Molecular dynamics simulation of nanoindentation on Al-$Cu_{50}Zr_{50}$ multilayers

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Abstract

We performed molecular dynamics (MD) simulation of nanoindentation on Al (metal)-$Cu_{50}Zr_{50}$ (metallic glass (MG)) multilayers aimed to investigate the effect of loading rate, MG thickness, and temperature on the load-displacement behavior and underlying deformation mechanisms. Simulation box size of (200×200×200) Å is used. At first Al–$Cu_{50}Zr_{50}$-Al crystalline model is constructed with the bottom layer (Al) of 70 Å (FCC crystal structure and lattice parameter = 4.01 Å), the middle layer $Cu_{50}Zr_{50}$ of 60 Å (FCC Cu, a = 3.61) and the top layer (Al) of 70 Å in height along y–direction under periodic boundary conditions and comprises of 538538 atoms. $Cu_{50}Zr_{50}$ region is created by randomly replacing copper atoms by zirconium atoms. $Cu_{50}Zr_{50}$ MG is obtained by rapid cooling from 2000 K to room temperature at a cooling rate of 8.6×10^{11} Ks^{-1} (timestep=0.002 ps). EAM (Embedded Atom Method) potential is used. The layered interface models are then equilibrated at 300 K for 500 ps using NVT to relieve internal stresses. Nanoindentation is carried out using a spherical diamond indenter on the MG region at different loading rates in the range of 0.5-5 Å/ps and different temperatures (10-300) K under NPT ensemble and S P S boundary conditions along x, y and z directions. At temperature of 50 K and loading rate of 0.8 Å/ps, we observed a peak load of 88 nN. Further, we found that with increase in loading rate, the peak load increases. Stiffness is calculated form the unloading curves and is found to increase with increase in MG thickness. As anticipated, the increase in temperature decreases the strength of the multilayers. The atomic displacement vector plots reveal MG as obstacles to the movement of dislocations nucleated at the interface. The results provide significant insight into the elastic behavior, deformation mechanisms at the nanoscale.

Key words: Molecular dynamics; Interface; nanoindentation; Dislocations; atomic displacements.

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Introduction

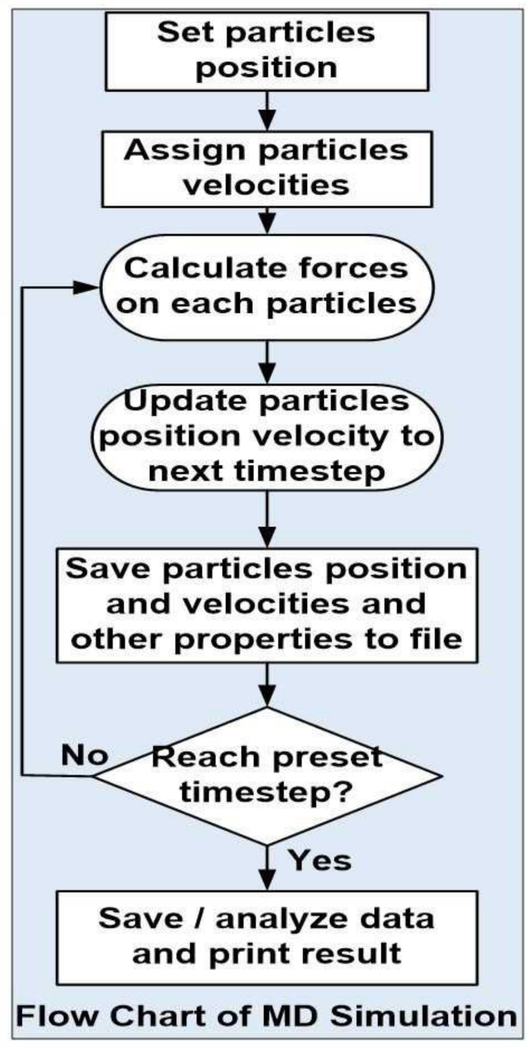
- Al-based metal matrix composites are of great interest owing to their remarkable mechanical properties, such as low density, high elastic modulus, strength and good wear resistance, which make them attractive for applications in the aerospace, automotive and defence.
- Metallic Glass reinforcement has better compatibility with the Al matrix and results in better interface bonding than conventional ceramic particles.
- The interface plays a vital role in determining the mechanical properties of the composite. This is because of large surface occupied by the interface. Therefore the interface between the matrix and the reinforcement plays a crucial role in determining the resultant properties of the composite and the strength of the composites depends on the strength of the interface.

Aim and Objective

- Creation of the Al(metal)-$Cu_{50}Zr_{50}$(metallic glass) multilayers model interface.
- Carry out nanoindentation deformation studies of the interface at different temperature in the range of 10-300 K and different loading rates in the range of 0.5-5 Å/ps.

Computational Details

- MD simulation of nanoindentation via LAMMPS (Large Scale Atomic/Molecular Massively Parallel Simulator)
- Simulation box size of (200×200×200) Å is used. At first Al–$Cu_{50}Zr_{50}$-Al crystalline model is constructed with the bottom layer (Al) of 70 Å (FCC, a = 4.05 Å), the middle layer $Cu_{50}Zr_{50}$ of 60 Å (FCC Cu, a = 3.61) and the top layer (Al) of 70 Å in height along y–direction under periodic boundary conditions and comprises of 538538 atoms.
- $Cu_{50}Zr_{50}$ MG region is created by rapid quenching route (cooling rate=8.6×10^{11} Ks^{-1}).
- EAM (Embedded Atom Method) potential is used. The layered interface models are then equilibrated at 300 K for 500 ps using NVT to relieve internal stresses.



