

NANO-INDENTATION OF ALUMINIUM REINFORCED METALLIC GLASS COMPOSITES: A MOLECULAR DYNAMICS STUDY

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Abstract

Molecular dynamics (MD) simulations are performed for nanoindentation on metal (Al)-metallic glass ($\text{Cu}_{50}\text{Zr}_{50}$) reinforced composites to investigate the mechanical properties and the effects of volume percentage on behavior of the load-displacement curves. The interaction among Al-Cu-Zr is modelled using a EAM (Embedded Atom Method) potential. Simulation box size of $100 \text{ \AA}$ (x) $\times$ $100 \text{ \AA}$ (y) $\times$ $100 \text{ \AA}$ (z) is modelled for investigating the properties of the sintered models by altering the volume percentage on the scale of 5%–20%. Nanoindentation is done along y-direction with a spherical diamond indenter at temperature of 300 K with constant indentation speed of 100 m/s. NVT ensemble is used with a timestep of 0.002 ps. Investigations on the effect of volume percentage show that as volume percentage of Metallic Glass (MG) increases, the corresponding Load required to penetrate inside the sample also increases. As a result of this Hardness also increase as volume percentage varies from 5% to 20%.

Keywords: Molecular Dynamics, Sintering, Nano- Indentation, Metal Matrix composites (MMC's), Volume percentage.

1. Introduction

The exceptional mechanical properties of aluminium based MMC's (metal matrix composites) are of great interest due to reduced density, high strength, enhanced elastic modulus as well as better wear resistance, and these exceptional mechanical properties make these MMC's captivating for utilization in automotive, defense and aerospace [1]. At ambient as well as elevated temperatures, ceramic materials like Al_2O_3 or SiC shows an outstanding combination of both stiffness and specific strength, which make these as commonly used reinforcements [2,3]. Ceramic reinforcement materials have porous interface due to their low wettability, which is a major problem because of increased corrosion sensitivity and ebbed mechanical properties of the composite [4]. Cu-Zr metallic glass (MG) as a reinforcement material in Al-alloy matrix is being used for the first time [5]. In recent times, Al alloy matrix is being reinforced with various types like Ni, Fe, Al, Cu and Zr based of MGs particles. They reports all in all enhancement in properties of Al alloy [5–7]. As a result, MG reinforcements as a potential substitute for ceramic reinforcements could be considered in MMC's.

Consolidation of powders with the help of thermal energy, which usually happens at about 2/3 of the melting temperature, is called sintering. In present work sintering is preferred



over other manufacturing process because of the lower transition temperature of MG then the melting point temperature of the metal (Al). The other main advantages of this process over other manufacturing methods are less energy consumption, high ability to get complex shapes, dimensional precision in final product, excellent surface finish, repeatability and high reliability. Thus, sintering is one of the most economical manufacturing processes, especially in mass production [8]. In the present work Al based MMC's reinforced with Cu based MG ($\text{Cu}_{50}\text{Zr}_{50}$) nano-particles will be developed by sintering route through Molecular Dynamics (MD) simulations with volume percentage of MG to be 5% and 20% and termed as Model-I and Model-II respectively. Nano-indentation tests are done on this models to investigate the deformation behavior and response on the mechanical properties of the composite such as maximum load, hardness and elastic modulus through load-displacement plots [9].

2. Simulation method

2.1. Interatomic potentials

In MD simulations the interactions between atoms are calculated through the interatomic potential functions. Since in this work sintering of aluminium reinforced MG composites is investigated, there is a need for proper potential functions for the interactions between Copper and Zirconium atoms in Metallic glass and aluminium with Metallic glass. In order to obtain the forces between atoms, EAM potential is employed [10].

In present study we have done MD simulation using LAMMPS (Large Scale Atomic/Molecular Massively Parallel Simulator) an open source simulator developed by Sandia Laboratory is being employed [11]. The interaction among Al-Cu-Zr is modelled using a Zhou et al. EAM potential. For force calculations a cut-off distance of 7.1 Å is used. The potential is valid and other details of parameters can be obtained from Ref. [12]. Moreover, the potential is used by several researchers. Phase transitions in nanoparticles like FeCo and FeNi have been studied by Meng et al. [13]. Zhou et al. potential is used to study oxidation of Al layers on $\text{Ni}_{65}\text{Co}_{20}\text{Fe}_{15}$ surface [14]. Moreover, effect of temperature and strain rate on metal- metallic glass interface has been modelled using the above potential [15].

