



Size distribution of shear transformation zones and their evolution towards the formation of shear bands in metallic glasses



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ARTICLE INFO

Article history:

Received 5 March 2016

Received in revised form 26 April 2016

Accepted 1 May 2016

Available online 20 May 2016

Keywords:

Shear transformation zone

Shear band

Metallic glasses

Molecular dynamics simulations

ABSTRACT

The room temperature tensile deformation behavior of two metallic glasses (MGs), $\text{Cu}_{64}\text{Zr}_{36}$ and $\text{Cu}_{40}\text{Zr}_{60}$, was investigated, by employing molecular dynamics simulations, with a view to examine the evolution of plastic deformation at the atomistic scale. It was found that after reaching the maximum stress, atoms in areas with lower packing efficiency, which have liquid-like polyhedral atomic configurations, exhibit larger displacement. On further deformation, the atoms in rigidly packed regions, which have solid-like polyhedral atomic configurations, also start partaking in the plastic deformation, especially within the shear band region. The average shear transformation zone (STZ) size, defined by the coordination neighborhood of highly strained atoms, was found to increase from 17 ± 3 to 106 ± 6 atoms within the strain range of 7–12%, which spans the shear band initiation to mature formation, in both MGs examined. A detailed examination of the distributions of the number and the size of STZs as a function of strain reveals that the formation of the shear band is linked with the occurrence of a few super-sized STZs.

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1. Introduction

The unit processes and mechanisms responsible for plastic deformation in metallic glasses (MGs) are researched extensively by using experimental, theoretical and computational tools in the past couple of decades [1–8]. Briefly, the current understanding is as follows. The unit carriers of plasticity, which are analogous to mobile dislocations in crystalline metals, are the shear transformation zones (STZs) [2,3]. These STZs are clusters of atoms that undergo collective shuffle/displacement from their mean positions, so as to accommodate strain and in the process relax the applied stress. While consensus in published literature on the size of the STZs is still elusive [4–8], it is generally agreed that the STZs get activated in those regions where the atomic packing is less efficient, i.e., local free volume content is more [9,10]. At high temperatures, i.e., when the temperature of deformation is higher than the glass transition temperature, STZs carry the entire deformation and plasticity is homogeneous [1]. At lower temperatures, on the other hand, when the applied stress is sufficiently large, plastic deformation manifests in the form of localized flow bands or shear

bands [11–13]. While a number of different aspects of these bands were extensively investigated, it remains unclear as to how the deformation localization evolves from STZs. The work reported in this paper attempts to address this through molecular dynamics (MD) simulations, which facilitate the visualization and study of deformation starting from the atomic level to the initiation and mature formation of a shear band. Another objective of the present study is to relate various events in the macroscopic stress-strain response (especially the occurrence of strain localization) of an MG with the internal atomic-level structural evolution in it [10]. Recently, the internal structural evolution in the early stages of shear banding in $\text{Cu}_{64}\text{Zr}_{36}$, was investigated by Cao et al. [10]. By monitoring the local structural evolution during mechanical deformation, they demonstrated as to how the atomic-level structure controls the shear band initiation and thus the mechanical properties. They suggest that the atoms with Voronoi index [0,0,12,0] play the most important role during the shear banding. However, the structure of $\text{Cu}_{64}\text{Zr}_{36}$ is relatively special amongst Cu-Zr alloys in the sense that they contain a large number of [0,0,12,0] clusters as compared to other Cu-poor alloy compositions, and hence are not representative of the deformation processes that occur in all MGs. To address this deficiency, we use MD simulations to investigate the shear localization behavior of Cu-rich ($\text{Cu}_{64}\text{Zr}_{36}$) as well as Cu-poor ($\text{Cu}_{40}\text{Zr}_{60}$) MGs. In the course of investigation the following issues are also addressed in

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detail: (1) Which kind of atomic packing facilitates relatively easily shearing? (2) What is the size distribution of STZs? (3) How do STZs evolve into a shear band?

