밀도 분산에 의한 Zr-Cu 비정질 금속에서의 소성변형능 향상

Enhancement of Plasticity of Highly Density-fluctuated Cu-Zr Amorphous Alloy

***#Junyoung Park[1], Yoji Shibutani[2]**

*#J. Park(pcello@kumoh.ac.kr)[1], Y. Shibutani[2]

[1]Kumoh National Institute of Technology, Dept. Mech. Eng., [2]Osaka University, Dept. Mech. Eng.

Key words : Zr-Cu binary amorphous alloy, highly density-fluctuated state, Zr2Cu-nanocrystals, shear band

1. Introduction

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, these strain localizations are directly related to strength and fragility of metallic glasses. Unstable and abrupt failure due to just a few shear bands is usually found on uniaxial tensile or bending test[1]. It is important to understand the mechanism of shear band formation since abrupt failure related to fragility prevents amorphous materials from being used in industrial applications. It is also well known that strain localization is connected with local viscosity.

In order to avoid the fragility, a lot of experimental researches have been investigated up to date on amorphous composite materials containing nanocrystals [1]. Ironically, nanocrystals embedded by metallic glasses promote shear band formation and terminates within themselves. Consequently, structural-inhomogeneity induced by nanocrystals makes deformable-homogeneity (retarded strain localization by multiple shear bands), but, structural-homogeneity induced by pure amorphous structure makes deformable-inhomogeneity (abrupt strain localization by just a few shear bands).

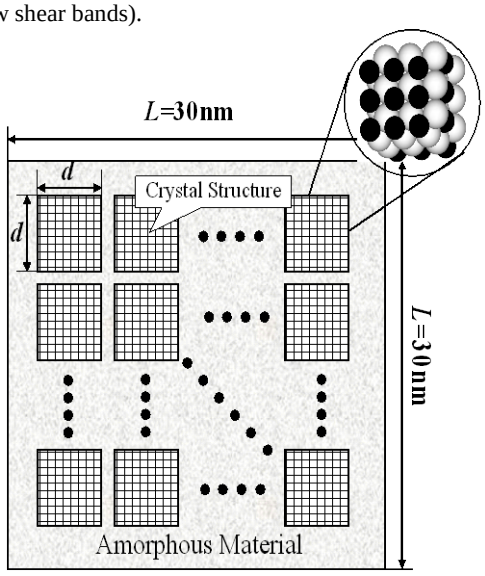
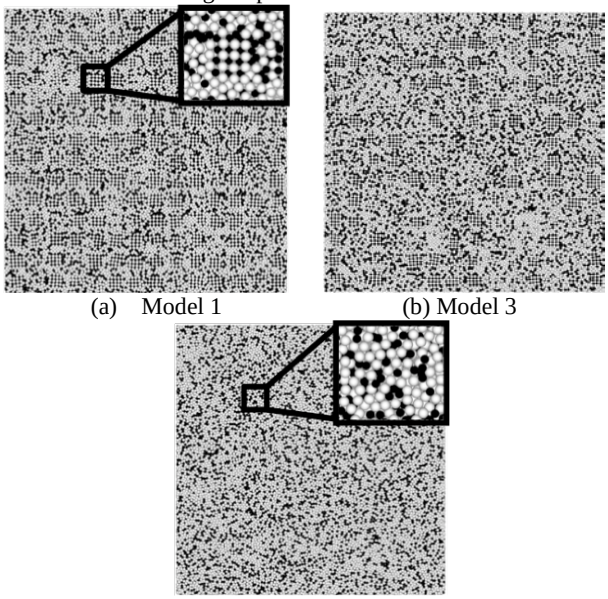


Fig. 1 Schematic of mixed models where L is about 30nm, d is 1.3nm. The total number of inserted crystals is 196. At each column and row, 14 crystals are positioned.

2. Computational Model Setup

To make computational model, we choose about 100,000-atoms $Zr_{67}Cu_{33}$ system with pure amorphous structure as an initial amorphous structure at the first step. The fully relaxed structure for 200ps has the size of about 30nm x 30nm x 22nm. Besides, Zr_2Cu crystals with perfect C11b structure (one of body-centered cubic structures) found easily in the experiment of binary system and with size of about 1.3nm x 1.3nm x 22nm are prepared as an initial crystal structure [2]. 196 nanocrystals (14 rows and 14 columns) are evenly distributed on amorphous basis as seen in Fig.1. The initial volume fraction of nanocrystals is around 17%, based on the number of atoms with crystal structure. The mixed structure is relaxed for 200ps at 300K again before receiving heat treatment. Based on the characterizations of the present computational models, the mixed structures with artificially inserted nanocrystals are relaxed at below melting temperature.



