Scripta Materialia 135 (2017) 41–45

Contents lists available at ScienceDirect

Scripta Materialia

journal homepage: www.elsevier.com/locate/scriptamat

Regular Article

Mechanical properties of spinodal decomposed metallic glass composites

Yongwei Wang [a,c], Mo Li [b,c,*], Jinwu Xu [a]

[a] School of Mechanical Engineering, University of Science and Technology Beijing, Beijing 100083, China
[b] State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing, Beijing 100083, People's Republic of China
[c] School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332, United States

A R T I C L E I N F O

Article history:
Received 27 February 2017
Accepted 12 March 2017
Available online xxxx

Keywords:
Metallic glass composite
Free volume
Plasticity
Shear band
Spinodal decomposition

A B S T R A C T

Controlling and manipulating heterogeneity through spinodal decomposition is one of few effective ways in making better metallic glass matrix composites. Here using a finite element modeling we investigate how the geometry, orientation, size, and statistical and spatial distribution of varying free volume heterogeneities in spinodal decomposition affect mechanical properties of the composites. Among the plethora of factors, orientation and statistical distribution of free volumes in the spinodal microstructures are identified as two key ones critically influencing the mechanical responses. The size effect is also discovered and found to be governed by the minimum size in shear banding initiation and propagation.

1. Introduction

Introduction of various heterogeneities into metallic glass (MG) is an effective way to improve the mechanical properties of the monolithic samples known for their undesired brittleness and lack of toughness, including crystalline or amorphous particles [1], fibers [2], or layers [3]. Through blocking and altering the shear localization behavior, the inclusions with different structure and mechanical properties can enhance the plasticity and strength of the MGs. However, such practice encounters tremendous technical difficulties. The foremost is controlling dispersity of the heterophases in MG matrix. Due to surface tension and size, small particles and fibers tend to bundle together, which causes stress concentration and undesired failure. The difficult undermines the ability to effectively utilize these inclusions and manipulate the properties of MG composites. The important factors are inclusion shape, size, and orientation, which is known to play important roles in determining the overall mechanical properties of any composites [4]. As a result, most MG composites made so far are still in *ad-hoc* fashion [5–10].

To overcome these difficulties, new approaches are developed, one of which is through chemical spinodal decomposition (CSD). The CSD utilizes the chemical instability of the multicomponent alloys: when cooled some chemical elements separate in either liquid or solid state and form heterogeneous regions from nanometers to microns in size which exhibit different geometric shapes and structures, and most importantly are dispersed homogeneously [11–15]. For example, perfect spherical shaped second phase form in some metallic glass melts and are dispersed homogeneously [16–20], which is nearly impossible by physically mixing such small particles into the MG matrix. The CSD regions with different chemical composition and structure have different mechanical properties and free volume (FV) density from the matrix that can be exploited in making composites [20–24]. For example, if the decomposed region is crystalline, the FV concentration is close to zero; otherwise the regions exhibit continuous variation of FVs associated with the chemical composition change [25–31]. These finely dispersed heterogeneities lead to great improvement in mechanical properties of MG composites [20–31]. However, the underlying mechanisms and the critical factors in making this promising MG composite remain unidentified and quantitative knowledge is lacking for exploring and designing new MG composites.

In this work, we shall investigate how these homogeneously dispersed regions or heterogeneities affect mechanical response of MG composites in terms of FV which is a characteristic quantity to gauge the variation of the structure and chemical compositional change in amorphous solids. Here we deal specifically with the bi-continuous dispersed microstructures from the CSD (Fig. 1(a)). As shown below, this choice allows us to study not only how specifically the CSD affects the mechanical properties but also reach out for a broad range of attributes of the heterophases in MG composites with complex microstructures such as the variation of FVs, size and shape and most importantly, the orientation of the inclusions that is absent in spherical particulate inclusions. This study will also help us to understand the role played by orientation of the "grain boundaries" in nanoglass which are similar to the

