Improvement of Plastic Deformation in Hetrogeneous Atomic Cu-Zr Amorphous Alloy with Distributed Nanocrystals

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Abstract

This study explores the influence of volume fraction of nanocrystals of Cu-Zr amorphous alloys on shear band formation. As the number of crystals with very tiny size increases, the strain localization, i.e. shear band, decreases without large drop of flow stress. The DPRs also depict no sudden drop and relatively high values. The strain state during the deformation represents a few shear bands at low volume fraction while there are no distinguishable shear bands at high volume fraction of nanocrystals.

1. Introduction

Unlike crystalline materials, metallic glasses exhibit a remarkably high elastic modulus and strength on mechanical deformation. Although their mechanical behaviors have been extensively studied, the precise nature of the deformation mechanism in these amorphous metals still remains unclear [1, 2].

The deformation of metallic glasses is mainly driven by inhomogeneous deformation, a kind of strain localization called shear band. Except at temperature sufficiently high to allow homogeneous deformation, shear bands are directly related to strength and fragility of metallic glasses. Unstable and abrupt failure due to few shear bands is usually found on uniaxial tensile test while multiple shear bands showing apparently plastic deformation occur on uniaxial compression test or bending test[3~10]. It is important to understand the mechanism of shear band formation since abrupt failure is related to fragility prevents amorphous materials from being used in industrial applications.

In order to avoid the fragility, a lot of experimental researches have been investigated up to date on amorphous composite materials containing nanocrystals [8]. It is also reported that crystalline phases in metallic glasses enhance ductility or plastic strain up to 35%, because the crystalline phases can promote multiple shear bands [5-10]. Ironically, nanocrystals embedded by metallic glasses promote shear band formation and terminates within themselves. It means the nanocrystalline not only enhances the generation of shear band, but also prevents the propagation of shear band. It is believed that this dual nature is why the amorphous composite materials with nanocrystals have more ductility.

Therefore, it is much interested in realizing the variation of fragility at amorphous composite materials with nanocrystals. In this work, we investigated the influence of volume fraction of nanocrystals to shear band formation using molecular dynamics. This choice is motivated by a number of recent publications for strain

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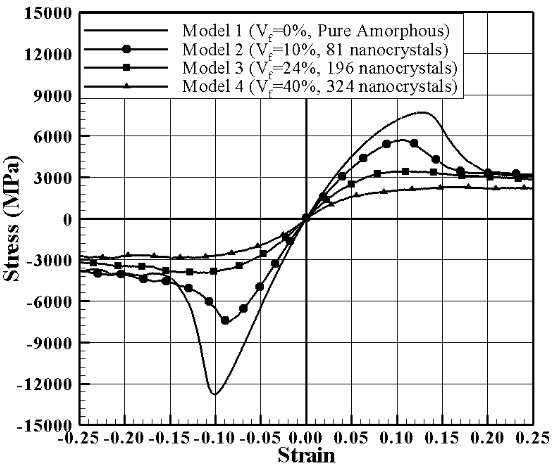


Fig. 1. Stress-Strain curve for the models with the different volume fraction of crystals.

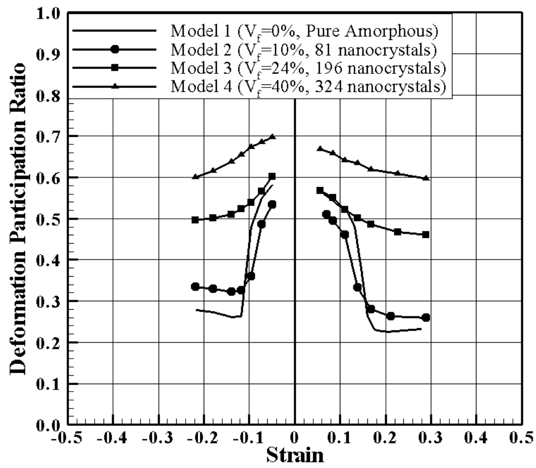


Fig. 2. Curve for DPR. vs. Strain. The volume fraction is proportional to the DPR.

localization using molecular dynamics simulation [11-15]. These researches find the mechanism of shear band formation is related with the quasi-crystal like short range order, the mass density of pure amorphous materials and the number of nanocrystals.

