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Variation of glass transition temperature of $Al_{90}Sm_{10}$ metallic glass under pressurized cooling

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ABSTRACT

In this paper, the role of hydrostatic pressure in $Al_{90}Sm_{10}$ bimetallic glass formation has been studied using molecular dynamics simulations with Embedded Atom Method (EAM) potential. The bimetallic glass is prepared by subjecting the $Al_{90}Sm_{10}$ alloy to hydrostatic pressure (P = 0, 2, 4, 6, 8 GPa) during cooling the melt (cooling rate~1 K/ps) and the variation in glass transition temperature is determined. It is observed that the glass transition temperature rises as applied hydrostatic pressure increases.RDF analysis indicates the enhancement in local ordering of the $Al_{90}Sm_{10}$ alloy with increasing applied pressure. Voronoi analysis of the bimetallic glass reveal that the glass-transition temperature behavior seems to be greatly influenced by distorted ICO-like structures Z14 < 0, 2, 8, 4 > , Z13 < 0, 1, 10, 2 > , Z13 < 0, 2, 8, 3 > . However, population of T6 motifs (3661 motifs) remains constant irrespective of the variation in applied hydrostatic pressure. This work as a whole provides an insight towards co-relation between glass transition process and applied pressure during cooling along with underlying physics for $Al_{90}Sm_{10}$ bimetallic glass.

1. Introduction

Amorphous Metallic alloys or Bulk Metallic Glass (BMGs) have been drawing much attention in the past few decades due to their corrosion resistant [1], high specific strength [2, 3], ultrahigh fracture toughness [4], excellent thermoplastic formability [5, 6] and superior biocompatibility [7]. Among the BMGs Al–based rare earth amorphous alloys (Al-R) with high Al content (> 80%) have attracted tremendous interests of the scientific community due to their superior strength-to-weight ratio and high fracture strengths in addition to the mentioned above properties [8–10]. An insight of the structure of these undercooled liquids is vital for developing an understanding of such unique behavior of the Al-R amorphous alloys based on structure property correlation. Al—Sm binary alloy has glass forming ability for widest range of compositions (i.e. from 8 to 16 atomic percent of Sm) [11] among all the Al-R systems and therefore it gets significant focus from the researchers. Experimental studies have been carried out by the investigators to determine the glass transition temperature of $Al_{92}Sm_8$ produced by different processing routes [12] and study the effect of quenching conditions on devitrification behavior of Al_xSm_{100-x} [13]. Attempts have also been made by the researchers to analyze the transformation kinetics and microstructural evolution during initial crystallization [14] and investigating the local structure in rapidly quenched Al_xSm_{100-x} employing transmission electron microscopy (TEM) and high energy synchrotron X-ray Diffraction (HEXRD) [15]. Additionally, Wang et al. [16] have studied the evolution of microstructure as a function of velocity or interface undercooling for Al_xSm_{100-x} systems. At higher cooling rates the size of the crystals or amorphous structure so formed are very small to be resolved by conventional TEM or XRD [14]. Therefore, it becomes challenging for the scientific communities to study the structural evolution of the binary Al—Sm alloys via experimentation. Moreover, Molecular Dynamics (MD) has proven to be a powerful tool for investigating the structures and properties of the BMGs, owing to its ability to provide detailed atomic trajectories [17] and dynamic characterization of structural evolution [18]. In addition, identification of the short range ordering (SRO) phenomenon during the fast solidification and the role of various process parameters on glass formation of Al—Sm metallic glasses during rapid quenching can be investigated by MD simulation. Sun et al. [18] have carried out ab-initio MD (AIMD) simulation to investigate the variation of SRO and (Medium Range order) MRO with varying cooling rates and have reported the significant enhancement of the SROs and MROs with decreasing cooling rate. Bokas et al. [19] have stated based on their study that the glass forming ability of the Al—Sm amorphous alloys increases with increasing Sm percentage until 10 atomic percent. They have also reported that addition of any further Sm decreases the

