Journal of Alloys and Compounds 586 (2014) S262–S266

Contents lists available at SciVerse ScienceDirect

Journal of Alloys and Compounds

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

Simulation of shear banding in bulk metallic glass composites containing dendrite phases

H.Y. Zhang, G.P. Zheng *

Department of Mechanical Engineering, Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong

ARTICLE INFO

Article history:
Available online 27 March 2013

Keywords:
Metallic glasses
Metal matrix composite
Mechanical properties
Computer simulations

ABSTRACT

The mechanisms of shear banding in Zr-based bulk metallic glasses (BMGs) containing dendrite phase such as β-Zr_2Cu are numerically investigated using the phase-field simulation approaches. The growth of dendrite is simulated based on Elder's solidification theory. The interactions between the shear bands and the dendrites are studied using the phase-field model for shear banding in BMGs. It is found that the properties of dendrites such as the rotation angle representing their dispersion patterns and their fracture energy significantly affect the branching, multiplication and detour of shear bands, which result in the improved ductility of the composites. The simulation evaluates quantitatively the properties of dendrites that determine the features of shear banding in the composites.

1. Introduction

In the past decades, bulk metallic glasses (BMGs) have attracted much attention because of their distinguished mechanical strength, excellent corrosion resistance and thermo-plastic deformation properties [1]. However, shear banding or localized shear deformation at room temperature has prevented BMGs from applications in many areas [2–4]. In order to improve the room-temperature ductility of BMGs, several kinds of BMG matrix composites containing quasicrystals or intermetallic crystalline phases have been developed [5–9]. Significant improvements on the ductility have been reported in BMG matrix composite where *in situ* formed dendrite phases are introduced [10–12]. Although recent experimental and simulation studies have revealed that the restriction of shear banding and the bifurcation of shear bands which could be related with the presences of dendrites in the BMG matrix composites may play important roles in their improved ductility, how the relevant parameters of this crystalline dendritic phase such as its volume fraction, shape and dispersion pattern affect the mechanical properties of BMG matrix composites in microscopic or mesoscopic scales are yet to be resolved.

In this work the mechanisms of shear banding in the Zr-based BMG containing dendritic phase are numerically investigated based on the phase-field models [13]. As observed in experiments, the geometries such as the arms of the dendrites could significantly affect the deformation behaviors of the BMG composites. Previous simulations [14] on the shear banding and mechanical properties of BMG composites fail to account for such geometric details of the dendrites. It is essential to consider the geometry and microstructural details of the dendrite since the sizes of the arms of the dendrite are comparable with that of shear bands, which ultimately determined the shear banding behaviors of BMG composites under mechanical deformation. Hence in this work we will analyze the interaction of shear bands with dendrites' microstructures and how ductility could be improved in connection with such interaction.

This paper is organized as follows. In Section 2, we briefly describe the simulation methods, including the phase-field models for the simulation of dendrite phase formation processes [15], simulation of shear banding in BMG and crack propagation in crystalline phase. In Section 3, the simulation results will be discussed to reveal the details of interaction between shear bands and dendrites. From the simulation, the effects of the properties of dendrites such as their patterns, geometry and mechanical properties on the ductility of the BMG composites can be revealed in the mesoscopic scales.

2. Models and simulation methods

Phase-field modeling methods are employed to investigate shear banding in BMGs, dendrite phase formation and crack propagation in crystalline dendritic structures. Details are described as follows.

2.1. Phase-field modeling of shear banding in BMGs

According to the phenomenology model for shear banding in BMGs [13], the shear band is considered as a consequence of the structural transformation of deformation defects, which represent the loosely packed atomic structures consisting of excess volumes that are more vulnerable to internal rearrangement than the ideal close packed glassy structures. Whether it is activated thermally or mechanically, the shear band shall be presented as a result of accumulation and nucleation of

* Corresponding author. Tel.: +852 27666660.
E-mail address: mmzheng@polyu.edu.hk (G.P. Zheng).

0925-8388/$ - see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.jallcom.2013.03.159

the deformation defects. The normalized density of deformation defects defined as $w(\boldsymbol{r})$ is chosen as the order parameter describing the deformed glassy structures. Based on the above-mentioned definitions, the ideal un-deformed state can be described as the structure with $w(\boldsymbol{r}) = 0$, and the presence of ordering of deformation defects can be represented as $w(\boldsymbol{r}) > 0$. The shear band can be described as the states when the density of deformation defects reaches a critical value, defined as $w(\boldsymbol{r}) \geqslant 0.8$, while the fracture occurs when $w(\boldsymbol{r}) \to 1.0$. Based on these phenomenological accounts for the deformation and fracture characteristics of BMG, the free energy density of *deformation defects* can be written by a Ginzburg–Landau formulism as:

$$f_w = \frac{a}{2}w^2 + \frac{b}{3}w^3 + \frac{c}{4}w^4 + \ldots, \tag{1}$$

where a, b and c are coefficients depending on local strain energy and temperature.