2. Computational details

Molecular dynamics simulations of the $\text{Cu}_{64}\text{Zr}_{36}$ and $\text{Cu}_{40}\text{Zr}_{60}$ MG systems were performed using the embedded atom method (EAM) potential [14] in the large-scale atomic massively parallel simulator (LAMMPS) [15]. Each model system, with the dimensions of 28.2 nm (X) \times 56.4 nm (Y) \times 5.6 nm (Z), which contains approximately 500,000 atoms, was generated using the “melt–quench–duplicate” procedure [10,16–20]. Briefly, the procedure is as follows: First, a cubic cell containing about 10,000 atoms was melted at 2000 K and zero pressure for 2 ns to ensure homogeneity, during which periodic boundary conditions (PBCs) were applied in all three dimensions. Subsequently the cells were quenched from 2000 to 50 K over 19.5 ns at a cooling rate of $\sim 10^{11}$ K/s. The final dimensions of the post-quenched cubic cells were measured to be $5.6 \times 5.6 \times 5.6 \text{ nm}^3$. This cell was then replicated in X and Y dimensions, such that samples of size 28.2 nm (X) \times 56.4 nm (Y) \times 5.6 nm (Z) were generated. They were then relaxed for 100 ps at 50 K before tensile loading at a constant strain rate of $1 \times 10^8 \text{ s}^{-1}$ to a maximum strain, ϵ_m , of $\sim 14\%$, at 50 K. During deformation, PBCs were applied in Y and Z directions, while the surface in the X direction was allowed to deform freely, so as to closely mimic the geometrical constraints on a thin film. The time step during deformation was chosen as 1 fs. To visualize plastic shearing during deformation, the local shear invariant von Mises strain of each atom in the sample was calculated using the equation: $\eta_i^{\text{Mises}} = \sqrt{\frac{1}{2} \text{Tr}(\eta - \eta_m I)^2}$, where η and η_m are local Lagrangian and hydrostatic strains for that atom, respectively [21]. To calculate η_i^{Mises} of each atom, individual atomic positions after deformation are compared with their respective configurations in the undeformed state. To identify and follow the evolution of plastic deformation we track atoms with $\eta_i^{\text{Mises}} > 0.2$. These atoms will be referred to as the sheared or S-atoms here afterwards.

3. Results and discussion

3.1. Formation and evolution of S-atoms

Fig. 1(a) shows the tensile stress (σ)–strain (ϵ) responses obtained on the $\text{Cu}_{64}\text{Zr}_{36}$ and $\text{Cu}_{40}\text{Zr}_{60}$ MG samples. After the initial elasticity, which lasts up to a strain of $\sim 4\%$, nonlinear deformation starts. Both the MGs show a peak in stress, σ_m , with σ_m in $\text{Cu}_{64}\text{Zr}_{36}$ being nearly 1.5 times higher than that in $\text{Cu}_{40}\text{Zr}_{60}$. The reduction in σ with ϵ beyond the peak is gradual in the latter case whereas a steep reduction in σ is noted in $\text{Cu}_{64}\text{Zr}_{36}$ at $\epsilon \sim 11\%$. This corresponds to the process of shear localization into a narrow band [10,16–20]. While shear bands also form in $\text{Cu}_{40}\text{Zr}_{60}$ sample, the stress decay in it is more gradual. Beyond σ_m , the S-atoms start appearing in the samples, which are illustrated in Fig. 1(b) and (c) through snapshots taken at three different ϵ values. At $\epsilon = 9.2\%$ for $\text{Cu}_{64}\text{Zr}_{36}$ and 8.6% for $\text{Cu}_{40}\text{Zr}_{60}$, which correspond to the initial stage of plastic deformation, referred to as ϵ_i here afterwards, the fraction of S-atoms to the total number of atoms, F_S , is only $\sim 0.5\%$. At this stage, they are found to be uniformly distributed in both the samples. Two additional snapshots, representing either side of the rapid stress drop in the σ – ϵ curve are shown in Fig. 1(b) and (c). The corresponding strains are referred to as ϵ_o and ϵ_e . For $\text{Cu}_{40}\text{Zr}_{60}$, we use the linear fits to find that ϵ_o and ϵ_e correspond to 9.8% and 12.1% respectively. The steep drop in stress, accompanied with clustering of S-atoms in a narrow region (inclined at $\sim 45^\circ$ to the loading axis) of the sample at the ϵ_o , is a signature of shear localization that can potentially evolve into a shear band (SB). Indeed, in the next deformation snapshot taken at ϵ_e , a mature shear band can be clearly seen in the aforementioned narrow region of both samples. Note that the thickness of shear band in $\text{Cu}_{64}\text{Zr}_{36}$ is smaller than that in $\text{Cu}_{40}\text{Zr}_{60}$. By this stage, the majority of