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diffusion coefficient of the central Al-atoms of the ICO-like structures subsequently leading to insignificant enhancement in glass forming ability of the Al−Sm binary alloys. MD simulations have been performed [20] at solid-liquid interfaces to examine the structural differences at the interface of undercooled $Al_{90}Sm_{10}$ alloy. Sun et al. [21] have carried out genetic algorithm based study to understand the underlying structural order transcending at liquid glass and crystalline states of $Al_{90}Sm_{10}$ alloy. AIMD simulations have been carried out by Zhang et al. [22] to capture short range to medium range co-relation of the system. They have found out that that interpenetrating structures of the Sm centered structures is less favorable in the $Al_{90}Sm_{10}$ alloy owing to the intrinsic repulsion between the Sm atoms. It is evident from the literature that no work has been reported on the effect of pressure during quenching on the glass transition behavior of the Al−Sm alloys.The present study aims to investigate the implication of applied hydrostatic pressure on glass forming process by considering its influence on glass transition temperature. Moreover in this study we have attempted to report the underlying mechanism (in particular to the cluster evolution) of the glass transition behavior in $Al_{90}Sm_{10}$ alloy based on voronoi cluster analysis and radial distribution function (RDF) plots.

2. Simulation details

MD simulations are performed employing Finnis-Sinclair empirical potential [23] developed for Al−Sm MGs (Sm concentration up to 25 atomic percent) in isothermal- isobaric (NPT) ensemble to model the interatomic interactions for $Al_{90}Sm_{10}$, using LAMMPS software package [24]. The system is initially constructed with 62,500 atoms under periodic boundary conditions arranged on fcc (face centered cubic) lattice in a cubic box with the dimensions of $10 \times 10 \times 10$ nm^3 (refer Fig. 1 (a)). A constant integration time step of 2 fs is considered for the simulation study. Al and Sm atoms are randomly distributed throughout the sample such that the ratio of Sm to Al atoms is 0.11. The energy minimized configuration of the sample is achieved by the conjugate gradient algorithm. Simulations are performed in NPT ensemble where the temperature and pressure are controlled using Nose-Hoover thermostat and barostat respectively [25, 26]. The sample is subsequently melted and equilibrated for 50 ps at 1750 K several hundred degrees above the melting temperature of $Al_{90}Sm_{10}$ [13]. Latterly, all the systems are quenched to 300 K at a rate of 10^{12} Ks^{-1} under varying hydrostatic pressure i.e. 0 GPa, 2 GPa, 4 GPa, 6 GPa and 8 GPa. A schematic representation of the amorphisation process has been illustrated in Fig. 1(b). To identify the evolution of various cluster arrangement during amorphisation various techniques (as implemented in the OVITO [27] software) are employed to visualize and analyze the simulation results like Centro-symmetry Parameter (CSP) estimation [28],Voronoi Polyhedra analysis [29] and Radial Distribution Function (RDF) analysis. The amorphisation of the $Al_{90}Sm_{10}$ sample has been demonstrated by the color coded CSP values as the process proceeds (refer Fig. 1).