According to the characteristics of shear band, the regions around the deformation defects still remain elastic, and the strain energy $e[\varepsilon_{ij}]$ can be written as $e[\varepsilon_{ij}] = 0.5C_{ijkl}\varepsilon_{ij}\varepsilon_{kl}$, where ε_{ij} is the component of the strain tensor, and C_{ijkl} is the component of the stiffness matrix. In a glassy solid where deformation defects such as free volumes are presented, the free-energy density of the deformation defects f_w has to be taken into account in the local strain energy $f(w, \varepsilon_{ij})$ which contributes to the free energy density F of the glassy solid: $f(w, \varepsilon_{ij}) = e[\varepsilon_{ij}] + f_w$. Because the deformation defect density is very small at the elastic region, the coefficients of Eq. (1) can be expanded by the plastic work $\Delta e = e[\varepsilon_{ij}] - e_0$ under plastic deformation, where e_0 is the strain energy at the elastic limit. Assuming the leading error term $\Delta e \cdot w^4$ or $(\Delta e)^2 \cdot w^2$ in Eq. (1) after such expansion, the local strain energy is written as:

$$f(w, \varepsilon_{ij}) = e[\varepsilon_{ij}] + \frac{a_0}{2}w^2 + \frac{b_0}{3}w^3 + \frac{c_0}{4}w^4 + \left(\frac{a_1}{2}w^2 + \frac{b_1}{3}w^3\right)(e[\varepsilon_{ij}] - e_0),$$

where the coefficients a_0, b_0 and c_0 depend on external state variables except the strain, and $a_0 = a'(T_g - T)/T_g$ where T_g is glass transition temperature and a' is a constant. a_1 and b_1 are constants.

Under external load, the free energy of the system is an integral of the kinetic energy, the free-energy density and the gradient of the density of deformation defects over the whole volume of the solid as:

$$F = \int \left\{ \frac{\rho_0}{2}[\dot{\vec{\boldsymbol{u}}}]^2 + f(w, \varepsilon_{ij}) + \frac{\kappa}{2}|\vec{\nabla} w|^2 \right\} dV, \tag{2}$$

where ρ_0 is the mass density of the sample; $\boldsymbol{u}$ is the displacement field; V is the volume of metallic glass, and κ is the interfacial energy between the ideal glassy regions and the deformation defects [13]. The equations of motions for $\boldsymbol{u}$ and w can be described as the variation of the free-energy of the system according to the Ginzburg–Landau theory,

$$\rho_0 \frac{\partial^2 \vec{\boldsymbol{u}}}{\partial t^2} = -\nabla \cdot \left[\frac{\delta F}{\delta \varepsilon_{ij}}\right] = \mu \nabla \cdot \left[\left(1 + \frac{a_1}{2}w^2 + \frac{b_1}{3}w^3\right)\nabla \vec{\boldsymbol{u}}\right], \tag{3a}$$

and,

$$\tau_w \frac{\partial w}{\partial t} = -\frac{\delta F}{\delta w} = \kappa \nabla^2 w - (a_0 w + b_0 w^2 + c_0 w^3) - w(a_1 + b_1 w)(e[\varepsilon_{ij}] - e_0), \tag{3b}$$

where τ_w is the characteristic time for deformation defects activation. By solving Eq. (3), the dynamic process of deformation of BMG can be described [13].

Zr-based (Zr–Ti–Ni–Cu–Be) BMG with dimensions of $20 \times 20 \times 2\ \mu m^3$ is chosen as the BMG matrix in the simulation. An initial crack with length of 0.4 μm, as shown in Fig. 1a, is introduced. The materials properties of Zr-based BMG are as follows [16]. $T_g = 625$ K; Young's modulus $E = 95$ GPa; Possion's ratio $\nu = 0.36$; $\rho_0 = 6050\ kg/m^3$; elastic strain limit under uniaxial tension is $\varepsilon_{limit} = 2\%$, and $e_0 = 38\ J/m^2$; $\tau_w = 0.25$ ns.

2.2. Phase-field modeling of dendrite formation

In order to investigate the interaction between the shear bands and the crystalline dendrites, formation of β-Zr_2Cu dendrite phase from the melts of alloys has to be simulated first. Dendritic structure is commonly seen in the solidification of alloy, and its shape is usually very complicated. The phase-field model based on Elder's solidification theory [15] has been successfully developed to describe the dendritic pattern formation.

