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Dynamic characterization of Cu-Zr binary bulk metallic glasses (A Molecular Dynamics Study)

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Abstract

In the present study, molecular dynamics simulation employing embedded atom method (EAM) potential is performed to investigate the formation and characterization of CuZr bulk metallic glasses (BMGs). To elucidate the effect of component concentration of three samples of BMGs including $Cu_{25}Zr_{75}$, $Cu_{50}Zr_{50}$ and $Cu_{75}Zr_{25}$ that are formed by melt quenching. The local structure of BMGs is analyzed by means of radial distribution function (RDF) and local atomic number density ρ . The mechanical behavior of three compositions is investigated using uniaxial compressive loading at a constant strain rate, It is revealed from the results that yield strength increases with increasing Cu-concentration. Thermal expansion of CuZr BMGs is examined and variation in length and volume is measured. The analysis revealed that $Cu_{25}Zr_{75}$ and $Cu_{50}Zr_{50}$ exhibited the typical expansion behavior while $Cu_{75}Zr_{25}$ showed an anomalous behavior.

Key Words: molecular dynamics simulation; embedded atom method; bulk metallic glasses; Share bands and anomalous expansion

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1. Introduction

Bulk metallic glasses BMGs have emerged as material of great interest in recent decades. Their good processing ability, glass forming ability and remarkable stability against crystallization made them potential candidate for the industrial applications. There are many advantageous properties like fatigue resistance, corrosion resistance, high strength and elastic strain limit have gained enormous consideration from the scientific and industrial point of view [1]. From last two decades, mechanical behavior of BMGs is the central point of research both theoretically and experimentally [2]. They exhibit very high strength owing to inexistence of 'crystal-slip' mechanism [3]. It is found that at high stresses and low temperatures BMGs show inhomogeneous plastic deformation because of the evolution of localized shear bands. BMGs undergo plastic deformation, when stress goes beyond yield stress, due to formation and propagation of shear bands [4]. The inexistence of dislocations, grain boundaries and shear band propagation is considered as the cause of plastic flow in BMGs. It strongly connects with the mechanical characteristics and fracture mechanism in BMGs [5]. Failure or fracture appears at once only after first shear band evolution, however ductility is observed in BMGs at room temperature during deformation under compression (or by rolling or indentation). Thus destructive failure is escaped and sample shows plasticity to some extent due to formation of multiple shear bands [6].

Mechanical behavior of Zr based BMG is investigated under compressive loading at room temperature employing constant strain rate. It is found that Zr based BMG exhibited high yield strength upto 1.8 Gpa but limited plasticity before fracture [7]. Molecular dynamics (MD) simulation indicated that pervading key note of short range ordering in BMGs is responsible for their enormous strength [8]. Results of simulation on Cu-Zr BMGs revealed that relative to $Cu_{50}Zr_{50}$ composition $Cu_{36}Zr_{64}$ showed less plastic deformation but greater activation energy under compressive loading [9]. Large yield strength but little ductility of less than one percent is reported for BMGs at room temperature. However, it is found that Cu-Zr base BMG exhibits both high yield strength and enlarged ductility along with plastic strain upto 16% [10]. One of the most significant thermodynamic characteristic is thermal expansion and is greatly associated with the amorphous structure of BMGs [11]. BMGs compared to crystalline solids, show different thermal expansion behavior that may limit their practical applications. Therefore, it is very important to investigate the thermal expansion behavior of BMGs [12].

The aim of this work is to form and characterize the structural, mechanical and thermal behavior of Cu-Zr BMGs. The local structure of BMGs is analyzed by means of RDF and local atomic number density and the mechanical behavior is explored using uniaxial compression. Thermal behavior of Cu-Zr BMGs is investigated through resulting length, volume and thermal expansion coefficient.