3. Result and discussion

3.1. Variation of glass-transition temperature with pressure

In order to identify glass transition temperature (T_g), variation of volume as a function of temperature during the cooling process has been plotted in Fig. 2. As mentioned in the previous section the sample is melted at 1750 K, several hundred degrees above the melting temperature of $Al_{90}Sm_{10}$,1200 K [13]. Several investigators have also employed similar temperature range [19, 22, 23] for carrying out the simulation based study of glass transition behavior of Al−Sm alloys.Then the varying volume values obtained is linearly fit and the glass transition temperature (T_g) is manifested by the intersection of the two lines as at T_g slope changes, and the method is commonly used in literature [30]. Fast cooling of molten alloy does not provide enough time duration for required movement and reorientation of the atoms in liquid phase necessary for long range ordering, thus leading to formation of an amorphous phase with excess free volume in the system [31, 32]. The T_g obtained for $Al_{90}Sm_{10}$ alloy at 0 GPa pressure is 645 K (refer Fig. 2 (a)) similar to findings reported by Mendelev et al. [23], where the value of T_g is reported to be 693 K. The slight variation in T_g from that reported in the literature than that attained in this study might be due to the variation in the simulating parameters such as the temperature up to which the sample is heated, the cooling rate or the holding time at the high temperature before carrying out the cooling process. However, the T_g reported in this study is closer to that experimentally (T_g = 445 K) determined [12] for $Al_{92}Sm_8$ alloy. The deviation in the experimental-based and simulation-based study values

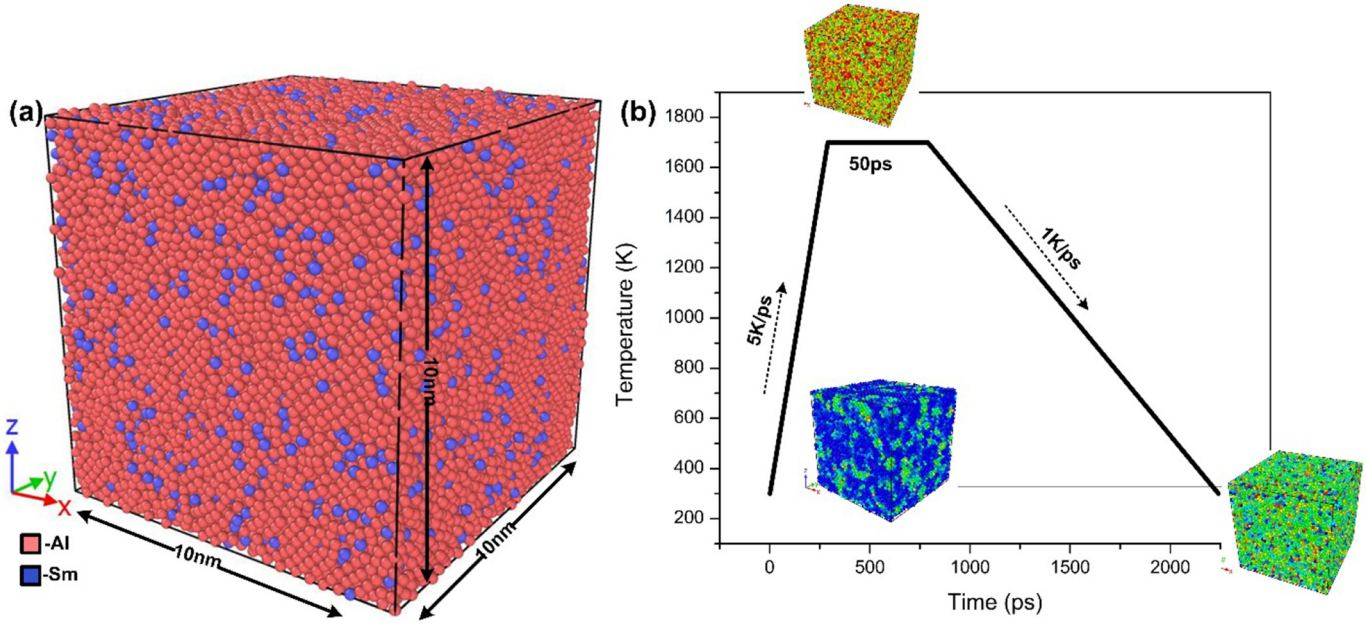

Fig. 1. (a) Three-dimensional $Al_{90}Sm_{10}$ metallic glass specimen color-coded according to particle type (b) Variation of temperature during the heating and cooling process along with snapshots of the specimen at different stages color coded according to Centrosymmetry Parameter values (CSP).