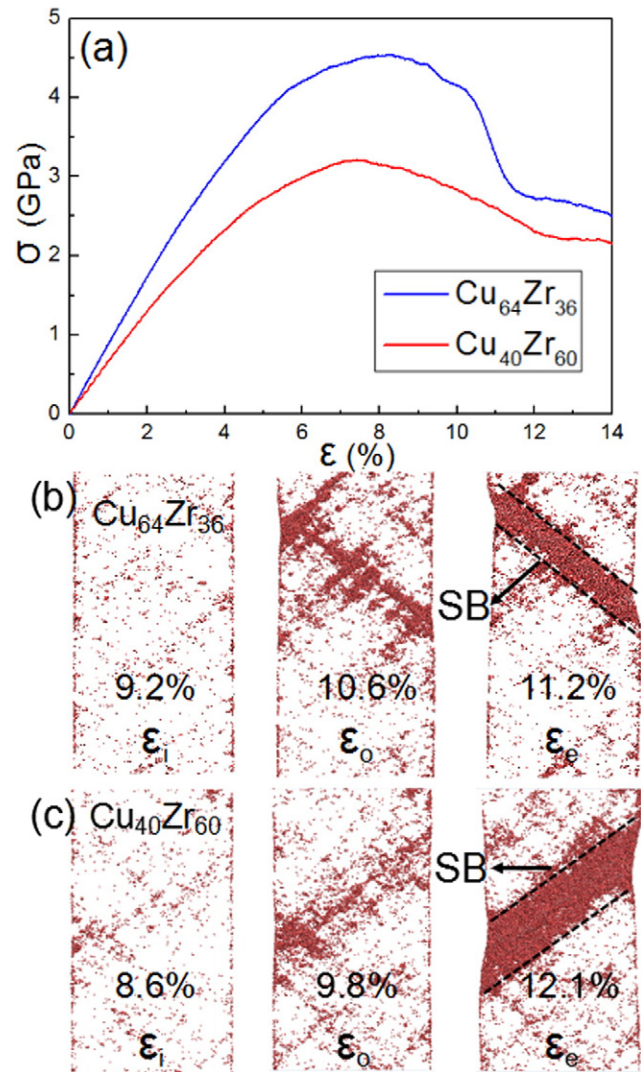


Fig. 1. (a) Stress–strain (SS) curves, (b) Deformation maps at three strains corresponding to ϵ_i , ϵ_o and ϵ_e for $\text{Cu}_{64}\text{Zr}_{36}$ and $\text{Cu}_{40}\text{Zr}_{60}$ MGs, respectively. The red points represent S-atoms and the black dash lines mark the shear banded area.

the S-atoms are located within the shear band region. These three specific deformation states denote the life cycle (from nucleation to maturing) of a SB.

Fig. 2 shows the evolution of S-atoms in both the alloys as a function of strain. As both MG samples contain similar atomic numbers, the fraction of S-atoms, $F_S = N_S/N_T$ (N_T = total number of the MGs) rather than the number of S-atoms, N_S , are presented and discussed here afterwards. F_S remains negligibly small below the linear elastic limit and remains so even when the σ – ϵ responses become non-linear, until ϵ reaches $\sim 6\%$. Further deformation to a strain of 8% , which is the strain corresponding to σ_m , results in a slow increase in F_S in both samples. Thereafter, the two alloys diverge significantly in terms of their F_S vs. ϵ behavior. While both are classical S-shaped, the one obtained on $\text{Cu}_{64}\text{Zr}_{36}$ shows a near-vertical raise within a narrow strain range, whereas $\text{Cu}_{40}\text{Zr}_{60}$ shows a more gradual increase. Further, the former appears to reach a plateau, while F_S in the latter continues to increase with ϵ .

The evolution of F_S with ϵ is closely related to the stress response of the whole sample, more so during the formation of a SB. Since plastic deformation is a stress relaxation process, the S-atoms, which mediate plasticity, are expected to carry large local strain. In that context, the increasing number of S-atoms during the SB formation, is the cause for the observed stress drop in the σ – ϵ curves. This is further illustrated by

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