2. Simulation methodology

Classical MD simulations have been performed using the Large-scale Atomic or Molecular Massively Parallel Simulator (LAMMPS). Glass formation has been achieved through melt quenching technique. In the first step we construct a simulation cell consisting of 6084 Cu atoms possessing B_2 crystal structure. The Cu atoms are then randomly substituted with Zr atoms in order to achieve the desire $Cu - Zr$ configuration with various concentrations. A generalized renowned type of EAM potential created by Finnis Sinclair [13] is used for the interatomic interactions.

$$E_i = F_\alpha \left(\sum_{j \neq i} \rho_{\alpha\beta}(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij})$$

where F is function of atomic electronic density ρ and is called embedding energy. ϕ represents pair interaction between atoms, and α and β are the element kinds of atoms i and j . Periodic boundary conditions are applied in all dimensions to describe the bulk volume and to eliminate the surface effects. We adopted Verlet's algorithm with a time step of 1fs for the integration of equation of motion. Conjugate gradient method is employed to minimize the energy of sample. The sample is equilibrated at this minimum energy at 300 K. The sample is then heated upto 2000 K (above its melting temperature) so that the atoms are able to leave their initial positions. To achieve good glass forming the cooling rate is kept high so that crystallization may cease and reordering of atoms may be avoided. Sample is allowed to equilibrate at this temperature for 500 ps and then quenched down to 300 K using temperature step of 200 K through a cooling rate of the order of 20 K/ps. The sample is equilibrated after each temperature step for 250 ps so that all the atoms may achieved homogenous temperature. Finally the sample is equilibrated at 300 K for total time of 1 ns [14]. The initial crystalline structure and final BMGs of $Cu_{50}Zr_{50}$ sample is

shown in figure 1(a & b) respectively. During the simulation process (isothermal-isobaric) NPT ensemble have been employed. In this technique time integration on the Nose Hoover style non Hamiltonian equations of motion has been performed. Thermostating is performed by adding some dynamic variables coupling with velocities of the particles and barostating is achieved by adding some dynamic variable in the dimension of simulation domain.

3 Results and discussions

3.1 Characterization of Cu₅₀Zr₅₀ Bulk Metallic Glasses

To characterize the bulk metallic glasses we choose Cu₅₀Zr₅₀ configuration. The sample is prepared using above mentioned methodology through melt quenching technique. The resulting Cu₅₀Zr₅₀ bulk metallic glass is shown in figure 1(b).

Figure 1: (a) initial crystalline $Cu_{50}Zr_{50}$ structure at 300 K (b) final amorphous $Cu_{50}Zr_{50}$ (BMG) structure at 300 K, where blue and yellow colors represent Cu and Zr atoms respectively.

The difference between initial crystalline $Cu_{50}Zr_{50}$ and final amorphous $Cu_{50}Zr_{50}$ (BMG) structure is obvious from figure 1. In crystalline $Cu_{50}Zr_{50}$ structure figure 1(a) all atoms are arranged in regular manner while in amorphous $Cu_{50}Zr_{50}$ BMG structure figure 1(b) the atoms are at random positions.

The radial distribution function (RDF) analysis is a useful approach for collecting structural information about the systems, especially liquids and glasses. Figure 2 represents the

RDF curves for initial $\text{Cu}_{50}\text{Zr}_{50}$ configuration at 300 K indicating crystalline state and final amorphous $\text{Cu}_{50}\text{Zr}_{50}$ configuration at 300 K.

Figure 2: RDF plot for the initial and final configuration of $\text{Cu}_{50}\text{Zr}_{50}$ sample.

In case of crystalline $\text{Cu}_{50}\text{Zr}_{50}$ structure for small value of r the function is zero because the atoms can approach to a certain limited distance. It shows a rise at a nearest-neighbor distance of 2.5 Å, falls down to zero, and further peaks appear at distances relating to second neighbors and so on. For amorphous $\text{Cu}_{50}\text{Zr}_{50}$ (BMG) the first and second peaks of RDF show a slight shift towards right in comparison with crystalline counterpart. This is in accordance with the fact that amorphous materials have usually lower density than that of crystalline materials. The second neighbor peak in the amorphous $\text{Cu}_{50}\text{Zr}_{50}$ (BMG) material is splitted and slightly broader than the corresponding peak in the crystalline $\text{Cu}_{50}\text{Zr}_{50}$ material. Splitting of the second peak is characteristic of an amorphous structure. But the very strong 3rd neighbor peak of crystalline $\text{Cu}_{50}\text{Zr}_{50}$ is almost entirely missing from amorphous $\text{Cu}_{50}\text{Zr}_{50}$ structure RDF [15].

