Role of free volume on the plasticity in Cu-Zr amorphous binary alloy

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Abstract

The role of free volume on the room temperature plasticity of $Cu_{50}Zr_{50}$ metallic glass was investigated through spherical nano-indentation simulation studies by Molecular Dynamics simulations. Excess free volume was generated by randomly deleting the atoms in the glassy structure. In the present investigation ~ 4% excess free volume was created in the $Cu_{50}Zr_{50}$ model metallic glass comprising of 2457 atoms followed by nano-indentation. The load-displacement plot shows that free volume contributes for plastic deformation. The metallic glass that had excess free volume (4%) yielded at lesser load compared to the metallic glass model devoid of excess free volume.

Introduction

- Metallic glasses are metallic materials with disordered atomic structure. Unlike crystalline materials they do not possess long-range atomic order. Disordered structure is obtained on rapid cooling from the liquid melt and hence suppressing nucleation and growth of crystalline phase.
- The deformation mechanism in metallic glasses is different from that of crystalline materials due to the disordered atomic level structure. Metallic glass packing models (Saksl et al., 2003; Miracle, 2004) suggest that the atomic structure comprises of atomic clusters plus the empty space between them.
- The empty space between these clusters is termed as 'free volume' in which atomic rearrangements occur without affecting the surroundings significantly by application of temperature or stress and these are the preferred regions for destabilization of the glassy structure.
- The proposed microscopic mechanism which governs both homogeneous and inhomogeneous flow is the atomic jump, and macroscopic flow occurs as a result of a large number of individual atomic jumps (Spaepen, 1977).
- The other mechanism of deformation is shearing of shear transformation zone (STZ) as proposed by Argon (1979) which is formed around a free volume site. Shear bands have been observed in deformed samples of metallic glasses (Hajlaoui et al., 2008). Some proposed that movement of shear bands results in plastic.

Objective of the present investigation

- Molecular dynamics simulation deformation studies by nano-indentation have been carried out on two glassy $Cu_{50}Zr_{50}$ model alloys one with devoid of excess free volume and the other with excess free volume in order to see the influence of free volume on the flow behvior.

MD simulation procedure

- Molecular Dynamic (MD) simulation deformation studies have been carried out on LAMMPS (Large Scale Atomic/Molecular Massively Parallel Simulator) platform .

1. Creation of Crystalline $Cu_{50}Zr_{50}$ alloy model containing 2457 atoms →
2. Heating of the alloy to 2300 K. Holding for 160 ps followed by quenching of the liquid alloy from 2300 K to 300 K at a cooling rate of 10^{12} K/s to obtain glassy alloy. The above heating holding and quenching are carried out using NPT ensemble, periodic boundary and zero bar pressure →
3. Few atoms are randomly removed from the glassy structure to create excess free volume →
4. Nano-indentation (indenter radius 10 Å; indenter velocity 2 Å/ps) of the quenched structures (with excess and devoid of excess free volume) at room temperature using NVT ensemble

Results and Discussion

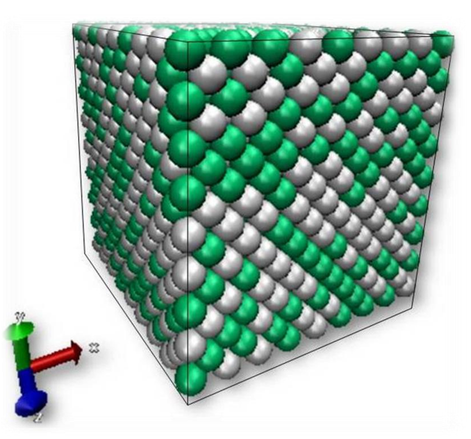

Fig. 1a: VMD (Visual Molecular Dynamics) snap shot of $Cu_{50}Zr_{50}$ crystalline alloy

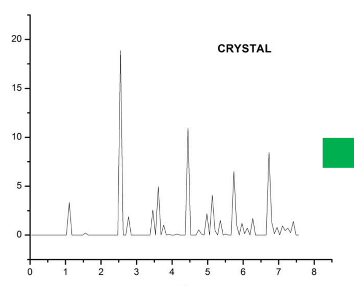

Fig.1b: Radial distribution function plot of Cu-Zr pair in $Cu_{50}Zr_{50}$ crystalline alloy