(a) Model 1 (b) Model 3

(c) Model 5

Fig. 2 Atomic configurations of all as-relaxed models before uniaxial loading. Models 1 and 3 still have some crystals even after quenched, while Models 5 is almost reduced to amorphous structure. White denotes Zr, and black does Cu.

To adjust the several density-fluctuated states from the artificially made-amorphous composites, the as-relaxed model is quenched at quenching rate of 2.6×10^{12}K/s from 600K (Model 1), 1000K (Model 2), 1200K (Model 3), 1400k (Model 4) and 1800K (Model 5), which range from the superliquid state to below the glass transition temperature. After quenching process, the temperature keeps a constant 300K for 400ps or more. Refer to Fig. 2.

3. Results and Discussion

To quantify the amount of crystal-based local structure, the percentage of atoms with BCC structures are measured by weighted Voronoi analysis considering the size of atoms [3]. As mentioned above, the inserted crystal structure, C11b, is a kind of BCC structure. The BCC structures are considered as Voronoi polyhedron only with (04460) or (06080) denoted by Schläfli notation. The percentage of atoms with BCC structure and the averaged density of the whole system are shown in Fig. 3. Each point is corresponding to each model. For examples, the leftmost points are model 1 with 600K quenched temperature. As seen in the figure, density curve shape is identical to that of the percentage of atoms with BCC, because the density of crystal is larger than that of amorphous. Models 1 (600K) and 2 (1000K) have high BCC

percentage and high density, 17% and 6737kg/m^3 as expected. However, models 4 and 5 have relatively low BCC percentage and density below 2% and 6720 kg/m^3, respectively, which densities are much closer to that of pure amorphous structure (6719 kg/m3) made by quenching over melting temperature.

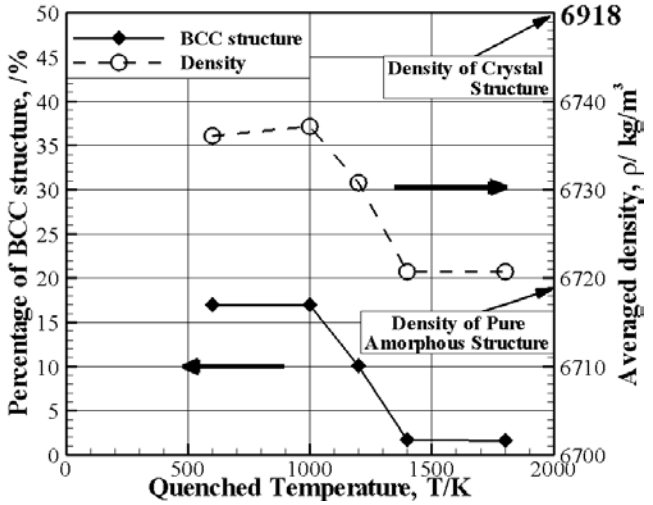


Fig. 3 Percentage of atoms with BCC structures and density of whole cell versus quenched temperature.

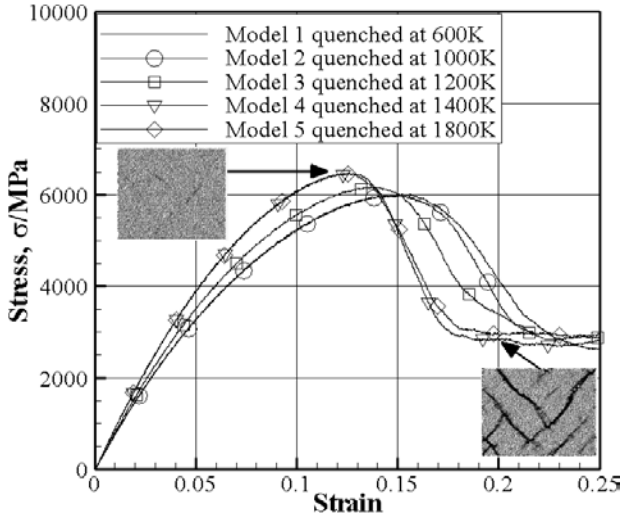


Fig. 4 Nominal stress-strain curves for the models with the different quenched temperature.

