Molecular Dynamics Simulation of Structural Characterization of Elastic and Inelastic Deformation in ZrCu Metallic Glasses

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1. Introduction

Bulk metallic glasses (BMGs) have attracted much attention as novel potential engineering materials because of their specific mechanical properties [1–3]. However, compared with their crystalline counterparts, many extraordinary behaviors in glasses are still poorly understood [4–6]. One of the most well-known features is the very high elastic strain limit of BMGs, which is about one order of magnitude higher than that in conventional crystalline metals and alloys [7–9]. However, it is known that the global plasticity of BMGs is very low [10, 11], which is caused by avalanche of shear transformation zones (STZs). The shear transformation zone (STZ) was hypothesized as the small cluster containing tens of atoms confined within elastic medium [11]. High-purity metallic-glass materials only show the elastic deformation or very limited plastic deformation under unconstrained conditions [12]. It is of great significance to understand the microcosmic differences between elastic strain and plastic strain. Therefore, studying structural characterization of elastic and inelastic deformation in BMGs at the atomic level is particularly important.

Recently, some researchers provide some details on the elastic deformation of amorphous solids [13–16]. For instance, Hufnagel reports the use of high-energy X-ray scattering to measure strain in a Zr_{57}Ti_{15}Cu_{20}Ni_{8}Al_{10} bulk metallic glass in situ during uniaxial compression in the elastic regime [15]. In addition, much work has been devoted to the inhomogeneous plastic responses (shear transformation events) in MGs [17–21]. However, the exact correlation of the degree of elastic and inelastic deformation with the internal structure in MGs at the atomic level is still unresolved. This condition can be attributed to the very limited existing experimental method for detecting atomic motion. Considering the experimental difficulty of directly measuring the movement of an atom or determining which local structures are prone to form, we have focused on computer simulation of simple alloy systems. This technique eliminates some of the problems encountered in experiments and studies the deformation processes at the atomic level.

Given the lack of a structural indicator for making a distinction between elastic and inelastic deformation, understanding the microscopic deformation mechanism in MGs on the whole is difficult [22]. In this letter, the nanoscopic deformation behaviors in a ZrCu metallic-glass model during loading-unloading process under uniaxial compression have been analyzed on the basis of the molecular dynamics (MD). And we employ the reversible degree of shear origin zones (SOZs) as structural indicator to distinguish the elastic and inelastic deformation processes in MGs.
2. Theoretical Model and Calculation Details

2.1. Preparation of ZrCu MG. In our molecular dynamics (MD) simulations, the model system of ZrCu MG was supplied in a large-scale atomic/molecular massively parallel simulator (LAMMPS) [23]. The force field used in this work is a realistic embedded atom method (EAM) potential [24], which is suitable for computing pairwise interactions for metals and metal alloys. The dimensions of the model structures used in the calculations are 17.1 nm × 25.6 nm × 4.3 nm in the x-, y-, and z-directions, respectively. The structures contained approximately 100,000 atoms. The model was heated from 300 K to 2500 K at a constant rate of 10 K ps⁻¹. To make the state of the system as natural as possible, we relaxed the liquid system for 50 ps at 2500 K within the NPT ensemble (namely, constant number, constant pressure, and constant temperature, and the temperature was controlled by Nose-Hoover thermostat method) under periodic boundary conditions. Next, we cooled the system from 2500 K down to 100 K in 100 K decrements at a constant quenching rate of 5 K ps⁻¹ at zero external pressure in the NPT ensemble.

2.2. Compression of ZrCu MG. Afterwards, compression at a constant strain rate of 1 × 10⁸ s⁻¹ along the y-direction was loaded at a constantly low temperature of 50 K. Periodic boundary conditions were imposed in the y- and z-directions and free surfaces in the x-direction to allow the occurrence of shear offset on the free surfaces. To simulate plane strain state, we maintained the pressure of the z-direction at zero.

3. Results and Discussion

3.1. The Compressive Stress-Strain Curve of ZrCu MG. The compressive stress-strain curve of ZrCu MG is shown in Figure 1. The yield stress is linear when the strain is <4%, suggesting an elastic deformation stage. The simulation result is in good agreement with the result obtained by Cao [25]. With increased strain, the rise of stress values becomes slow, showing a platform corresponding to the inelastic deformation. The stress reaches a maximum of 2.3 GPa at a strain of about 6%. To clarify the microstructure evolution at different stages of the system, 2% and 5% compressive strain of the system at the imposed y-direction, respectively, are analyzed.

