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The effect of void defects on the shear band nucleation of metallic glasses

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ABSTRACT

Molecular dynamics simulations were employed to investigate the effect of void defect on the shear band nucleation in a $Cu_{64}Zr_{36}$ metallic glass. Unlike uniform samples, the samples with void defects can form shear bands at a much lower strain. Finite element simulation revealed stress concentration near the voids, which can explain the early formation of shear bands. The shear band behaviors are also influenced by the size, shape and distribution of the defects. These findings can provide simulation support to understand the shear band heterogeneous nucleation process of metallic glasses in the real case.

1. Introduction

The shear band behavior is a topic of intense research in the mechanical study of metallic glasses (MGs). The shear band nucleation process closely relates to the yielding process of MGs; the later shear band slide and arrest behaviors control the plastic behaviors of MGs; and the final fracture of MGs is usually triggered by shear band delamination [1–5]. However, due to the unclear amorphous structure of MGs, the exact deformation mechanism and the process of how the shear bands form and slide in MGs are still under debate. Contradictory results can be observed in different researches. For the elastic limit of MGs, some molecular dynamics (MD) and experiments at submicron scale indicated that the critical strain for shear band nucleation in MGs could be as high as 5–10% [6,7]. However, in experiments, bulk MGs (with a size beyond 1 mm) usually yield at a much lower strain near 2% [8,9], which raised the speculation that the existence of defects could facilitate the heterogeneous nucleation of shear bands [6,10–16]. This understanding is in accordance with some theoretical and experimental expectations that the microstructure of MGs is inhomogeneous [17–26]. On the other hand, introducing pores as the second phase into MG matrix has been proved to be an effective way to enhance the ductility [27–29]. MG foams or cellular structures may be ductile in appropriate conditions.

The concept of inhomogeneous structure or defects has been accepted in not only MGs but also other modern materials. In crystalline alloys, the defects at nanometer scale are known as dislocations, vacancies, interstitial atoms, and so on. At larger scale, there also exist defects such as casting flaws, shrinkage porosity and surface imperfection. Numerous numerical simulations have been proceed to study the effect of void in crystalline alloys, since the nucleation, growth and coalescence of voids were believed to be responsible for the fracture of many ductile materials [30–33]. In MGs, the exact form of defects is hard to be defined, due to the amorphous microstructure and uncertain atomic packing. Many previous MD simulations of shear bands in MGs considered homogeneous sample without any defects. This situation can only be used to understand the homogeneous nucleation scenario of shear bands. In the real case, defects such as voids do exist in the shear bands of MGs [34], and can affect the plastic deformation and fracture [35]. It should also be noted that the MD simulations are always with much smaller dimension, artificial boundary condition, and unrealistically high strain rate. Therefore, the MD simulation predictions will show a distinct mismatch with the experimental results of MGs. So far, with many theoretical studies and simulations on shear band nucleation in MG being proposed [36–40], the researches on shear bands heterogeneous nucleation and the evolution of defects (or voids and inhomogeneous regions) are still required [35,41,42].

In this study, MD simulations were applied to explore the shear band nucleation process from void defects in a $Cu_{64}Zr_{36}$ MG. The results show that by adding a 3 nm radius spherical void defect to a uniform glassy matrix, the critical shear band nucleation strain could decrease from ~10% to ~6%. By changing the size of the void, the critical strain would change accordingly. The evolution of local strain, stress and shape of the void during the deformation process was further discussed. These results support that void defects indeed could facilitate the shear band nucleation in MGs, and could be a reference for further research on optimizing the plastic deformability of MGs.

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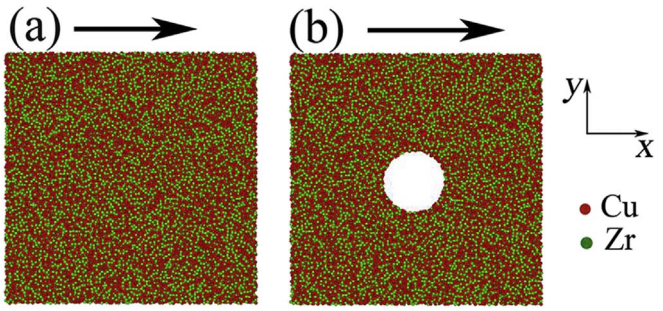

Fig. 1. (a) Illustration of the solid MD model. (b) Illustration of the hollow MD model with a 3 nm radius spherical void in the center. The Cu and Zr atoms are represented with red and green colors, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

2. Simulation

A binary metallic glass $Cu_{64}Zr_{36}$ was employed in the MD simulations, which was a widely used system in previous MD studies on the structure and property investigations of MGs [43–46]. The model considered a cubic sample consisting of 864,000 ($244 \times 244 \times 244$ Å^3) atoms interacted by the Cleri-Rosato potential [47]. To obtain an original amorphous structure, the model was heated to 2000 K (which is hundreds Kelvins higher than the melting point of $Cu_{64}Zr_{36}$ alloy [43]), relaxed for 250 ps, and then cooled down to 10 K at a cooling rate of 4×10^{11} K/s. Next, the atoms in a spherical volume with a radius of $r = 3$ nm were removed from the center of the model (at $x = 122$ Å, $y = 122$ Å, $z = 122$ Å). The cross-sections of the original solid model and the hollow model are shown in Fig. 1(a) and (b), respectively. To study the shear behavior, we performed simple shear to both the models along the *xy* direction at a strain rate of 10^9 s^{-1} with a stepwise shear strain increment of $\Delta\gamma = 0.1\%$. Periodic boundary conditions (PBCs) and zero pressure were employed in all the three directions of the models in the simulations.