In order to observe the density variations in the initial and final configurations of $\text{Cu}_{50}\text{Zr}_{50}$, we divide the simulation box along z -direction into small slices, each of volume V_i . Within these slices of width 0.1 nm, the local atomic density and cross sectional area are

measured for Cu and Zr constituents. Comparison of local atomic density of initial and final configurations of $\text{Cu}_{50}\text{Zr}_{50}$ is shown in figure 3.

Figure 3: Atomic density as a function of position (z) for initial and final configurations of $\text{Cu}_{50}\text{Zr}_{50}$ sample.

It is clear from the graph that long range density oscillations are observed in the initial configuration of $\text{Cu}_{50}\text{Zr}_{50}$ sample and this is characteristic of a crystalline material. Final configuration does not show such long range density fluctuations rather their fluctuations decay into an almost constant and featureless total number density and this behavior is expected for a totally disordered structure.

The $\text{Cu}_{50}\text{Zr}_{50}$ (BMG) is deformed under uniaxial compression along z-direction at 300 K by applying a constant strain rate of $0.4 \times 10^9/\text{s}^{-1}$ along z-direction. Periodic boundary conditions are implemented in all directions. To allow free movement in x and y direction, pressure is kept at zero bar in these directions. Figure 4 (a to f) displays the snapshots of the deformation in $\text{Cu}_{50}\text{Zr}_{50}$ BMG at different time steps.

Figure 4: Deformation of $\text{Cu}_{50}\text{Zr}_{50}$ BMG at various time steps. (a) 2.5 ps (b) 250 ps (c) 500 ps (d) 750 ps (e) 1000 ps and (f) 1227 ps respectively. Blue color represents Cu atoms and yellow color refers to Zr atoms.

The resulting stress-strain curve for $\text{Cu}_{50}\text{Zr}_{50}$ BMG at a strain rate of $0.4 \times 10^9/\text{s}^{-1}$ is displayed in figure 5.

Figure 5: Uniaxial compressive loading stress VS strain for $\text{Cu}_{50}\text{Zr}_{50}$ BMG at $0.4 \times 10^9/\text{s}^{-1}$ strain rate.

It is evident from the stress strain curve that $\text{Cu}_{50}\text{Zr}_{50}$ BMG initially show elastic behavior (i.e stress increases with increase in strain) with a yield strength of 2.18 GPa. After that it exhibits plastic deformation without any work hardening. The plastic region of compressive stress-strain curve represents serrated flow, which is suggestive of the evolution/propagation of multiple shear bands during the process of compressive loading. Similar behavior (serrated flow above the yield point of MG under compressive loading) is observed in Zr-based and Pd-based

BMGs [16]. Largely, this serrated flow can be attributed to the shear band formation. Nearly one observable serration can be described as a shear band event [17] that may involve one or more than one shear bands [18]. From the stress-strain curve it can be noticed that there is no dramatic change in maximum stresses occurring in plastic region, however decrease in minimum stresses is observed as deformation progresses [18].

Elastic behavior (i.e. the stress reloading) observed in the plastic region doesn't contribute to plastic deformation. The plastic strain only results from the load drop i.e. shear band propagation. In BMGs, plastic deformation begins with the beginning of shear localization. The shear band development is related with free volume creations. At low temperature, free volume created by an external load at a specific site when achieves a certain value results in the nucleation of shear band at this site. This shear band formation causes load drop. Very high expansion speed of the shear band makes it stable soon after its formation and consequently the load drops ceases. For further deformation, new shear bands are needed as the present shear bands are immovable. For nucleation of new shear bands, stress is restored to yield point. New shear band causes load drop again. The repetition of this process gives rise to serrations in stress strain curve [19].