Flow Chart of MD Simulation

Results

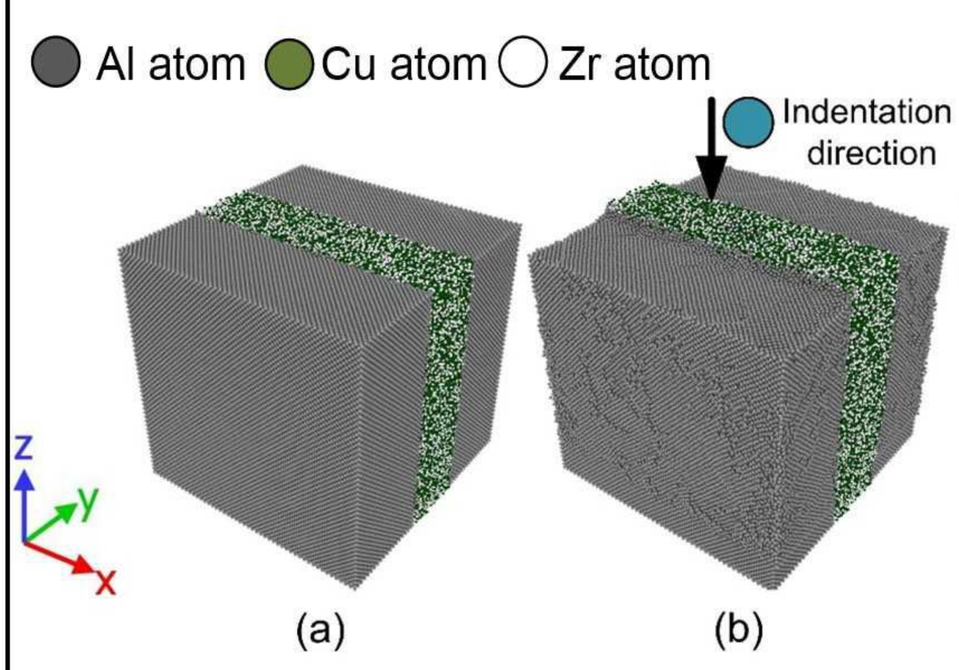


Fig1 (a) Initial sample, (b) Sample after Indentation

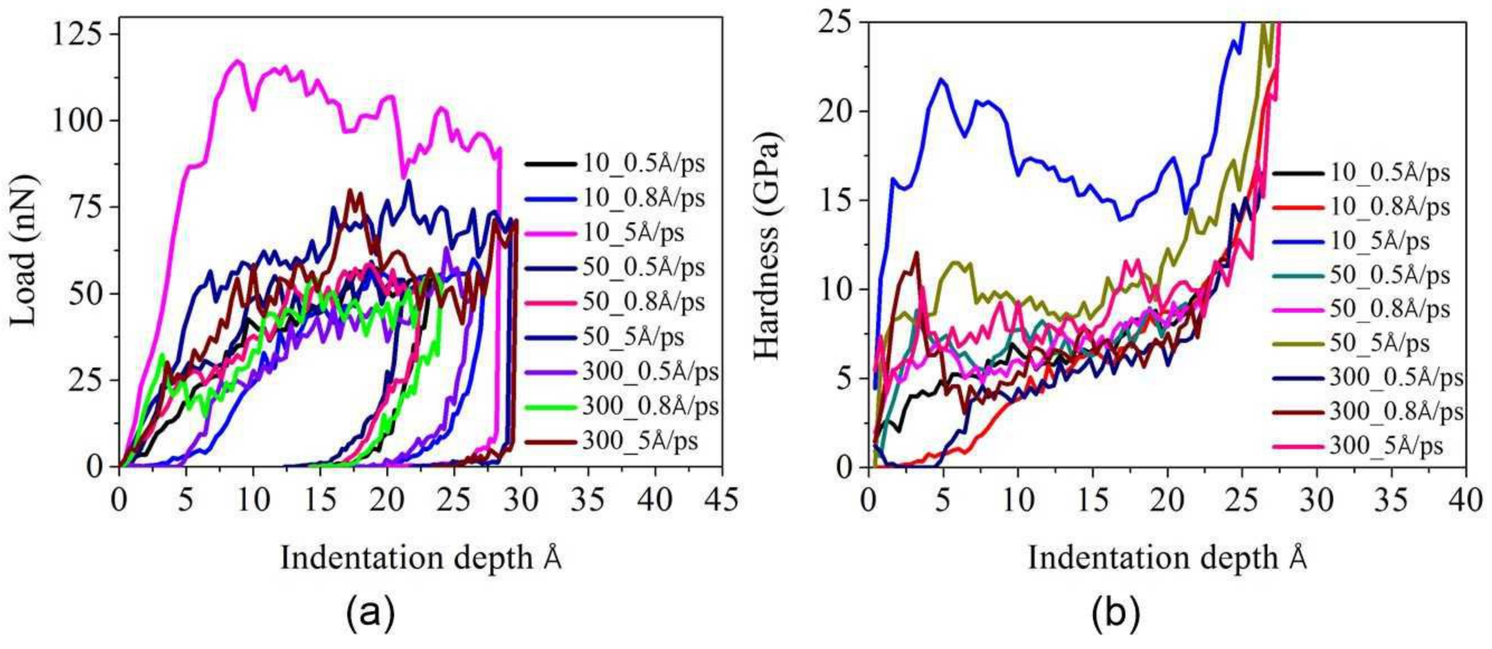


Fig 2 (a) Load Vs Indentation depth (b) Hardness Vs Indentation

Conclusions

- As loading rate increases, the peak load increases. At temperature of 10 K and loading rate of 5 Å/ps, we observed a maximum peak load of 117 nN.
- As the temperature increases, the strength and hardness of the multilayers composite decreases.

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