3.2. Change in x-Displacement under Relaxation Process of Elastic and Inelastic Deformation. To display the relaxation process of elastic and inelastic deformation, we used the degree of x-displacement of each atom as the structural indicator, as shown in Figure 2. It is important to note that there are also y-displacement and z-displacement, and we just put the x-displacement as a representative to characterize the relaxation process. Figures 2(a)–2(d) show the relaxation process by monitoring x-displacements after unloading 2% stress. Figures 2(d')–2(d‘) reveal the relaxation process under 5% strain. In Figure 2(a), some x-displacements exist after compressing the ZrCu system. However, after 150 ps relaxation (Figures 2(b)–2(d')), x-displacements gradually disappear, suggesting that the x-displacements of each atom are reversible at the elastic deformation stage. On the other hand, the x-displacements of the system with 5% strain are strongly evident, as shown in Figure 2(a'). After 150 ps relaxation, the x-displacements gradually recover but numerous x-displacements still exist in the system, as shown in Figure 2(d'). Figures 2(a')–2(d') suggest that these x-displacements are irreversible at a strain of 5%, which correspond to the inelastic deformation stage. This observation also indicates that some atoms cannot go back to the initial location at the inelastic deformation stage. The author Zhang et al. also reported that the instantaneous elastic strain is observed to vanish immediately as the applied stress is removed (unloading process), while inelastic strain that decays beyond the simulation timescale is still remained [26]. This validates our results and implies that, with the increase in strain, some atoms deviate from their original positions, causing the local structure to be destroyed. Even after a long period of relaxation, these atoms cannot be restored to their original locations. To eliminate system size effects, we also structured a bigger model whose dimensions were 27.5 nm × 5.5 nm × 55 nm in the x-, y-, and z-directions, respectively, containing approximately 500,000 atoms. And we found that the main results presented above do not change.

3.3. Change in \( \eta_i^{\text{Misses}} \) under Relaxation Process of Elastic and Inelastic Deformation. To further explain the phenomenon of the x-displacement in the relaxation process, we use the atomic local shear strain \( \eta_i^{\text{Misses}} \) as a structural indicator to monitor deformation processes [27]. We use relaxed glass prior to performing uniaxial compression deformation in the y-direction as a reference. Atoms in Figure 3 are colored according to their atomic shear strain \( \eta_i^{\text{Misses}} \). Regions that have undergone larger shear strain (light blue) have a relatively large \( \eta_i^{\text{Misses}} \).

Shear origin zones (SOZs) are the regions in a metallic glass where strain becomes inhomogeneous [28]. A typical experimentally observed shear band width in a metallic glass
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Figure 2: Relaxation process observed by monitoring x-displacement after unloading the stress of ZrCu MG. (a)-(d) compressed by 2% strain. (a')-(d') compressed by 5% strain. The red region represents the atoms moving along the positive x-direction, and the blue region represents the atoms moving along the negative x-direction.

is on the order of 10 nm to 20 nm [29], but the size of SOZs is about 1 nm to 2 nm. Therefore, SOZs are smaller than shear bands. In Figure 3(a), some SOZs can be clearly observed after 2% strain compression of the ZrCu systems. However, after 150 ps relaxation (Figure 3(d)), fewer SOZs are observed, suggesting that the formation of SOZs is reversible at the elastic deformation stage. In Figure 3(a'), many SOZs can be observed after 5% strain compression of the ZrCu systems. After 150 ps relaxation (Figure 3(d')), many SOZs are still observed, suggesting that the formation of SOZs is irreversible at the inelastic deformation stage. The quantity and size of the SOZs in Figure 3(a') are larger than those of the SOZs in Figure 3(a). This observation indicates that new SOZs form with increased strain and the origins increase in size. With increased strain, these SOZs interact with one another and develop into shear bands. Smaller amounts of SOZs can be seen in Figure 3(d), whereas numerous SOZs can be observed in Figure 3(d'). This observation implies that, with increased SOZ size to a certain value, the formation of SOZs becomes irreversible. Hence, we propose that elastic deformation is related to these SOZs in MGs. The degree of SOZs in MGs can be controlled, and the plasticity of metallic glass can be improved [28].