* Corresponding author at: School of Mechanical Engineering, University of Science and Technology Beijing, Beijing 100083, China.
E-mail address: mo.li@gatech.edu (M. Li).

http://dx.doi.org/10.1016/j.scriptamat.2017.03.019
1359-6462/

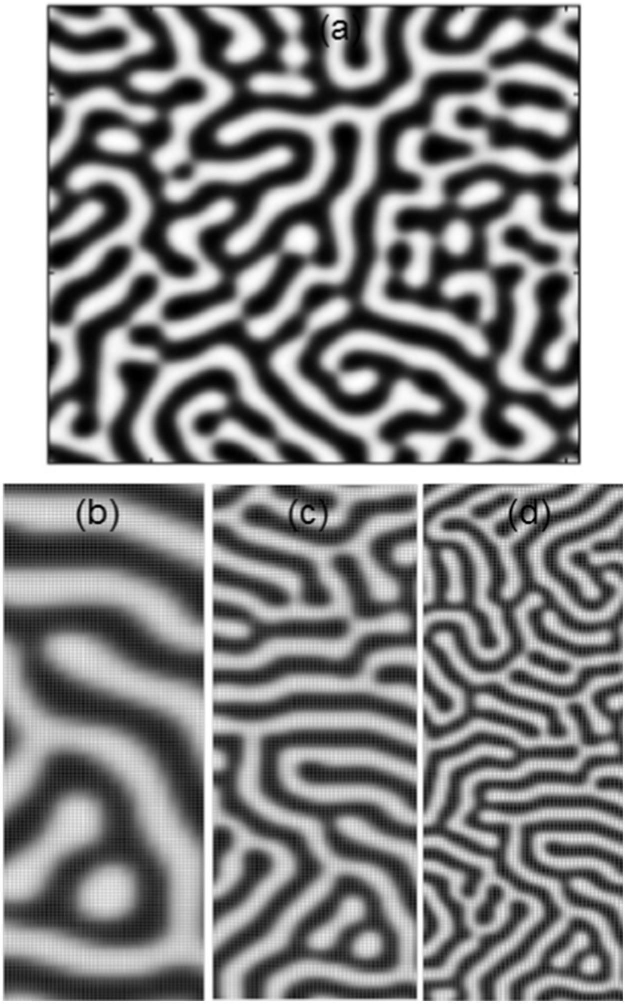

Fig. 1. (a) The micrograph of a bi-continuous statistical microstructure pattern of a CSD binary MG system from phase field modeling. Samples with characteristic sizes have different resolutions, (b) coarse, (c) medium, and (d) fine, against the same underlying finite element mesh grid (the thin grid lines) size (150 × 50 grids).

CSD microstructures with interconnected boundaries [32] but their ramification remains unknown in the overall mechanical properties.

Among many factors, two basic ones, *spatial* and *statistical* distributions of FVs, stand out and need to be implemented to model the complex MG composite with the CSD bi-continuous microstructures. The spatial distribution is provided by the *micrograph* of the spinodal decomposed two-phase microstructure obtained from phase field modeling (Fig. 1(a)). The microstructure is digitized with certain mesh points (see Fig. 1(b)-(d)). The values of the grey scale from the CSD micrograph is used to assign relative FV density on each grid point. The FV density value is generated separately from a *statistical distribution* from the following three different transformations of a beta distribution function *beta* [33], *beta*(50,50) × 0.04 + 0.03, *beta*(1,1) × 0.04 + 0.03 and *beta*(0.1,0.1) × 0.04 + 0.03 labeled as A, B and C type respectively. The FV distribution in A type of samples resembles a truncated Gaussian, B a random distribution, and C a bimodal distribution, all of which have the same mean at 0.05. Since the difference between the maximum and minimum FV values in A and B distributions is small, FV distribution at the diffuse *interface* in the CSD patterns has small gradient, whereas C has the interface with sharp FV gradient [34]. As shown in Fig. 1 the white regions have higher FV density values and the darker regions lower values which vary continuously throughout the samples according to the CSD pattern.

