Computational Materials Science 155 (2018) 129–135

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Local atomic environment and shear banding in metallic glasses

Marcela Tercini, Roberto Gomes de Aguiar Veiga, Alejandro Zúñiga*

CECS, Federal University of ABC, Santo André, SP, Brazil

ARTICLE INFO

Keywords:
Metallic glass
Deformation
Shear band
Molecular dynamics
Atomic environment

ABSTRACT

In this work we studied the compression behavior of a $Cu_{45}Zr_{45}Al_{10}$ metallic glass and the relationship between the local atomic environment and shear banding using molecular dynamics. The $Cu_{45}Zr_{45}Al_{10}$ metallic glass was first produced using the quenching technique and then deformed in compression for up to 20% at a strain rate of $10^8\ s^{-1}$. Both the compression stress-strain curve and analysis of the local shear strain show that shear banding is initiated at approximately 5%, while Voronoi analyses indicate that the most significant structural change as a function of compression strain is a decrease in the amount of Cu-centered ⟨0, 0, 12, 0, 0⟩ icosahedra. Additionally, we propose a novel quantitative tool for characterizing the local atomic environment in the metallic glass: the local density of atoms that satisfy a given condition. By using this tool for three different conditions we observed a strong spatial correlation between shear banding and the distribution of distorted Cu-centered ⟨0, 0, 12, 0, 0⟩ icosahedra.

1. Introduction

Metallic glasses (MGs) are metallic alloys with an amorphous structure that only possess short and medium range order [1,2]. In general MGs have a unique combination of exceptional properties such as low elastic modulus, high elastic limit, and high elastic strain limit [3,4]. In particular, Cu-Zr and Cu-Zr-Al metallic glasses have been widely studied due to their excellent glass forming ability and high ductility in compression [5,6]. It has been long recognized that the mechanical behavior of MGs is different from that of traditional (crystalline) alloys since plastic deformation in MGs is not governed by dislocation movement but strain localization instead. Strain localization in MGs is initiated with the formation of shear transformation zones (STZ) that evolve into well-developed shear bands (SB) [7]. Shear transformation zones generally appear at the softest regions of the glass during the beginning of the plastic regime, turning these regions more susceptible to flow [7]. It has been also shown that the short range order of a metallic glass greatly influences the formation of shear transformation zones and shear bands [8]. Therefore, a great deal of effort has been made to try to understand the relationship between short range order and strain localization. However, short range order is difficult to study experimentally due to the limitations in spatial and temporal resolution of the available experimental techniques [9]. For that reason, atomic simulations in general and molecular dynamics in particular have been used extensively in the study of deformation in metallic glasses.

Several simulation studies have shown that local icosahedral arrangements play a key role in the formation of shear bands. This is not surprising since icosahedra are the most common polyhedra in Cu-Zr metallic glasses (they act as barrier for crystallization during solidification) [8]. Similarly, an increase in the concentration of icosahedral environment has been associated with an increase in resistance to plastic flow [10]. Another important concept used to characterize the influence of the local atomic environment on the formation of shear bands is that of local fivefold symmetry (LFFS). The LFFS quantifies the fraction of pentagons in a given Voronoi polyhedron (or atomic environment) [11]. Some studies have shown that shear band formation is related to local distributions of the LFFS [11,12], and that regions with high degree of LFFS have low free volume [13]. A related metrics used to study the local symmetry in disordered systems is the bond orientational order parameter, which quantifies the organization of clusters based on angular relationships and it is widely used to characterize symmetry in liquids or glasses [14]. Therefore, local environment and symmetry in MGs can be studied using several metrics or parameters and a deeper understanding of these structural parameters can be the key to understanding plastic deformation in MGS [13]. In this work we studied the deformation of a $Cu_{45}Zr_{45}Al_{10}$ metallic glass in compression using molecular dynamics. We also propose a new quantitative tool (local density of atoms that satisfy a given condition) as a means to study local variations of key structural parameters in our metallic glass as a function of compression strain. The use of these local density maps allowed us to spatially correlate shear banding with

* Corresponding author at: Avenida dos Estados, 5001, Bairro Santa Terezinha, Santo André, CEP 09210-580 SP, Brazil.
E-mail address: alejandro.zuniga@ufabc.edu.br (A. Zúñiga).

https://doi.org/10.1016/j.commatsci.2018.08.025
Received 20 June 2018; Received in revised form 10 August 2018; Accepted 12 August 2018

