Intermetallics 83 (2017) 70–82

Contents lists available at ScienceDirect

Intermetallics

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

Tensile stress-strain response of metallic glass matrix composites reinforced with crystalline dendrites: Role of dendrite morphology

Mayuresh K. Shete [a], Tanmay Dutta [a], I. Singh [a], R. Narasimhan [a, *], U. Ramamurty [b]

[a] Department of Mechanical Engineering, Indian Institute of Science, Bangalore 560012, India
[b] Department of Materials Engineering, Indian Institute of Science, Bangalore 560012, India

A R T I C L E I N F O

Article history:
Received 13 October 2016
Received in revised form
25 November 2016
Accepted 5 December 2016
Available online 21 December 2016

Keywords:
Metallic glasses
Microstructure
Inhomogeneous deformation
Brittleness and ductility
Shear band
Finite-element modeling

A B S T R A C T

Bulk metallic glass composites (BMGCs) consisting of soft crystalline phases (commonly referred to as dendrites) in a metallic glass matrix have shown enhanced tensile ductility compared to conventional bulk metallic glasses (BMGs). Experiments and atomistic simulations suggest that a large number of geometrical parameters such as aspect ratio, spacing and orientation of dendrites as well as their spatial distribution can affect the mechanical response of BMGCs. However, the precise mechanism by which these parameters influence shear band initiation and propagation is not well understood. Therefore, continuum simulations of tensile loading on BMGCs with different morphologies are performed in this work. The results show that aspect ratio of dendrites has weak effect on the mechanical response up to the peak stress stage. However, it influences ductility considerably, albeit in a different manner for BMGCs with high and low hardening dendrites. The present analysis suggests that a BMGC capable of displaying mildly strain hardening response with large strain to failure can be designed by using closely spaced dendrites of high aspect ratio, and aligning them parallel to the maximum tensile stress direction.

1. Introduction

Bulk metallic glasses (BMGs) possess an impressive combination of mechanical and physical properties, which make them candidates for advanced structural applications [1–3]. A serious impediment for widespread deployment of BMGs, however, has been their negligible tensile ductility, which is due to unhindered propagation of single or few shear bands (SBs) [3,4]. Therefore, a major research challenge has been to enhance the room temperature ductility of BMGs. Amongst the different strategies that are being examined to enhance the ductility, the composite route, wherein dendritic crystalline phases are carefully introduced into the glass matrix, offers the most promise [5–11]. Experiments show that presence of matrix-dendrite interfaces in such bulk metallic glass composites (BMGCs) promotes nucleation of multiple, distributed shear bands which either get deflected by [7,12–14] or penetrate through the dendrites [7,14–18]. This, in turn, results in more homogeneous plastic deformation and enhanced energy dissipation leading to improved mechanical response and fracture toughness [5,8,11]. Indeed, Hays et al. [5] found extensive necking with plastic strain of 15% at necked region and overall plastic strain of ~5% prior to failure in Zr-based BMGC specimens. Necking was also observed in the tension experiments of Qiao et al. [16] and Szuecs et al. [19].

Given that the BMGCs do indeed have a microstructure, it is natural to expect that their mechanical performance can be affected by a number of different microstructural parameters such as shape, size, morphology, elastic properties, yield strength, hardening behavior and volume fraction of the dendrites, V_f. A number of experimental [6,8,11,19] and simulation [17,18,20–22] works were carried out to investigate these, a few of which are summarized below. Lee et al. [6] found that tensile ductility of La-based BMGCs enhances considerably when V_f was increased beyond 40%. They also reported non-linear behavior after yielding and ultimate strength followed by strain softening in the BMGC with $V_f = 50\%$. Hofmann et al. [8] also studied effect of V_f on mechanical response of Zr- based BMGCs and found that strain to failure enhances with increase in V_f. In addition, they reported that the fracture surface in BMGC with V_f of 42% is macroscopically flat whereas the specimen with a higher V_f of 67% exhibits zigzag fracture surface. It must be mentioned that BMGCs consisting of dendrites with different sizes and inter-dendrite spacing in addition to different V_f were used in the experiments of Hofmann et al.

* Corresponding author.
E-mail address: narasi@mecheng.iisc.ernet.in (R. Narasimhan).

http://dx.doi.org/10.1016/j.intermet.2016.12.006
0966-9795/

[8]. Thus, the observations made by them are a result of the synergistic interactions between V_f and the morphological changes to the dendrites. In order to understand the role of morphology on deformation response of BMGCs, Narayan et al. [11] performed tension experiments on BMGCs manufactured through different processing routes. By this means, they could vary the morphology while keeping V_f fixed. They observed that BMGCs with coarser dendrites and fine spacing in between them lead to an overall better mechanical response.

The above summary of experimental results indicates the importance of the inter-dependence of various ‘microstructural’ parameters, as well as the necessity to develop a detailed understanding of the role of each individual parameter. It must be mentioned that in recent works, Lee et al. [23] and Zhang et al. [24] have devised a method of varying the dendrite size while keeping their volume fraction, V_f fixed. Thus, in Ref. [24] it was shown from semi-solid treatment, β−Ti dendrites in a Be-rich matrix can be made finer while keeping their volume fraction approximately constant by increasing the cooling rate. However, since the number of morphological and constitutive parameters associated with the crystalline dendrites is large, it would still be difficult to vary all of them in a systematic manner. In this regard, numerical simulations can provide critical insights on the individual roles of these microstructural parameters on the deformation mechanism operative in BMGCs. Biner [20] explored the influence of mechanical properties, volume fraction and morphology of ductile reinforcements on the ductility of BMGCs by performing unit-cell based finite element analysis using a pressure sensitive and rate dependent porous plasticity model. They observed that while the ductile reinforcements may alter the morphology of SBs, the overall failure behavior is controlled by the glass matrix. Consequently, only a marginal improvement in the ductility in BMGCs was noted. It must be mentioned that volume fractions of reinforcement considered in Ref. [20] were less than 15%.