3.3 Effect of component concentrations

We chose three different compositions $Cu_{25}Zr_{75}$, $Cu_{50}Zr_{50}$ and $Cu_{75}Zr_{25}$. Similar to $Cu_{50}Zr_{50}$ (BMG) formation, $Cu_{25}Zr_{75}$ and $Cu_{75}Zr_{25}$ are also prepared by heating the sample substrates of $Cu_{25}Zr_{75}$ and $Cu_{75}Zr_{25}$ upto 2000 K (above melting temperature) and finally quenching the samples to 300 K. To study the effect of component concentration on glass formation and stability of BMGs, RDFs of $Cu_{25}Zr_{75}$, $Cu_{50}Zr_{50}$ and $Cu_{75}Zr_{25}$ are compared. RDF curves may give useful knowledge to certify the impact of various concentrations of components on final structures and stability of BMGs in this respect. To explain the possible variation in the final structures of three samples, the curves of RDF are plotted against interatomic distance in figure 6. The RDF curves for $Cu_{25}Zr_{75}$, $Cu_{50}Zr_{50}$ and $Cu_{75}Zr_{25}$ are shown by black, red and blue colors respectively.

Figure 6: RDF plot for $\text{Cu}_{25}\text{Zr}_{75}$, $\text{Cu}_{50}\text{Zr}_{50}$ and $\text{Cu}_{75}\text{Zr}_{25}$ at 300 K.

Figure exhibits the clear difference among the final structures of $\text{Cu}_{25}\text{Zr}_{75}$, $\text{Cu}_{50}\text{Zr}_{50}$ and $\text{Cu}_{75}\text{Zr}_{25}$ BMGs at 300 K. The analysis of peaks of RDF curves of $\text{Cu}_{75}\text{Zr}_{25}$, $\text{Cu}_{50}\text{Zr}_{50}$ and $\text{Cu}_{75}\text{Zr}_{25}$ gives useful information about glass formation. The earliest peak of RDF is the highest for $\text{Cu}_{25}\text{Zr}_{75}$ composition, and show lowest value for $\text{Cu}_{75}\text{Zr}_{25}$ composition while $\text{Cu}_{50}\text{Zr}_{50}$ has a value in between. This shows that final configurations will be considerably different for the three compositions. It is found that peak height decreases with relative increase in Cu concentration, hence the structural stability and glass forming ability of sample increases with increasing Cu concentration. Comparison of the RDF curves shows that compositions do not affect the nearest neighbor distances. Similar behavior has been also observed before and after this shift has been characterized by densified atomic packing with increased Cu-content, because of improved topological atomic ordering [20].

To understand the effect of component concentrations on the mechanical behavior of Cu-Zr BMGs, $\text{Cu}_{25}\text{Zr}_{75}$, $\text{Cu}_{50}\text{Zr}_{50}$ and $\text{Cu}_{75}\text{Zr}_{25}$ BMGs are deformed under uniaxial compression at a strain rate of $0.4 \times 10^9/\text{s}^{-1}$ and the respective stress-strain curves for these BMGs are plotted in figure 7. Black, red, and blue colors represents the stress-strain curves for $\text{Cu}_{25}\text{Zr}_{75}$, $\text{Cu}_{50}\text{Zr}_{50}$ and $\text{Cu}_{75}\text{Zr}_{25}$ BMGs respectively.

Figure 7: Uniaxial compressive loading stress VS strain for $Cu_{25}Zr_{75}$, $Cu_{50}Zr_{50}$ and $Cu_{75}Zr_{25}$ at constant strain rate.

The comparison of these curves shows that yield strength is maximum for $Cu_{75}Zr_{25}$ BMGs, and minimum for $Cu_{25}Zr_{75}$ BMG. It is evident that yield strength increases with increasing Cu-concentration. Maximum plastic strain is observed for $Cu_{25}Zr_{75}$ BMG and minimum plastic strain is observed for $Cu_{75}Zr_{25}$ BMG. Hence ductility is found to decrease with increasing Cu-concentration in sample. It has been observed that plasticity depends on the packing density of amorphous alloys. Alloys with lower packing density (lower short range ordering and increased percentage of free volume) exhibits enhanced plasticity and vice versa. In Cu-Zr alloys it is found that packing density increases with increase in Cu content [11]. This is the reason for low ductility in $Cu_{75}Zr_{25}$ BMG. Also it is clear from the curves that the sample with the highest Cu concentration (i.e. $Cu_{75}Zr_{25}$ BMG) fractures first. While $Cu_{25}Zr_{75}$ BMG prove to be more ductile and fails lastly. Tendency to fractures increases with increasing Cu-concentration in sample; we can conclude that brittleness increases with increasing Cu concentration.