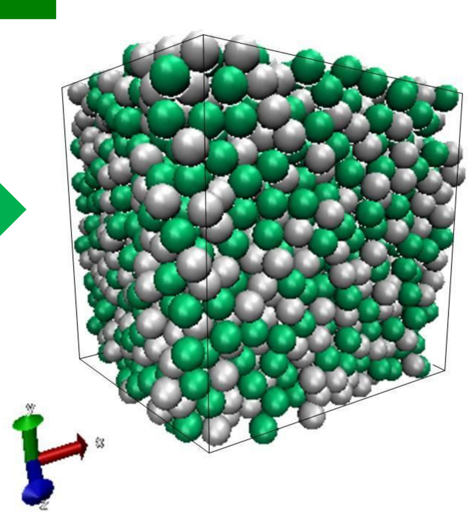

Fig.2a : VMD snap shot of $Cu_{50}Zr_{50}$ glassy alloy

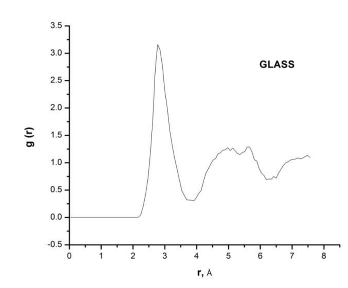

Fig. 2b: Radial distribution function plot of Cu-Zr pair in $Cu_{50}Zr_{50}$ glassy alloy

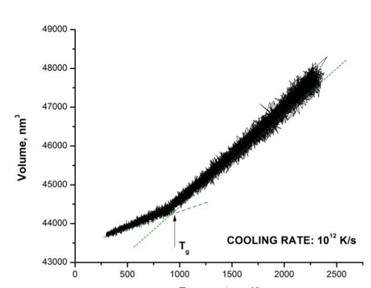

Fig. 2c: Volume –Temperature plot during rapid cooling

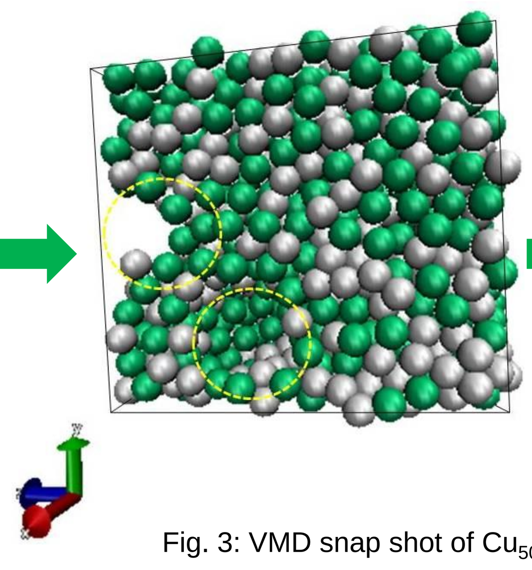

Fig. 3: VMD snap shot of $Cu_{50}Zr_{50}$ glassy alloy with excess free volume (encircled regions indicate free volumes)

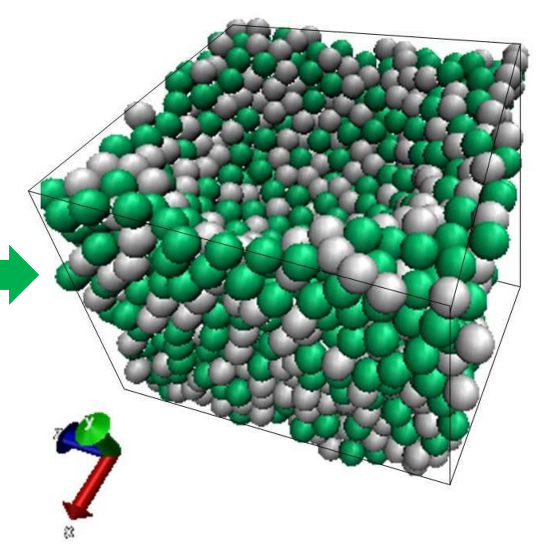

Fig. 4: VMD snap shot of $Cu_{50}Zr_{50}$ glassy alloy after indentation

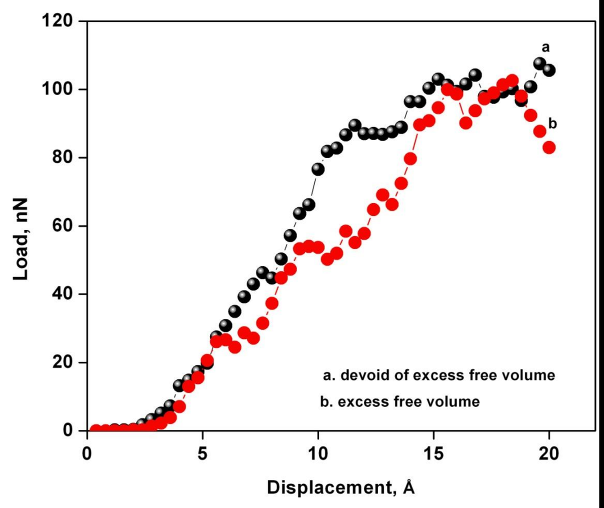

Fig. 5: Load-displacement plot of $Cu_{50}Zr_{50}$ glassy structures with different free volumes

- It has been found that free volume significantly influences the deformation behavior of metallic glasses.

Conclusion

- Metallic glass with excess free volume yields at much lesser load compared to that devoid of excess free volume

References

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