2.2. Modelling

The atomic position snapshot of Al (metal)- $\text{Cu}_{50}\text{Zr}_{50}$ (MG) model before and after sintering is shown in Fig. 1(a) & 1(b), with dimension as 10 nm (width) × 10 nm (height) × 10 nm (thick). To acquire Al (metal)- $\text{Cu}_{50}\text{Zr}_{50}$ (MG) sintered model we start with construction of Al and $\text{Cu}_{50}\text{Zr}_{50}$ nano clusters. The centre is filled with $\text{Cu}_{50}\text{Zr}_{50}$ alloy clusters, which is achieved through randomly substituting 50% of Cu atoms by Zr atoms and rest with Al clusters. The separation

distance is set more than the equilibrium bond lengths, i.e., 3.5 Å. $\text{Cu}_{50}\text{Zr}_{50}$ MG is obtained by rapid cooling of $\text{Cu}_{50}\text{Zr}_{50}$ alloy from the temperature of 2300 K to 300 K at a cooling rate of 8.5×10^{11} K/s (timestep = 0.002 ps) with constant number of atoms (N), constant pressure and constant temperature (T) i.e NPT ensemble using the periodic boundary conditions. The sintered model then is equilibrated for 500 ps for relieving stresses generated during rapid cooling [3,5].

Indentation process was investigated using a spherical indenter of radius 15 Å. Fig 1(c) & 1(d) shows the model before and after indentations. The indenter deformability and thermal oscillations of indenter atoms were neglected. The hardness of Aluminium reinforced metallic glass composites is considerably lower than a diamond and therefore the rigid body model for the indenter is fully applicable in this model [16].

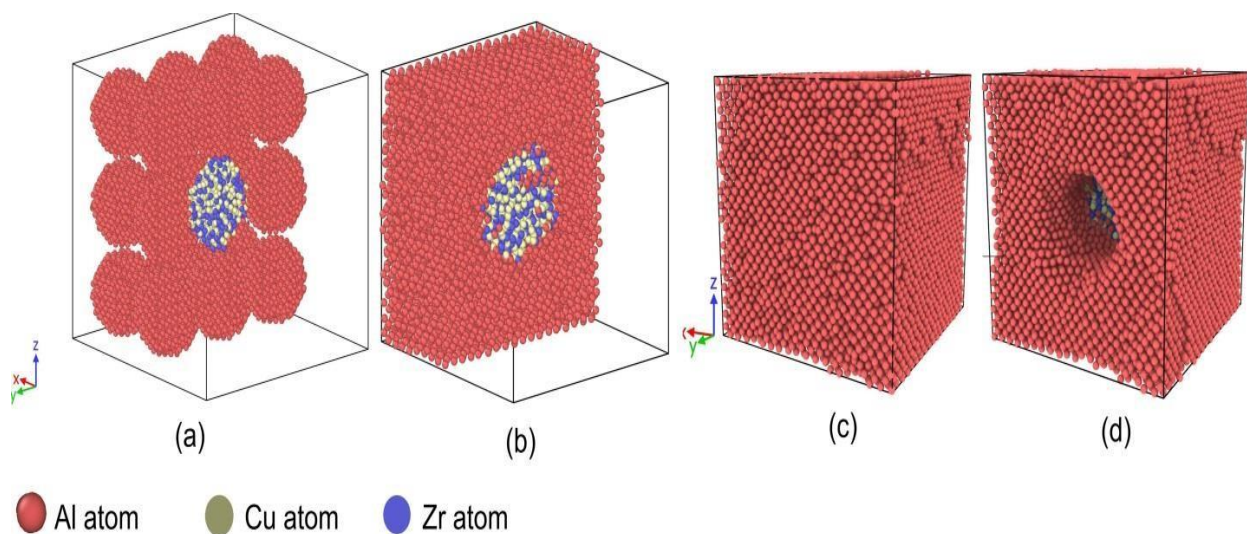


Figure 1: (a) initial model before sintering, (b) model after sintering, (c) model before indentation, and (d) model after indentation.

3. Results and discussion

Pressure sintering is used to model the two different models

1. *Model-I*: Volume percentage of MG in the model is taken as 5 %.
2. *Model-II*: Volume percentage of MG in the model is taken as 20 %.

Fig 1(a) & 1(b) shows the model-I with volume percentage of metallic glass to be 5%, before and after sintering. Fig 2(a) & 2(b) shows the model-I with volume percentage of metallic glass to be 20%, before and after sintering.