To study the effect of component concentration on the thermal expansion of Cu-Zr BMGs, we heat $\text{Cu}_{25}\text{Zr}_{75}$, $\text{Cu}_{50}\text{Zr}_{50}$ and $\text{Cu}_{75}\text{Zr}_{25}$ samples from 300 K to 900 K, above the glass transition temperature (≈ 700 K) [21] using MD simulation. Variation in length and volume is measured. Variation of length and volume with temperature is shown in figure 8 and 9 respectively.

Figure 8: Length VS temperature curve showing the variation in length of samples with temperature for $\text{Cu}_{25}\text{Zr}_{75}$, $\text{Cu}_{50}\text{Zr}_{50}$ and $\text{Cu}_{75}\text{Zr}_{25}$ BMGs.

Figure 9: Volume VS temperature curve exhibiting the variation of volume with temperature.

From the analysis of these curves, It can be revealed that $\text{Cu}_{25}\text{Zr}_{75}$, and $\text{Cu}_{50}\text{Zr}_{50}$ expand with the increase in the temperature. Expansion behavior of $\text{Cu}_{75}\text{Zr}_{25}$ is quite different as it show anomalous expansion. As BMGs are prepared through rapid quenching from melt at high cooling rates therefore $\text{Cu}_{75}\text{Zr}_{25}$ contain relatively higher excess of free volume. This is due to relatively higher glass forming ability of $\text{Cu}_{75}\text{Zr}_{25}$ compared to other configurations. When we increase the temperature of $\text{Cu}_{75}\text{Zr}_{25}$ BMGs from the room temperature the structural relaxation occurs in the BMG sample which gives rise to short range ordering. This topological short range ordering causes long range rearrangements of all the atoms through diffusion and atomic redistribution. This eventually results in the reduction of free volume present in the $\text{Cu}_{75}\text{Zr}_{25}$ sample. This relative reduction in length and volume is the direct consequence of annihilation of excess free volume and atomic redistribution due topological short range ordering. This results in anomalous thermal expansion of $\text{Cu}_{75}\text{Zr}_{25}$ and an irreversible increase in the density of sample. Figure 10 shows the linear expansion coefficient versus temperature curves of $\text{Cu}_{25}\text{Zr}_{75}$, $\text{Cu}_{50}\text{Zr}_{50}$ and $\text{Cu}_{75}\text{Zr}_{25}$ BMGs.

Figure 10: Variation of linear thermal expansion coefficients of $Cu_{25}Zr_{75}$, $Cu_{50}Zr_{50}$ and $Cu_{75}Zr_{25}$ BMGs with temperature.

It is clear from the graph that curves are approximately linear for $Cu_{25}Zr_{75}$, and $Cu_{50}Zr_{50}$ sample. This is described as the normal thermal expansion behavior. $Cu_{75}Zr_{25}$ BMG exhibits an anomalous behavior which can be clearly predicted from the negative values of thermal expansion coefficient. This occurrence of negative thermal expansion coefficient is also the result of reduction in volume and length due to atomic readjustment and topological short range ordering during the heating process.

Conclusions

In this study MD simulation is carried out to form and characterize Cu-Zr BMGs using LAMMPS (MD simulator). Three different compositions i.e. $Cu_{25}Zr_{75}$, $Cu_{50}Zr_{50}$ and $Cu_{75}Zr_{25}$ are prepared using melt quenching technique. It is concluded from the results of uniaxial compressive deformation of Cu-Zr BMGs that deformation mechanism of glasses is different from that of crystalline materials due to disordered structure. It is observed from the results that all BMGs samples exhibited shear deformation under compressive loading unlike brittle fracture during uniaxial tensile deformation, these BMGs exhibited limited plastic deformation in compression. The BMG with relatively higher Cu concentration has higher yield strength and lower probability of short range ordering and vice versa. The thermal expansion plot of three BMGs sample with various concentration shows that $Cu_{25}Zr_{75}$, and $Cu_{50}Zr_{50}$ expanded with the increase in the temperature. Expansion behavior of $Cu_{75}Zr_{25}$ is quite different as it show anomalous expansion. Initially it contract with the increase in the temperature due to lower density and free spaces in the glass at room temperature.

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