The order parameter $\varphi(\boldsymbol{r})$ is employed to represent the phase transformation during the formation of β-Zr_2Cu solid phase from the melts. It ranges from −1.0 to 1.0. $\varphi = -1.0$ corresponds to the liquid phase while $\varphi = 1.0$ represents the solid phase. The free energy functional of a binary alloy $f(\varphi, c, T)$ has been proposed as a function of $\varphi(\boldsymbol{r})$, the usual solute concentration field $c(\boldsymbol{r})$, and the temperature field $T(\boldsymbol{r})$. The equation can be described as [15]:

$$\Delta F = \int_v \left\{ \frac{|\varepsilon_c \nabla c|^2}{2} + \frac{|\varepsilon_\varphi \nabla \varphi|^2}{2} + f(\varphi, c, T) \right\} dV, \tag{4}$$

where $\varepsilon_c = \sqrt{H}W_c$ and $\varepsilon_\varphi = \sqrt{H}W_\varphi$ are the constants. $W_\varphi = 1$ nm and $W_c = 1$ nm are used to define the length scales of the solid–liquid interface and the compositional boundary, respectively. $H = 6.05 \times 10^{-13}\ J/m^3$ is the nucleation barrier which is assumed to be the same for Zr and Cu atoms [15]. Ginzburg–Landau formalism can be applied to Eq. (4) to establish the equations of motion for the phase fields $\varphi(\boldsymbol{r})$ and $c(\boldsymbol{r})$. β-Zr_2Cu dendrites with different sizes can be obtained by setting their surfaces as $\varphi(\boldsymbol{r}) = 0$. The temperature field is assumed to be homogeneous.

In this work, the properties of β-Zr_2Cu crystallites are chosen as follows [15]: the melting temperature $T_M = 1726$ K, the latent heat $L = 2.311 \times 10^9\ J/m^3$, the heat capacity $c_p = 5.313 \times 10^6\ J/(m^3K)$, the diffusivity $D_L = 10^{-5}\ m^2/s$. The Young's modulus is 121 GPa [17], and the Poisson's ratio is 0.28. Fig. 1b shows the geometry of a typical dendrite obtained from the simulation.

2.3. Phase-field modeling of crack propagation in crystalline phase

In the BMG composites, the adhesion between the secondary phase and the BMG matrix is assumed to be perfect, resulting in the continuous displacement at the dendrite-BMG interface. Shear bands in the BMG matrix may induce cracking in the crystalline dendrite phase. To simulate the cracking in dendrites obtained in Section 2.2, the order parameter ϕ describing the fracture state of the crystalline solid has to be introduced. It is defined that $\phi = 1$ represents unbroken solid while $\phi = 0$ denotes fully ruptured state.

The governing equation for the order parameter ϕ has been developed to analyze the unsteady crack motion during a brittle fracture [18]:

$$\tau_0 \frac{\partial \varphi}{\partial t} = D_\varphi \nabla^2 \varphi - V'(\varphi) - \frac{\mu_0}{2} g'(\varphi)(|\varepsilon_{ij}|^2 - e_c), \tag{5}$$

where $\tau_0 = 20$ ns is the characteristic time of fracture process and $D_\phi = 1 \times 10^{-5}\ J/m$ is the surface energy describing the fracture process zone. $\mu_0 = 100$ GPa is the shear modulus. $V(\varphi) = \frac{1}{4}\varphi^2(1 - \varphi^2)$ is a double-well function which determines the states of cracking as mentioned above, and $g(\phi) = 4\phi^3 - 3\phi^4$ aims to stabilize the unbroken state when the applied strain energy is smaller than the critical value e_c, which is used as a measure of the fracture energy of the crystalline dendrite phase.

The interaction between shear bands and dendrites in BMG composites can be described by solving Eqs. (3) and (5) with finite element methods. We use triangle meshes for the model systems. The sizes of meshes can be as small as 2 nm near the regions of initial crack and the tips of the dendrite arms.

3. Results and discussions

Fig. 1b shows the β-Zr_2Cu crystalline phase obtained from phase-field simulation. It can be found that the patterns of the dendrite phase are consistent with the β-Zr_2Cu dendrites observed in electron microscopy [12], in particular the secondary arms can be well distinguished from the primary arms of the dendrite.

For the Zr-based BMG composites containing β-Zr_2Cu dendrite phase whose fracture energy is approximated as $e_c = 48.4\ J/m^2$, the interactions between the shear bands and the secondary phases with four different rotation angles ($\theta = 0°$, 15°, 30°, and 45°) which describe the relative positions between the initial shear bands and the primary arms of dendrite, are shown in Fig. 2. If the rotation angle is $\theta = 0°$, the shear band gets close to the primary arm's tip of the dendrite. Then cracking occurs in the dendrite as shown in Fig. 2a. The cracking area of the dendrite is so large that shear bands are also generated in the BMG matrix close to the tip of the primary arms. It is noted that the interaction results in not only crack propagation in the dendrite, but also the extension of incident shear band in the BMG matrix. This interesting phenomenon suggests that under mechanical deformation the presence of dendrite phase in the BMG matrix leads to more fracture surfaces in the dendrite and more shear bands in the BMG matrix which could accommodate more plastic strains and the ductility of the composite could increase. In the case of the rotation angle $\theta = 15°$ as shown in Fig. 2b, when the shear band gets close to the secondary arms of the dendrite phase, its propagation direction is changed a bit by the secondary arms before it generates fracture surface in the primary arm. The crack passes through one of the primary arms of the dendrite and induces shear banding in the matrix, accompanying by an additional crack which passes through the other primary arm of the dendrite. More shear bands could also be generated in the BMG matrix close to the cracking areas of the primary arms. Similar with the case of $\theta = 0°$, the ductility may