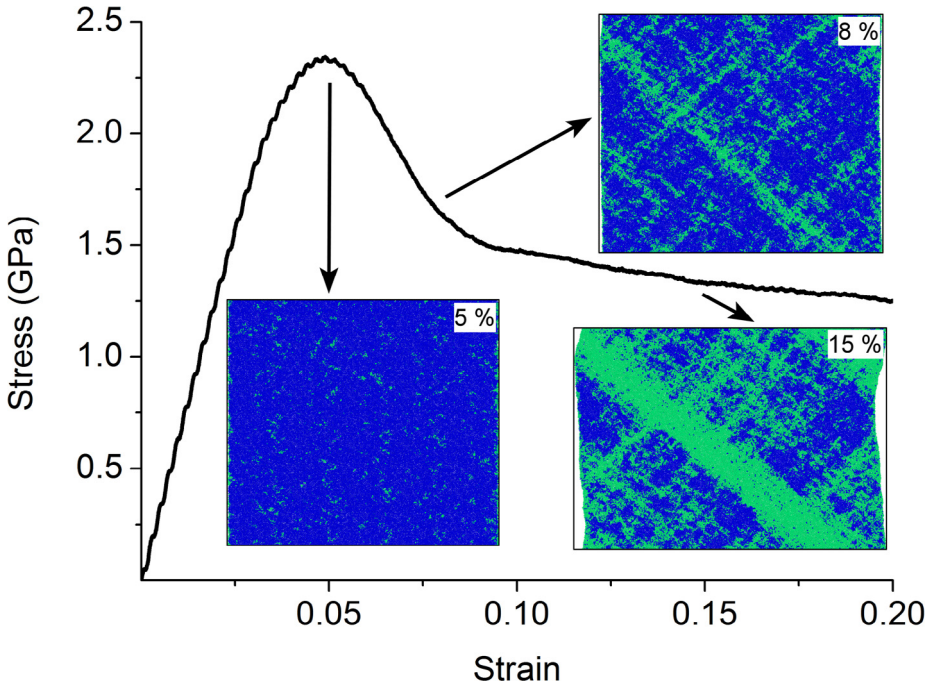

Fig. 1. Compression stress-stress curve and snapshots of the of local atomic shear strain for 5%, 8% and 15% compression strain.

changes in the local atomic environment.

2. Simulation details

A $Cu_{45}Zr_{45}Al_{10}$ amorphous model was produced *via* molecular dynamics using the quenching technique in the isothermal-isobaric (NPT) ensemble. First, a $Cu_{45}Zr_{45}Al_{10}$ crystal with a B2 structure and 54,000 atoms was heated to 2000 K in 10 ps, kept at that temperature for 50 ps and then cooled down to 300 K at a cooling rate of 0.17 K/ps. Finally, the system was maintained at 300 K for 50 ps to stabilize the amorphous structure. This 54,000-atom amorphous model was repeated five times in each direction to produce a 50 nm × 50 nm × 50 nm $Cu_{45}Zr_{45}Al_{10}$ simulation model containing 6,750,000 atoms. This large simulation box was then used to simulate a uniaxial compression test in the microcanonical (NVE) ensemble with periodic boundary conditions in the x and z directions, and non-periodic boundary conditions in the y direction. Prior to deformation the system was let to relax for 10^4 time steps (10 ps), ensuring that the total energy and the temperature both reached a steady state value. The uniaxial compression simulation was carried out at a strain rate of 10^8 s^{-1} for 2×10^6 time steps (2000 ps), which is equivalent to a total strain of 20%. All the simulations were performed using the Large-scale Atomic Molecular Massively Parallel Simulator (LAMMPS) software [15], the embedded atom potential (EAM) developed by Cheng et al. [16], and a time step of 1 fs. For analysis of the simulation results we used the Open Visualization TOol (OVITO) software [17].

3. Results and discussion

3.1. Stress-strain curve and shear localization

Fig. 1 shows the simulated compression stress-strain curve along with snapshots of the local atomic shear strain at different values of compression strain (5, 8 and 15%). The local atomic shear strain (η_i) is a good measure of the local inelastic deformation in amorphous materials and can be calculated as [18]:

$$\eta_i = \sqrt{\eta_{yz}^2 + \eta_{xz}^2 + \eta_{xy}^2 + \frac{(\eta_{yy}-\eta_{zz})^2 + (\eta_{xx}-\eta_{zz})^2 + (\eta_{xx}-\eta_{yy})^2}{6}} \quad (1)$$

where $\eta_{\alpha\beta}$ are the components of the strain tensor at atomic position $\mathbf{r}_i$. Regions of the snapshots of Fig. 1 where the local atomic shear strain is greater than 0.2 (or 20%) have been colored green, whereas regions where the local atomic shear strain is less than 0.2 have been colored blue[1] [19].

It can be observed that the flow stress in the stress-strain curve increased linearly until a maximum value is reached at 5% compression strain. At this point shear transformation zones can already be seen in the corresponding snapshot of local shear strain, indicating incipient shear localization. Some authors have related such incipient localization with atomic rearrangements associated with the mechanical instability of the potential energy landscape [20]. When our compression test reached ~8% strain, well defined regions of localized deformation (i.e. shear bands) are clearly seen, and the flow stress decreased compared to the maximum value reached at 5% strain. Greer et al. [7] argue that homogeneously nucleated STZ (as the ones seen in our simulation at 5% strain) can coalesce when a percolation threshold is reached, forming a shear band and inducing a decrease in the flow stress. Similarly, Homer [21] describes the following stages during deformation in amorphous metals: linear elastic response, STZ formation and clustering, shear band nucleation and growth, relaxation and thickening of the shear bands. In the relaxation and thickening stage, the stress to nucleate a shear band is significantly higher than the one needed to continue propagating the shear bands already formed. Therefore, the system tries to relax the flow stress via shear propagation and thickening as well as via interactions between the bands and the free surface. These interactions between shear bands and free surface play a key role in the relaxation of the flow stress. In fact, it has been experimentally observed that metallic glass nanowires exhibit a stress drop in the stress-strain curve due to shear band interaction with free surfaces [22]. The shear bands in our simulations are already interacting with the free surface at 8% compression strain, forming steps. At 15% compression strain, well defined and matured shear bands can be observed, along with a flow stress that decreases at a much lower rate (relaxation and thickening stage). All these observations are in good agreement with

[1] For interpretation of color in Figs. 1, 3–5, the reader is referred to the web version of this article.