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Non-localized deformation in metallic alloys with amorphous structure

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Abstract

In bulk or ribbon metallic alloys with monolithic amorphous structure, plastic deformation at room temperature is dominated by highly localized shear banding. Here we report suppressed shear localization under tension in a metallic glass (MG) embedded with pre-existing amorphous shear bands using large-scale atomistic simulations. It is demonstrated that pre-deformation lowers material strength and triggers enhanced strain fluctuation before sample yielding, leading to highly dispersed plastic shearing in the entire sample. Furthermore, the transition in deformation mode from highly localized shear banding to non-localized plastic deformation is associated with the competition between the yield strength of the material and the critical stress required for the formation of mature shear bands in the load-bearing materials. Given that a sufficient amount of glassy heterogeneities can be introduced into MGs under experimental conditions, the obtained results could provide a promising strategy for designing tensile ductile MGs with pure amorphous structure at room temperature.

Keywords: Metallic glass; Mechanical property; Plasticity; Molecular dynamics simulations

1. Introduction

Metallic glasses (MGs) possess attractive mechanical properties, such as high strength approaching the theoretical limit, large elastic strain limit and excellent corrosion resistance. The outstanding behavior is attributed to the unique liquid-like atomic structures without long-range atomic periodicity [1–3]. However, MGs in their bulk form suffer from a strong tendency for plastic strain localization in a narrow region called the shear band, and exhibit macroscopically catastrophic failure under tension at room temperature [4], significantly limiting their structural reliability. A great deal of effort has been made in recent years to improve the plasticity of MGs. Some monolithic MGs exhibiting obvious compressive plasticity were developed, possibly due to (a) a high Poisson's ratio with the relative ease of shearing over dilatation [5]; (b) in situ nanocrystallization during deformation [6]; and (c) more free volume by faster cooling [7] or minor alloying [8]. However, these MGs still show limited plastic strain under tension. In order to improve tensile ductility, MG/crystal composites have been designed by virtue of the interaction between the glass matrix and crystalline particles to inhibit the propagation of shear bands and to promote the formation of multiple shear bands. Remarkable tensile ductility of these composites has been successfully achieved [9–12].

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It has been argued that atomic-, nano- and micro-scale spatial fluctuations in material density and strength may play important roles in the deformation behavior of MGs [13–15]. Inspired by the concept of heterogeneous microstructures, pre-plastic deformation by compression and cold-rolling were performed to improve the plasticity of MGs during subsequent bending and compression tests, which is attributed to the introduction of pre-existing shear bands during pre-deformation [16,17]. The cold-rolled MGs even exhibited an obvious plastic elongation during tension [18,19], owing to the competitive movement of shear bands in different orientations. However, the underlying mechanism of how the pre-existing shear bands affect the deformation behavior of MGs, which is a key issue for understanding the mechanical behavior of monolithic amorphous materials, is still unclear. Since precise control of the spatial distribution of shear bands in real MGs is complex and difficult [20], it is worth conducting atomistic simulations to gain insights into the deformation mechanisms of MGs with pre-existing shear bands.

In the present work, we report large-scale atomistic simulation results of the tensile behavior of $Cu_{64}Zr_{36}$ (at.%) MGs embedded with pre-existing shear bands. We show that deformation mode switches from highly localized shear banding to non-localized plastic deformation at a critical content of pre-existing shear bands. We demonstrate that plastic shearing becomes more distributed in the sample and therefore more difficult to develop into a dominant shear band before sample yielding at high densities of pre-existing shear bands. Both the orientation and the spatial distribution of the pre-existing shear bands are essential to the onset of the transition. We emphasize here that the amorphous nature of pre-existing shear bands is the same as the glassy matrix, but essentially different from other kinds of spatial heterogeneities such as second-phase dendrites.

2. Methods

Molecular dynamics simulations of Cu–Zr MGs were conducted by using the embedded atom method potential [21]. The time step was chosen as 1 fs. A "melt–quench–duplicate–deform" procedure was adopted to generate pre-existing shear bands, as shown in Fig. 1. First, a cubic cell containing 64 at.% copper and 36 at.% zirconium was melted at 2000 K and zero pressure for 2 ns to ensure homogeneity, during which periodic boundary conditions were applied to all three dimensions. The cell was then quenched from 2000 K to 50 K over 19.5 ns at a cooling rate of 100 K ns^{-1}. The final dimensions of the cubic cell were measured to be $5.6 \times 5.6 \times 5.6\ nm^3$. Through duplication of the cubic cell, a sample with dimensions of $106.4 \times 117.6 \times 5.6\ nm^3$ was created. After 1 ns relaxation, uniaxial tensile loading was applied to the sample at a constant strain rate of $1 \times 10^8\ s^{-1}$ until a shear band (forming an angle of 49° with respect to the loading axis) was formed at a strain of 12%. The sample was then unloaded to a zero-stress state, which was used to construct MG samples with pre-existing shear bands. To confirm that no crystallization occurred during pre-deformation, three groups of atoms (with dimensions of $10 \times 10 \times 5.6\ nm^3$) were selected from the pre-existing shear band and the radial pair distribution functions (RDFs) were calculated, as shown in Fig. 2. It was seen that the RDFs are characteristic of amorphous materials.

Quasi-three-dimensional samples containing 0°, 49° and 90° pre-existing shear bands were extracted from the pre-deformed MG sample for uniaxial tensile simulations, as shown in Fig. 3. Details about the construction methods are given in Appendix A. To release the high excess energy associated with the artificial boundaries from sample preparation, the overlapping atoms on the boundaries should be removed (cutoff distance was chosen as 0.2 nm) and the system needs to be equilibrated before subsequent mechanical loading. To confirm the validity of our construction procedure, complementary simulations were carried out on two pure MGs, "Pure MG 1" and "Pure MG 2". The former sample is free of artificial boundaries since it was directly cut from the pre-deformed MG. Four internal boundaries exist in the latter sample, which was generated by putting small pieces of MGs together. The stress–strain curves from uniaxial tensile simulations are shown in Fig. 4. It is seen the effect of the artificial boundaries on the tensile behavior is negligible as compared with that of the pre-existing shear bands, which are fully illustrated below (see Fig. 5a).

All samples have dimensions of $47 \times 94 \times 5.6\ nm^3$, containing ~1,500,000 atoms. Atoms belonging to pre-existing shear bands are colored in red while others are colored in grey. The content of pre-existing shear bands in each sample was measured by the atomic percent of the red atoms, which allowed us to evaluate the critical amount of pre-existing shear bands for the deformation mode transition. Periodic boundary conditions were applied to the Y and Z directions, while free surface condition was applied to the X direction. The sample was relaxed for 100 ps before straining. During uniaxial tensile loading, a maximum strain of 20% was applied to the sample along the Y direction with a strain rate of $1 \times 10^8\ s^{-1}$. To visualize plastic shearing during deformation, the local shear invariant [22] η^{Mises} of each atom in the sample was calculated using $\eta^{\mathrm{Mises}} = \sqrt{\frac{1}{2} Tr(\eta - \eta_m I)^2}$, where η and η_m are local Lagrangian strain and local hydrostatic strain at that atom, respectively. Atoms with a value of η^{Mises} larger than 0.03 (resulting in shear bands with a width of ~10 nm in our simulations) are regarded as atoms in operating shear transformation zones (STZs).

3. Transition in deformation mode

Stress–strain curves for $Cu_{64}Zr_{36}$ MGs with various atomic percents of 0° pre-existing shear bands (aligned parallel to the loading axis) are shown in Fig. 5a. It is seen that