To investigate *size effect*, three types of samples from the same CSD pattern but with different resolutions are chosen: coarse, as type "1" (Fig. 1(b)), medium, as "2" (Fig. 1(c)) and fine, as "3" (Fig. 1(d)), while the size of the underlying finite element (FE) mesh grid (the thin grid lines) remains the same. Since the CSD patterns are in general elongated, its characteristic dimension or size is measured by the mean width of the interconnected FV regions. Therefore, type 1 is twice as large as type 2 which is twice as large as type 3.

From the combination of the *statistical distributions* of FVs (A, B, C) and *characteristic size* (1, 2, 3), we therefore have total of 9 types of samples. Two additional types of composite samples are also included in this work: the one with homogeneous spatial distribution of FVs which are labeled as "Random" [33] and the other with spatial orientation of the FV distributions in modulated patterns or layers which are labeled as "Gradient" [34]. In our naming scheme here the modulating FV regions are a special CSD patterns parallel to the loading direction (see Ref. 33). As we discuss below, this type of sample offers an extreme case with a spatial *orientation* as compared to the random orientation in the CSD bi-continuous statistical patterns (Fig. 1). Similarly, we also assign the three types of statistical FV distribution to these two cases, which gives rise to 6 additional types of samples. In the following, we shall name the 15 types of samples based on their spatial CSD patterns with different size and statistical FV distributions. For example, "A1" is for the samples with Gaussian statistical distribution of FV (A) on the coarse statistical CSD pattern (1) and "C3" is for the bimodal FV distribution (C) on a fine CSD pattern (3). The 6 special cases are named "A-, B- and C-Random" and "A-, B-, and C-Gradient" respectively. For example, the sample called "C-Gradient" has the CSD pattern parallel to loading axis (gradient) with the bimodal FV distribution (C).

With the initial interconnected CSD patterns of FV heterogeneities built in these samples, we can obtain the mechanical properties of the model composites by solving simultaneously the equations governing the change in FV and the strain and stress under external loading. This is done by implementing the UMAT subroutine in ABAQUS FE software and using the material parameters of bulk metallic glass $Zr_{41.25}Ti_{13.75}Ni_{10}Cu_{12.5}Be_{22.5}$. The total 7500 mesh elements are used (see Fig. 1(b)-(d)) in the cases reported here; a few cases with smaller and larger number of meshes are also used to test the size effect. To obtain the true plastic behavior, plane strain tension instead of compression is used with the effective strain rate of 0.1/s. Both free and periodic boundary conditions are used, but only the results from the latter are reported here. The reader is referred to Ref. 33–37 for more technical details.

The stress-strain relations for the samples are plotted in Fig. 2. To better our perception, the results are organized into three groups by different *colors*, red, blue and black for type A, B and C samples according to their FV statistical distributions, while the line thickness of the stress-strain curves is used for representing different CSD pattern sizes labeled as 1, 2, and 3. In the following, we present the results.

Size effect can be seen in the stress-strain relations with different line thickness of the samples in each group of samples with the same color for the underlying statistical FV distribution. For example, the A type of samples with the Gaussian-like FV distribution (red solid lines) in Fig. 2 shows little difference among themselves with coarse, medium and fine microstructures. The same weak size effect is seen for B and C types of samples (the blue and black solid lines with different line thickness). However, the *orientation* of the elongated CSD microstructure patterns emerges as a critical factor affecting the mechanical properties. The orientation is measured by the angle of a pattern with respect to the loading axis. Since the microstructures of the CSD patterns are continuous and tortuous, one cannot measure the angle as in straight lines. Instead, we deal with each continuous CSD pattern by first finding its center line (Fig. 3(a)-(c)); then divide each center line into segments with the length equal approximately to the mean width of the CSD pattern. Each segment is approximated as a straight line and its orientation angle is measured. The mean origination angle of each (continuous)