3.4. Change in the Fraction of FI in SOZs under Relaxation Process. To further explain the structural features of SOZs at different deformation stages of ZrCu metallic glass, the Voronoi tessellation method was used [30]. In this method, the simulation cell is divided into Voronoi polyhedra (VPs) around each atom. A VP is defined as the minimal polyhedron whose planar faces bisect at right angles the lines joining an atom to its neighboring atoms. The polyhedra can be characterized by the Voronoi index \([n_3, n_4, n_5, n_6]\), where \(n_i\) denotes the number of \(i\)-edged faces of the VP. An \(i\)-edged face reflects the local symmetry of the central atom with some nearest neighbor atoms in a certain direction.

In previous studies, the Cu-centered Voronoi polyhedron with index \([0, 0, 12, 0]\) (full icosahedron (FI)) has been found to be a key structural motif in amorphous Cu-Zr alloys [31]. FI units with high packing density and high shear resistance reportedly determine the plasticity of Cu-Zr glasses.

For our model ZrCu MG, we observed a clear difference between the responses of Cu atoms in Cu-centered full icosahedra [Cu-FI; Voronoi index \((0, 0, 12, 0)\) clusters] and those that do not have full-icosahedra surroundings (Cu-non-FI). The Voronoi tessellation analysis shows that 21.5% of Cu atoms are centers of full icosahedra in this sample. In our Voronoi analysis, the cutoff is chosen large...
Figure 3: Relaxation process observed by monitoring $\eta_i^{\text{Mises}}$ after unloading the stress of ZrCu MG. (a)–(d) compressed by 2% strain. (a')–(d') compressed by 5% strain. Regions that have undergone larger shear strain (light blue) have relative large $\eta_i^{\text{Mises}}$.

To check whether the drop of the numbers of the Cu-centered full icosahedra can recover to the initial fraction, the ZrCu systems compressed by 2% and 5% strain were analyzed, as shown in Figure 4(b). With increased relaxation time, the fraction of Cu-centered polyhedra of the ZrCu systems compressed by 5% returns to $\sim 19.3\%$ from $\sim 18.33\%$, whereas the fraction of Cu-centered polyhedra of the ZrCu systems compressed by 2% returns to $\sim 21.5\%$ from $\sim 21.1\%$. The fraction of Cu-centered polyhedra of the ZrCu systems before being compressed is $\sim 21.5\%$, as shown by the line of 0% strain in Figure 4(b). This fraction testifies the deformation along with decreasing the fractions of Cu-centered full icosahedra. Before $\epsilon = 4\%$, the decreasing process is reversible; after $\epsilon = 4\%$, the decreasing process becomes irreversible. This finding indicates that FI in SOZs is partially destroyed at the inelastic deformation stage. Interestingly, both fractions of Cu-centered polyhedra of the ZrCu systems compressed by 2% strain and 5% strain increase at the initial stage of relaxation. This phenomenon is facilitated by the additional energy introduced by the large stress overshoot caused by the high simulated strain rate. Therefore, the phenomenon leads to a recovery of the atomic structure, that is, a decrease in free volume and an increase in FI density.
Figure 4: (a) Fraction of Cu-centered full icosahedra at different strains during compression deformation. (b) Fractions of Cu-centered full icosahedra as a function of relaxation time. To show whether the drop of the numbers of the Cu-centered full icosahedra can recover to the initial fraction, relaxation of the sample compressed by 0%, 2%, and 5% compressive strain, respectively, is analyzed.

4. Conclusion

In conclusion, elastic deformation is related to the reversible degree of SOZs. We find that the formation of SOZs is reversible at the elastic stage but is irreversible at the inelastic stage. At the elastic deformation stage, the fraction of FI in SOZs remains at a high grade. However, the fraction of FI in SOZs quickly decreases with increased strain at the inelastic deformation stage, and the decreasing process is also irreversible. This finding implies that the FI structure is destroyed and that the local structural environments of the SOZs are changed. Therefore, we can change the degree of SOZ localization to adjust plastic deformation and accordingly provide foundations for basic research on and future applications of MG.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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