Zhou et al. [21] conducted atomistic simulations and reported that slender dendrites obstruct SB propagation more effectively than those with less aspect ratio (i.e., more spherical shape). Moreover, dendrites with parallel or perpendicular orientations with respect to loading axis are better at hindering SBs. They also noted that some SBs get arrested, few deflected along the matrix-dendrite interface while others penetrate through the dendrites. However, it is not clear from their work which parameters govern the SB penetration and deflection. Also, it is important to note that while MD simulations offer some qualitative insights, the length and time scales that are represented are quite small. In contrast to Zhou et al. [21], some continuum simulations have shown that dendrite shape has weak effect [17,18], while their size plays a greater role in improving the tensile ductility [17]. Thus, the role of dendrite shape on mechanical response of BMGCs is not well understood. Further, the constitutive model used in the work of Jiang et al. [17,18] was formulated within small strain framework. However, it must be noted that large displacement and rotation are expected due to interaction of SBs with the dendrites and, therefore it is more appropriate to use a finite deformation based plasticity theory. Recently, Shete et al. [22] studied the effect of volume fraction, V_f and strain hardening exponent, N of slender dendrites aligned with loading axis on the mechanical response of BMGCs through continuum simulations using a finite deformation plasticity model for metallic glasses. They showed that SBs penetrate through the dendrites for lower values of N, while they circumvent them for high N. In addition, increase in V_f stabilizes the plastic flow, while increase in N enhances the peak strength of the BMGC which approaches that of the parent BMG for high N of 0.3.

Although, some insights on mechanism of ductility enhancement in BMGCs have been gained through atomistic modeling and continuum simulations as discussed above, several questions remain unanswered. These are listed below:

- What is the effect of the aspect ratio of dendrites on the nucleation and propagation of SBs?
- Will aspect ratio of the dendrites affect the tensile response differently in BMGCs with high and low hardening dendrites? This is because the dendrites may redistribute the stress field in the surrounding matrix differently when they exhibit low and high hardening, thereby affecting the location of the SB nucleation sites. The magnitude of strain hardening of dendrites coupled with location of SB nucleation sites will influence the mechanism of shear band propagation in BMGCs.
- How does spatial distribution of dendrites influence the tensile ductility in BMGCs?

In order to address the aforementioned issues, plane strain finite element simulations of tensile loading on BMGCs of different morphologies are performed using a thermodynamically consistent finite strain based non-local plasticity model for metallic glasses. In order to systematically vary morphological features like dendrite aspect ratio, inter-dendrite spacing, spatial distribution of dendrites and obtain a clear understanding of their individual effects, idealized microstructures are considered. In addition, the role of strain hardening of dendrites of different aspect ratios is examined. Results show contrasting trend in ductility with change in aspect ratio of dendrites in BMGCs with high and low hardening dendrites. Also, composites displaying mildly strain hardening response with large strain to failure can be designed when dendrites with high volume fraction are aligned parallel to the loading direction.

2. Constitutive model and simulation aspects

The constitutive behavior of BMG matrix is represented through a finite deformation non-local plasticity theory proposed by Thamburaja [25], which has been shown to capture the mechanical response of BMGs [25–28], nanoglasses [29] and BMGCs [22] well. Moreover, use of a non-local model ensures accurate representation of strain localization which is insensitive to the finite element mesh employed in the analysis [30]. In the constitutive model proposed by Thamburaja [25], the free volume evolution $\dot{\xi}$, is governed by diffusion, creation by plastic shearing and hydrostatic stress, and annihilation by structural relaxation as:

$$\dot{\xi} = \dot{\xi}_o(s_1/s_3)\left(\nabla^2\xi\right) + \zeta\dot{\gamma} - \left(\dot{\xi}_o\overline{p}/s_3\right) - \dot{\xi}_o(s_2/s_3)(\xi - \xi_T). \tag{1}$$

Here, $\dot{\xi}_o = f_o \exp(-\phi/2\xi)$, where f_o is a reference frequency and ϕ a geometrical factor. Also, ξ is the current free volume, ξ_T the fully annealed free volume at temperature T, ζ free volume generation coefficient due to plastic shearing and $\overline{p}$ hydrostatic pressure. The constants s_1 and s_2 represent gradient and defect free energy coefficients (with units of energy per unit length and volume, respectively), whereas s_3 denotes the resistance to free volume generation. Further, in Eq. (1), $\dot{\gamma}$ is the rate of plastic shearing which is given by Ref. [25]:

$$\dot{\gamma} = \begin{cases} \dot{\gamma}_o\left(\dfrac{f^p}{c}\right)^{\frac{1}{a}} & \left(f^p = \overline{\tau} - \zeta\left(- s_1\left(\nabla^2\xi\right) + s_2(\xi - \xi_T) + \overline{p}\right) > 0\right) \\ 0 & (f^p \le 0) \end{cases}, \tag{2}$$

where, $\dot{\gamma}_o$ and $a > 0$ are the reference shear strain rate and strain rate sensitivity parameter, respectively. Also, $\overline{\tau}$ is the Mises shear