthogonal directions (x, y, and z) as well as uniaxial compression in the z direction after a equilibration step on the following systems: pure copper, pure silver, and 80-20 at.% Cu-Ag lamella with a silver layer depth of approximately 5 nm. EAM interatomic potential files from Y. Mishin^[4] were used. For the pure elements, cubes measuring 30x30x30 unit cells were generated. The bimetallic system consisted of a block measuring 30x30x12 silver unit cells and a 34x34x37 one of copper. All tests were conducted with periodic boundaries in all three axis.

The equilibration step allowed for the atoms to minimize its energy for 20 000 time steps of 1 fs (20 ns total) without any external forces at a temperature of 300 K. A uniaxial strain rate of 10¹⁰ 1/s was then applied for another 20 000 time steps. Stress/strain data in each axis was recorded during the experiment and plotted with Matlab. CFG files were also generated and passed to AtomEye for visualization.

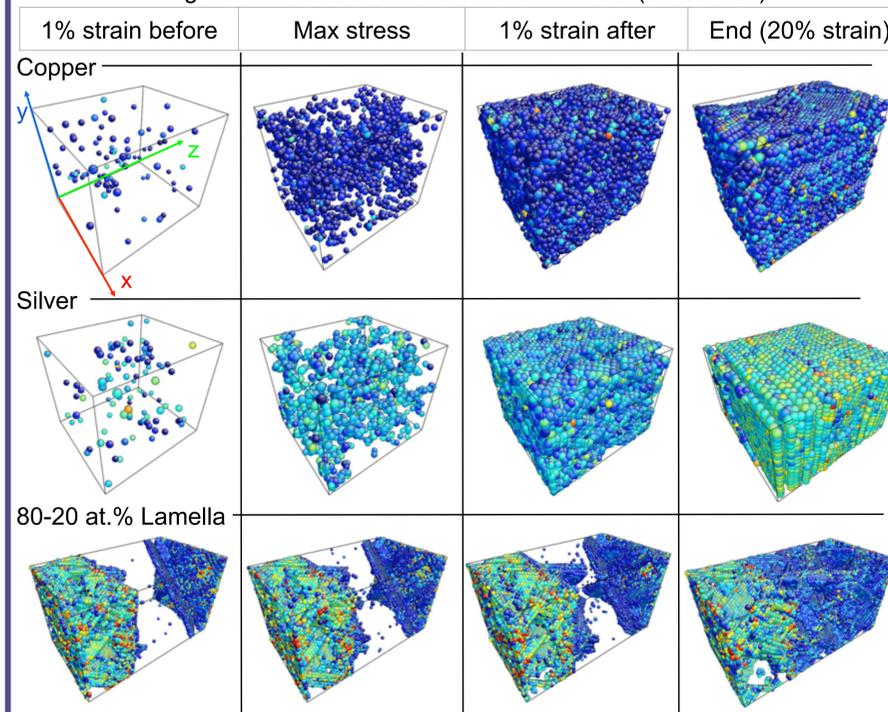
Results and Discussion



Note the high degree of similarity between the three axial tension tests for each specimen. For copper, it had a maximum stress of 10GPa at 13% strain. Silver was softer, with 6.5GPa at 12.25%. These tensile strengths are much higher than those found experimentally, where 0.20-0.35GPa for Cu and 0.14GPa for Ag are expected. The lamellar structure resembled Ag, with a maximum stress of 6.7GPa at 12% strain in all three axis.

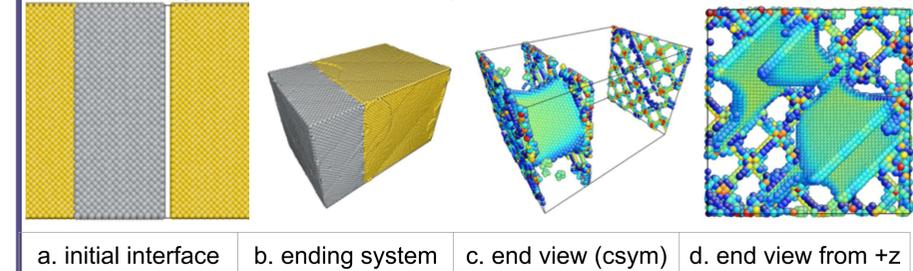
Peak compressive stresses (Cu: -3.8GPa, Ag: -2.3GPa, Lamella: -2.9GPa) occurred at 10% strain.

Figure 3: Visualization of the Tension Tests (Z direction)



The csym view was used for these images, brighter colors means higher csym values (more dislocation). Maximum stress occurs when many atoms are displaced, but have not yet fallen into a slip plane. In copper, many dislocations appear to form along the (111) and (010) planes, while in silver (001) and (100) are preferred. In the lamellar structure, there is less distinction between before and after max stress, which corresponds to the more rounded stress-strain curve. In lamellar max stress, there are likely many displaced Cu atoms that are just under the threshold, rendering them invisible. (111) was the preferred slip plane for the lamellar system.

Figure 3: Visualization Snapshots of Lamellar Minimization



Due to the process for creating a multi-species simulation, a small gap needed to be introduced at the interface. This gap was closed during the minimization. 3c shows a grid of stacking faults was formed following [110] directions in the (001) interfacial plane. Between these faults there were regions of atoms that had very low csym values. Within the silver block, dislocations grew into 2 pairs of parallel (111) slip planes. These dislocations initially formed along the edges of the defined region then moved and grew to be more central. The ends of these planes generally align with the faults already present at the interfaces. This grid of faults also proved to be the nucleating point for the dislocations when the specimen was in tension.

Conclusions

- LAMMPS MD simulation software was used to perform uniaxial tension and compression tests on copper, silver, and 80-20 at.% Cu-Ag systems.
- In nanocrystal copper and silver without defects, stress levels of 10 GPa and 6.5 GPa are required to generate mobile dislocations at strain levels of 13% and 12.25%, respectively.
- In CuAg lamellar System, minimization leads to formation of (111) stacking faults in the silver block. Dislocations move along (111) planes and are generated at the interface between two elements. Overall strength limited by silver in all three axis and the stress reached 6.7 GPa at 12% strain.

Future Work

Investigations into the peculiar stacking of the pure copper and silver systems could be performed by using other styles of computations besides the EAM files from Mishin. Given that this pair of elements is both commonplace and crucial to many places, it is worth investigating in detail other compositions and shapes, such as shelled nanowires or silver precipitates in a copper matrix. These simulations could also be made more realistic by introducing more atoms in different grains with a few defects, rather than a very limited number in a perfect crystal as was done here.

Acknowledgements

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