2. Computational Model

The 100,000-atoms Cu57Zr43 system with pure amorphous structure is chosen as a representative model (Model 1). The fully relaxed model with the size of about 31nm×31nm×17nm employs 2-D molecular dynamics study using modified Lennard-Jones potential fitted to the amorphous Cu57Zr43 system, in plane stress condition[16,17]. It means that z-coordination of each atom is fixed in 3-dimensional model. We choose the 3-D model to measure the atomic strain using the already developed program [18]. To the best of our knowledge, so far there is no study about shear band using full 3-dimensional model with full 3-D periodic boundary condition and under uniaxial loading. Although the reason is still uncertain, 3-D model used in molecular dynamics may be too pure to generate the shear band. In addition, the constraint of one dimension in 3-D can promote unstable state such as shear band, easily.

To make the amorphous composite materials with nanocrystals, we insert the nanostructures artificially with the perfect Zr2Cu crystal structure usually found in experimental studies [19] and the size of about 1nm×1nm, into model 1. The different numbers of nanocrystals are evenly distributed into the already-made amorphous structure before the relaxation: model 2 with 81 crystals corresponding to about 10%, model 3 with 196 crystals corresponding to about 24% and model 4 with 324 crystals corresponding to 40%. The data for model 1 and 2 came from the reference [15]. After the insertion, the crystal-inserted models are fully relaxed for 100ps, again under the periodic boundary condition. To make shear band, uniaxial tension and uniaxial compression are applied to each model. Deviatoric atomic strain is quantified by the atomic strain definition suggested by Mott and Argon [20]. In order to quantify the degree of strain localization, i.e. shear band, a quantity called deformation participation ratio (DPR) introduced by Shi and Falk is utilized [13]. The definition of DPR is the fraction of atoms that have an atomic deviatoric shear strain larger than that of the whole system. As the strain becomes localized, the DPR should be small.

3. Results and Discussion

Figure 1 shows stress-strain curves for the models with different volume fraction of nanocrystal under uniaxial compressive and tensile loadings. During deformation, the models with low volume fraction of nanocrystal reach to a maximum stress corresponding to 0.1 strain then suddenly drops. Unlike those with low

