Molecular Dynamic Simulation of the Stress in Metallic Alloys

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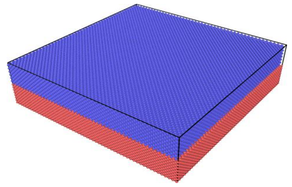
Introduction

Superalloys ability to withstand its mechanical strength at temperatures close to its melting point is the reason for the focus on this topic. Mechanical strength is dependent on deformation resistance, and deformation resistance is strongly influenced by dislocations in the structure.[1]



Side view of a nickel and aluminum bilayer. The blue atoms are nickel, and the red atoms are aluminum.

We use molecular dynamic simulations within LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) to investigate the stress and dislocations within Ni and Al heterostructures. An embedded atom method (EAM) potential developed by Mishin enables the construction of the lattice of Ni and Al.[2]

Methods

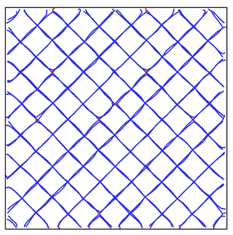
For each simulation, the atoms are analyzed by the DXA (Dislocation Extraction Algorithm) usging the visualizer package Ovito, that calculates the dislocation in the simulation by the equation below.[5]

$$\mathbf{b} = -\sum_{C'} \Delta \mathbf{x}'$$

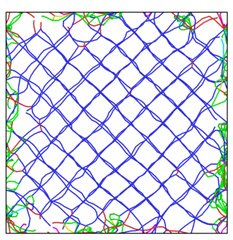
The Burger vector is equivalent to the sum of the change over time of the path of a dislocated crystal (C').

Relaxation→ Melting→ Cooling

In bottom left figure, 54 x 54 Angstrom Ni and Al bilayer with a depth of 14 Angstrom is relaxed. Dislocations are placed at 45 degree angles in the structure. In the right figure, the structure is heated to 1000K. Since the melting point of Ni is 1728K, the dislocations within the Ni structure are still visible.



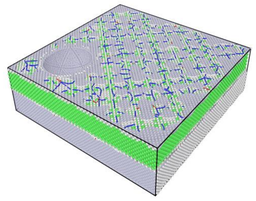
An image of the front view of the dislocation of a relaxed Nickel and Aluminum bilayer structure.



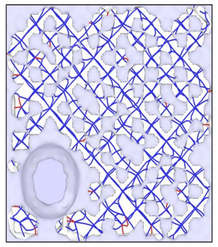
The representation of the dislocation. Colors blue, green, and red are perfect, Shockley, and other dislocations, respectively.

Nano-indentation

In both bottom figures the Ni and Al bilayer structure is indented by a sphere of radius 6 Angstrom.



The green atoms in the structure represents an face-centered cubic (FCC) structure which represents 75.3% of the structure.



This is a front view of the simulation. The white area represents the defect mesh in the relaxed structure.

Uniaxial Compression

In Figure 1[4], an 10 x 10 Angstrom with the depth of 10 Angstrom structure of Al is compressed to demonstrate dislocation hardening. In Figure 2, a similar simulation is created with Ni structure of similar dimension.

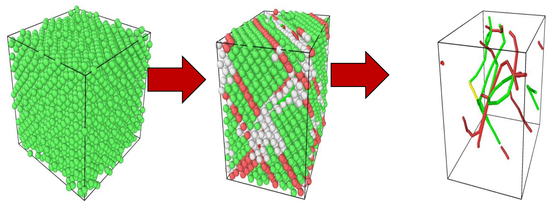


Figure 1. This is an image of the compression of Aluminum. As the Al structure is compressed, the Al FCC structure shifts to incorporate both a FCC and hexagonal close packed (HCP) structure. As the Al structure compresses, the amount of dislocations increase.

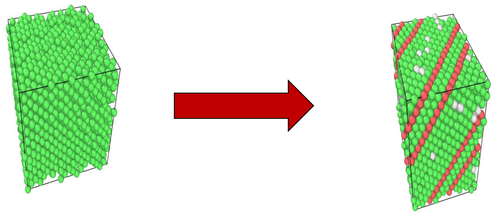
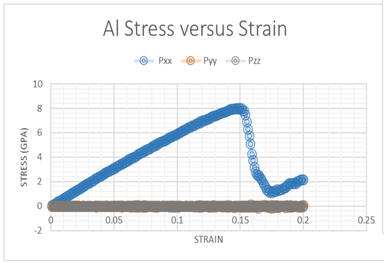
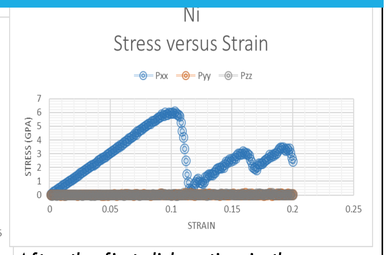


Figure 2. This is an image of the compression of Nickel. The dislocations appear and disappear throughout the simulation. This phenomenon is called dislocation starvation, and it is a hardening technique.[6]

Results



The peak of the stress and the strain is the point of dislocation[4].



After the first dislocation in the structure, the stress decreases. New dislocations are created with additional strain applied.

Conclusion

For simulations with fewer time steps and atoms, the DXA does not detect dislocation in the structure after cooling. For the 146,542 atom simulation with 2000 time steps heated to 1000K, 610 dislocation are detected. For the 146,542 atom simulation with 93 time steps, the simulation is confined to simulation box with boundary conditions of being periodic in the <x,y,z>. When a sphere of radius 6 Angstrom penetrates the simulation, it incorrectly produces 2 holes in reflection of each other. To correct the simulation, the simulation box is confined to the boundary condition of being non-periodic and shrink wrapped in the z-axis. A simulation of uniaxial compression was performed on Al[4] and Ni with the dimensions of 10 x 10 Angstrom with a depth of 10 Angstrom. For the 4,000 atom Ni simulation, the phenomenon, dislocation starvation, occurs. It results in a mechanically stronger Ni structure.

Acknowledgments

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References

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