During uniaxial tension, all curves reach the maximum then suddenly drop. The sudden drops are caused by the formation of shear band, as depicted in Fig.4. In Fig. 4, the maximum stress and the gradient of curve corresponding to the elastic modulus are apparently decreased as decreasing the quenched temperature, and the corresponding strain to maximum stress is increased as the percentage of BCC structure increases, that is, the plastic deformability is more improved. Consequently, resistance for deformation in the structural-inhomogeneity (for example, Models 1 and 2) will be achieved softly because the stored strain energy by the external work is already dissipated by atomic moving. However, it is harder for atoms to find big enough free volume to move in the structural-homogeneity (for example, Models 4 and 5). So, for the atoms to drop into the local minima will be limited during the deformation. Consequently, the structural-homogeneity will be able to keep the high energy state and strongly resist for deformation. Then, at the state with higher stress and smaller strain, it will be deformed abruptly, which means severe strain localization.

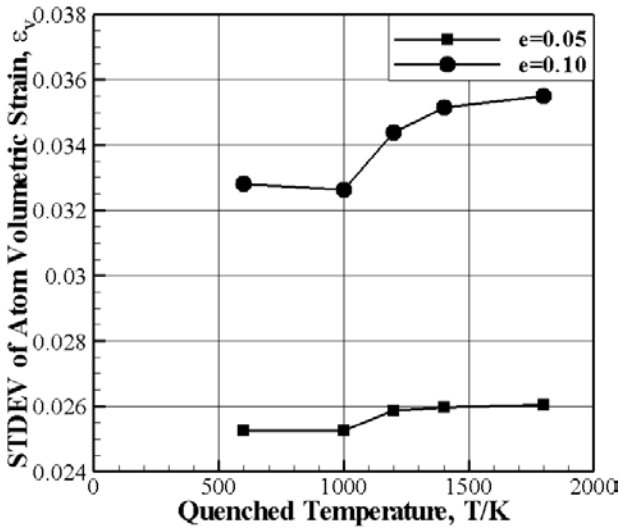


Fig. 5 Relationship between quenched temperature and standard deviation of atomic volumetric strain

Even at very low strain state (globally recognized elastic region) in Fig. 5 such as 0.05 strain, the structural-inhomogeneous models (models 1 of 600K and 2 of 1000K) have less deviation in both strain, atomic deviatoric strain and atomic volumetric strain, than the structural-homogeneous models (models 4 of 1400K and 5 of 1800K). At finite strain of 0.1, the trend becomes clearer. The structural-homogeneous model has large standard deviation. It makes sense because it has already reported in some paper that the amorphous structures with the larger number of crystals (structural-inhomogeneity) have richer multiple shear bands.

4. Conclusion

We perform molecular dynamics simulation for binary amorphous materials with highly density fluctuated structure induced by inserted nanocrystal structures. We found that structural-inhomogeneity induced by density-fluctuation makes deformable-homogeneity which means less deviation of atomic volumetric strain and deviatoric strain, while structural-homogeneity induced by pure amorphous structure promotes deformable-inhomogeneity which means more deviation of atomic volumetric strain even in elastic region.

후기

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MEST). (No.2009-0065745)

참고문헌

1. C.C. Hays, C.P.Kim, and W.L.Johnson, “Microstructure Controlled Shear Band Pattern Formation and Enhanced Plasticity of Bulk Metallic Glasses Containing in situ Formed Ductile Phase Dendrite Dispersions,” Phys. Rev. Lett., 84, 2901 (2000)
2. T. Nagase and Y. Umakoshi, “Phase stability of amorphous and crystalline phases in melt-spun $Zr_{66.7}Cu_{33.3}$ alloy under electron irradiation,” Scripta Mater., 48 (2003), 1237-1242
3. P. H. Mott, A. S. Argon and U. W. Suter, “The Atomic Strain,” J. Comput. Phys., 101 (1992), 140–150.
4. J. Park and Y. Shibutani, “Weighted Voronoi tessellation technique for internal structure of metallic glasses,” Intermetallics, 15 (2007), 187-192