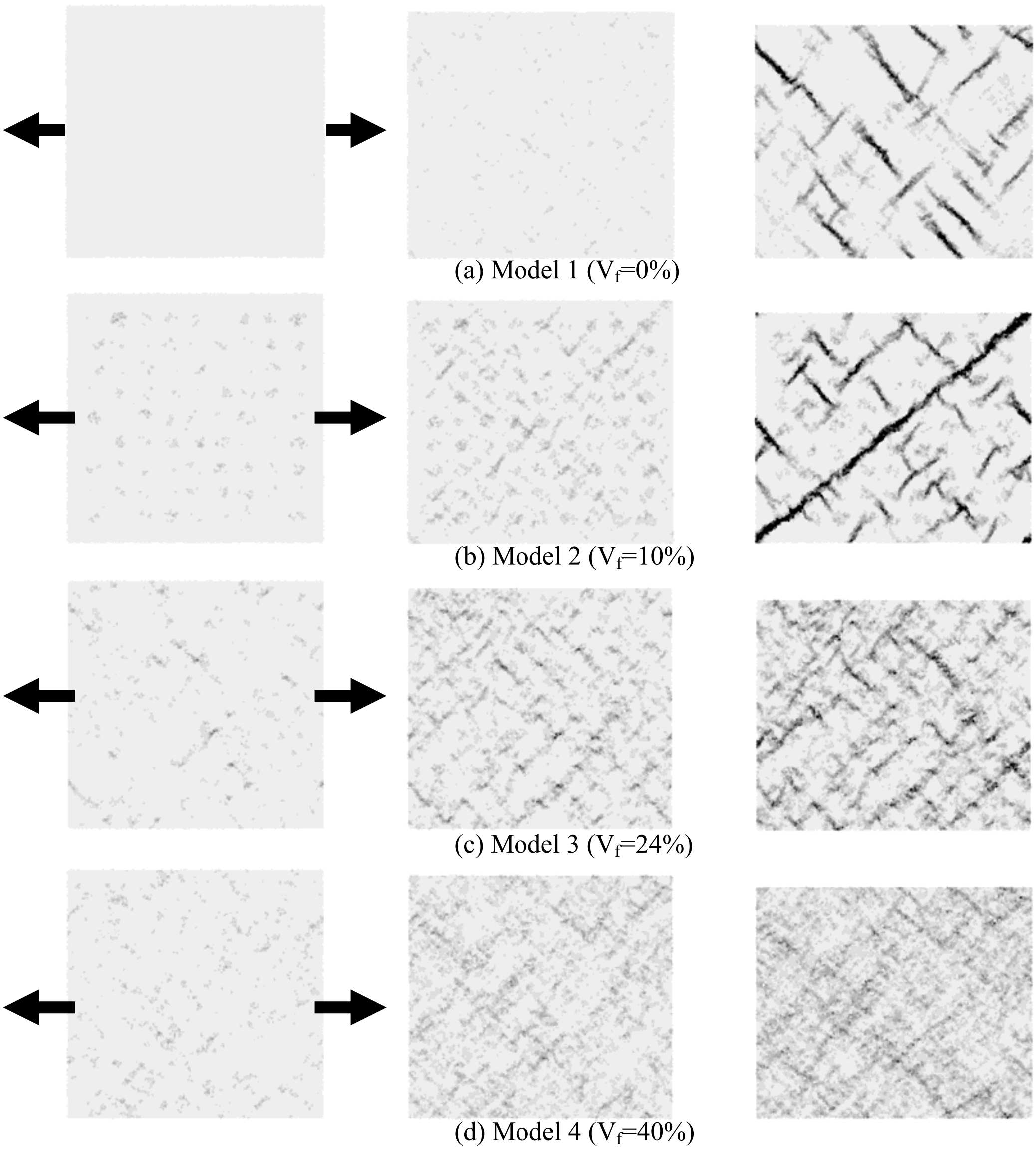
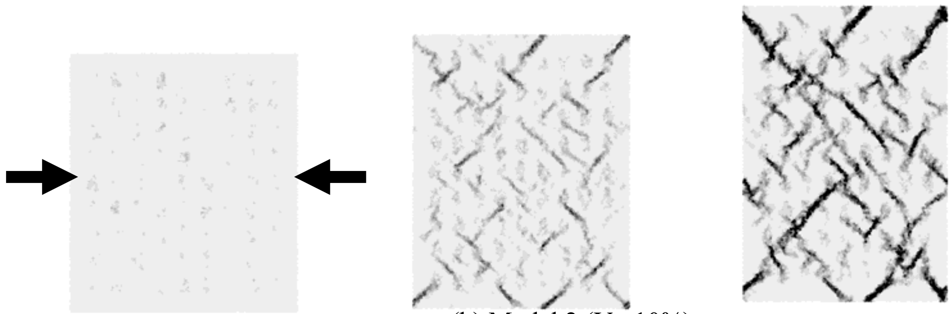


Figure 3. Shear bands represented by the deviatoric shear strain of uniaxial tension for each model, from left to right with ε_{11}=0.05, 0.10 and 0.15. Atoms are colored according to the value of the atomic deviatoric shear strain. Black represents a strain greater than 0.1 while white represents 0.0 strain.

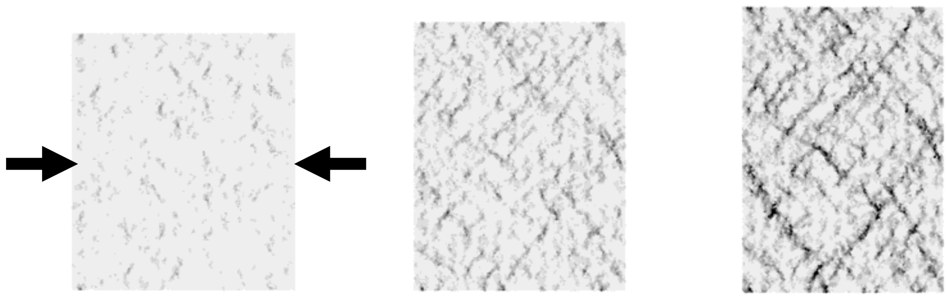
volume fraction, the models with high volume fraction show a typical stress-strain curve shape of crystalline materials, i.e. there are no overshoots on stress-strain curve for high volume fraction of nanocrystals. It means that yield point decreases as volume fraction of nanocrystal increases. Finally, the overshoot diminishes at high volume fractions. This can be expected because the amorphous materials with nanocrystals usually shows relatively lower yield point in experiments. We also found that the point with maximum stress is corresponding to the onset of shear band. More detail will be discussed in later. After the onset of shear band, the flow stress of all models keeps relatively constant.