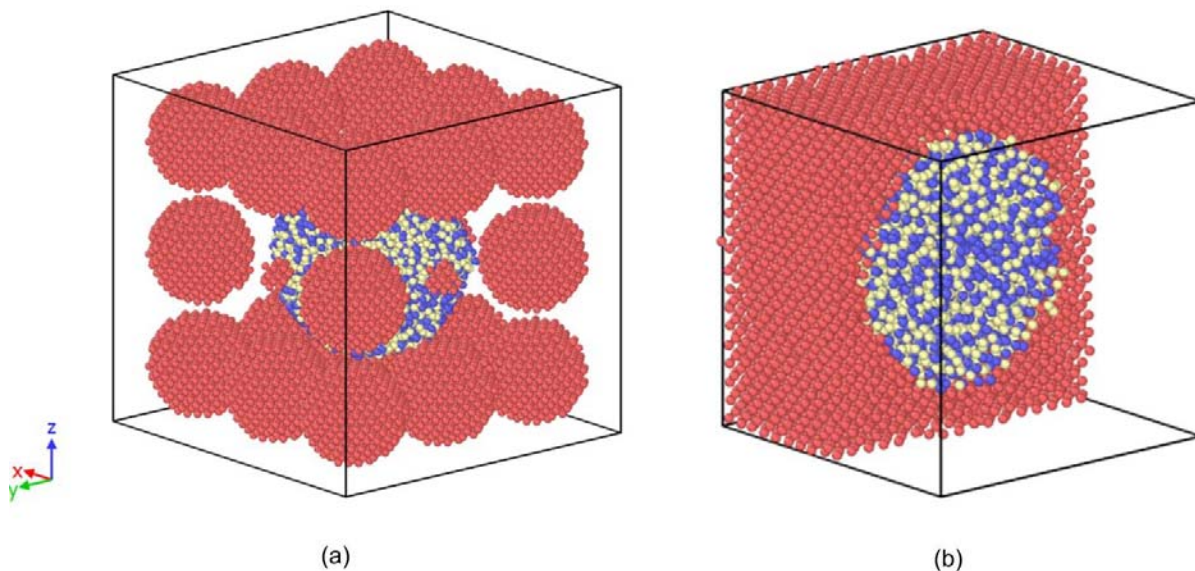


Figure 2: (a) initial model before sintering, (b) model after sintering, (c) model before indentation, and (d) model after indentation.

Nanoindentation process comprises of two stages in MD simulations, one being the equilibrium stage and other being the indentation stage. In equilibrium stage, the crystal surface and the indenter were positioned ~ 10 Å apart from each other and the system was simulated at 300 K for ~ 120 ps. In the indentation stage of the simulations, indenter is moved approximately 35 Å downward as per the modelled process at a perpetual speed of 100 m/s, and then retracted upwards at a perpetual speed of 50 m/s.

During displacement controlled indentations (depth-sensing approach), indenter is pressed against the surface up to a specified depth in the sample. The data of the load applied to the

indenter and the displacement of the indenter is represented in *Fig 3(a)*, which shows that, higher loads are required to penetrate inside the sample for higher MG vol%.

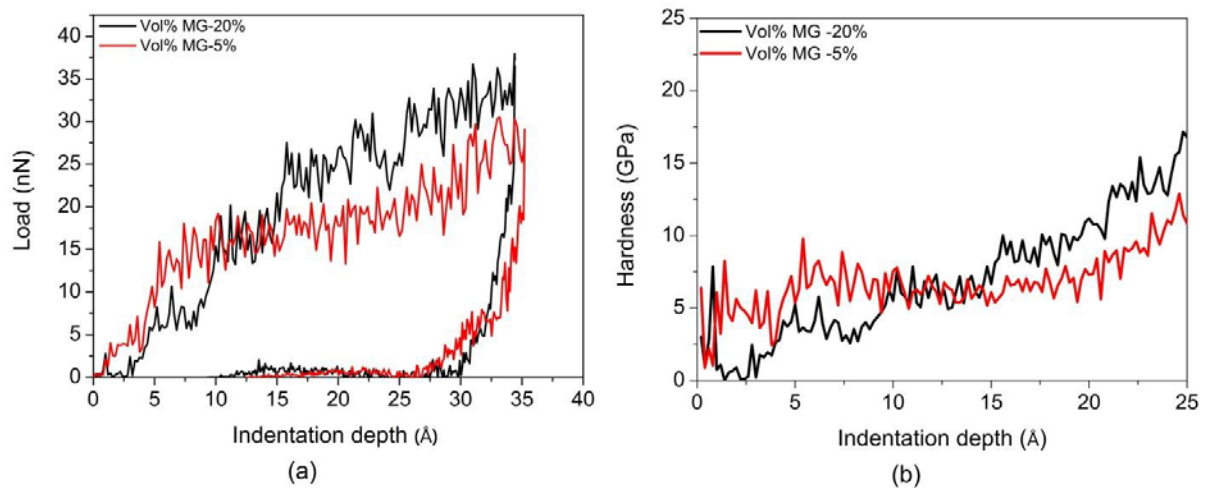


Figure 3: (a) Load-indentation depth plot (b) Hardness – indentation plot

Depending upon the Load vs indentation depth plot, Hardness has been calculated using the expression, $H=P/A$ (where H is hardness, P is load and A is projected area) and plotted in *Fig 3(b)*. Hardness increases as load required to penetrate inside the sample increases. Thus, as MG Vol% is higher, load required is higher and so is the hardness [17].

4. Conclusion

- As volume percentage of MG increases, the corresponding Load required to penetrate inside the sample also increases.
- Hardness of the sample increases with increase in volume percentage of MG and vice versa.

5. References

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