3. Results and discussion

Fig. 2 shows the simulated atomic local shear strain η^{Mises} distributions (the definition of η^{Mises} has been described in Ref. [48]) in the two models at different shear strains of $\gamma = 4$, 6, 8, 10 and 20%. With increasing strain, some locations of the models gradually reach relatively high local shear strain η^{Mises}. When the solid model reaches the strain of $\gamma = 10\%$, strain localization is observed in a narrow band parallel to the *x*-axis at $y = \sim 80$ Å with a thickness of about 10 nm, which is a signal of shear band nucleation. The shear band thickness is consistent with many simulations and our previous experimental inspection [34,49]. In the hollow model, the shear band initiates from the void at a lower strain of $\gamma = 6\%$ (Fig. 2(b)). During further shearing, the strain in the shear band region continues to increase, while the strain outside the shear band maintains relatively low value. At the strain of 20%, both the two models reach a local shear strain as high as ~100% in the shear band regions. The original spherical void in the hollow model has severely deformed and become very narrow. These results indicate that by considering a 3 nm radius void defect in this MG, the critical global strain of shear localization, i.e. the formation of shear bands, could be reduced from ~10% to ~6%.

Local softening is known as the main reason for the formation of shear bands in various materials [10]. In MGs and some other particle systems, shearing could cause volume expansion and softening, known as the shear dilatation effect [50,51]. Our previous experiments have pointed out that the packing density of the shear bands in MGs is a few percent lower than that of the MG matrix [52]. Here in Fig. 3(a), we show the evolutions of the average atomic Voronoi volume inside and outside the shear band at different global shear strains of the solid model. The red curve represents the atoms in the shear band region of $y = 30$–130 Å (consider the shear band center at $y = \sim 80$ Å and a thickness of about 10 nm), the blue curve represents the atoms outside the region. During early loading, the two curves almost coincide, indicating relatively uniform shear dilatation in the whole model. When the strain reaches 6%, a bifurcation occurs, where the atomic volume inside the shear band region continues to increase and the atomic volume outside the shear band region starts to decrease. Later, the atomic volume of the two regions gradually approaches two constants, respectively. This result could be explained by the shear dilatation effect. As the severely sheared locations dilate and become softer, the shear strain will localize into a shear band with relatively low density. Due to the formation of the shear band, the stress in the model will be partly released and therefore the dilatation outside the band can be partly recovered. During later shear band sliding, the shear dilatation effect and structure relaxation in the band are almost balanced. The global shear strain-shear stress curve of the model also shows that with the formation of the shear band, the overall global shear stress drops from the peak stress and approaches a constant near 0.8 GPa (The black curve in Fig. 3(b)).

In the real case, there could exist different kinds of defects at different scales in MGs, such as the surface imperfections and porosity in castings at micrometer scale, the soft spots [19,20] and liquid-like regions [17,18] at nanometer scale. During the sample fabrication process by rapid cooling, the gas in the alloy melt might precipitate and form

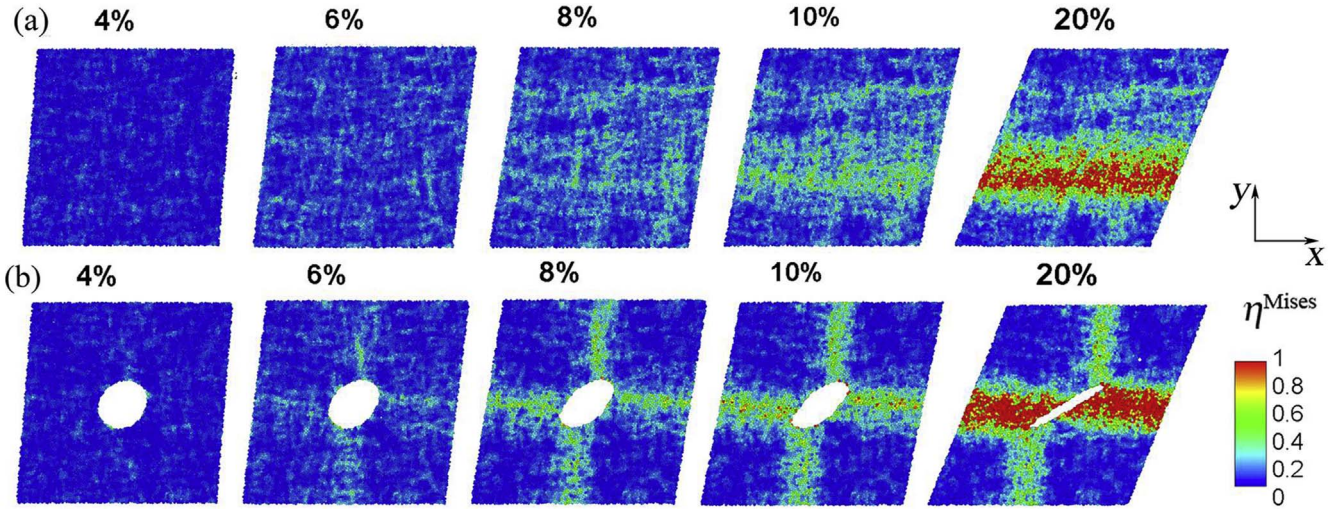

Fig. 2. Distribution of atomic local shear strain η^{Mises} in (a) the solid model and (b) the hollow model at strains of $\gamma = 4$, 6, 8, 10 and 20%.