In order to measure the degree of strain localization, the curves for DPR are depicted at Figure 2. While the models 1 and 2 with low volume fraction of nanocrystals have sudden drops at around 0.1 strain corresponding to the maximum stress and the onset of shear band, the models 3 and 4 do not show sudden drops. It means there is no severe strain localization at these models. While the magnitudes of flow stresses in Figure 1 show relatively small differences, the DPRs show large differences in Figure 2. It means that the strain localization can be prevented without a severe drop of flow stress. As seen in Figure 2, the model 3 and 4 do not show any sudden drop. The DPRs is continually decreasing during the

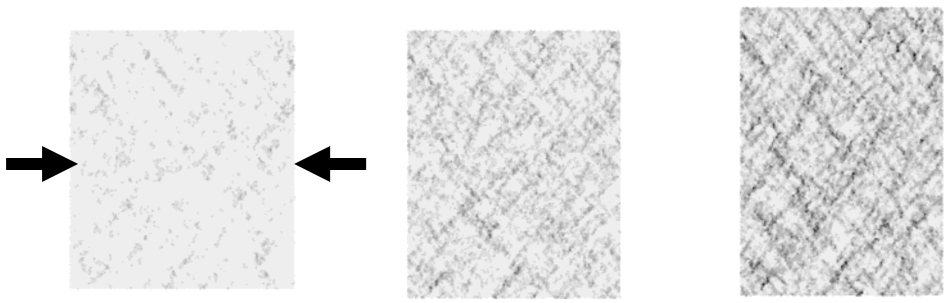
(a) Model 1 (V_f=0%)



(b) Model 2 (V_f=10%)



(c) Model 3 (V_f=24%)



(d) Model 4 (V_f=40%)

Figure 4. Shear bands represented by the deviatoric shear strain of uniaxial compression for each model, from left to right with ε_{11}=-0.05, -0.10 and -0.15. Atoms are colored according to the value of the atomic deviatoric shear strain. Black represents a strain greater than 0.1 while white represents 0.0 strain.

deformation. It is also noteworthy that strain localization of tension is more severe than that of compression, because the DPRs of tension at the same strain level is lower that that of compression. For example, DPR for 0.2 strain of Model 2 is around 0.28, while DPR for -0.2 strain is around 0.36. However, the differences between compression and tension diminish at high volume fraction of nanocrystals, for example, model 4 has the same value at 0.2 strain. The model with high nanocrystal volume fraction starts to show the same trend for both uniaxial tests.

Figure 3 and 4 depict the shear bands during tension and compression, respectively. In Figure 3, model 1 and 2 with low volume fraction of nanocrystals represents a few clear shear bands. In contrast, model 3 and 4 show homogeneous deformation rather than strain localization, i.e. shear band. Before 0.1 strain corresponding to maximum stress, shear bands starts to be generated in distinct regions. After 0.1 strain, the shear bands start to be propagated and connected to each other. Especially, the propagation makes a long shear band through the model at model 2. These propagations make the sudden stress drop in stress-strain curve. If the shear band occurs in many places, simultaneously, the deformation will be homogeneous as shown at model 3 and 4. Figure 4 depicts the strain states of each model in compression test. Like the cases of tension, model 1 and 2 shows clear shear bands corresponding to sudden drops of DPRs and stress. The deformations of model 3 and 4 also seem to be a homogenous deformation rather than strain localization. However, the number of shear band found in the model 1 and 2 is relatively greater than that of tension as found in the experimental studies [2,4-5].

4. Conclusion

Consequently, amorphous materials with high volume fraction of nanocrystals make homogeneous deformation during tension or compression without large decrease of flow stress. The DPRs also depict the improved states, i.e. no sudden drop and relatively high values. The strain state during the deformation represents a few shear bands at low volume fraction while there are no distinguishable shear bands at high volume fraction of nanocrystals.

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