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Research paper

A failure mechanism based constitutive model for bulk metallic glass

Rao Wei[a,b], Zhang Juan[a,b], Kang Guozheng[a,b,*]

[a] State Key Laboratory of Traction Power, Southwest Jiaotong University, Chengdu, Sichuan, China
[b] Applied Mechanics and Structure Safety Key Laboratory of Sichuan Province, School of Mechanics and Engineering, Southwest Jiaotong University, Chengdu, Sichuan, China

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ABSTRACT

The formation of micro-cracks caused by the nucleation and coalescence of nano-voids in the shear bands is regarded as a main failure mechanism of bulk metallic glasses (BMGs). Based on such a failure mechanism and the free volume theory, a 3-D constitutive model of BMGs is developed in this work within the framework of continuum mechanics; and the concentration of nano-voids in the BMG is introduced into the constitutive model as an internal variable whose evolution characterizes the nucleation and coalescence of nano-voids during the deformation. Moreover, to describe both the brittle and ductile failure modes presented during the tensile and compressive deformations of BMGs, respectively, a failure criterion is established by introducing a stress triaxiality, which can describe the failure characteristics of BMGs under different stress states. Finally, through the finite element implementation of the developed constitutive model, the effectiveness of the model is validated by comparing the simulated results with the experimental ones of BMGs; in addition, the nucleation and coalescence of nano-voids in the BMGs during the tensile and compressive deformations are also predicted, and the comparison of predicted results and experimental ones demonstrates the reasonability of the developed model.

1. Introduction

When certain molten metallic materials are rapidly solidified, some metastable metals with long-range disordered and short-range ordered microstructures are formed. Such metastable metals with a characteristic size larger than 1 mm are called as bulk metallic glass (BMG). Since its unique metastable structure, the BMG possesses many excellent mechanical properties, such as high yield stress and hardness, large elastic limit and relatively good toughness (Ashby and Greer, 2006). These excellent mechanical properties make the BMG have great potential applications in engineering. However, due to lacking the hardening mechanism, significantly narrow and single shear band would be easily formed during the deformation of BMGs. Thus, the BMGs exhibit a macroscopic brittleness and often fail catastrophically at room temperature when the applied maximum shear stress reaches to their yield stresses (Donovan and Stobbs, 1981; Hays et al., 2000). Because the inherent brittleness of BMGs restricts their applications in engineering structures, many researchers have used various methods to improve the ductility of BMGs and prevent their catastrophic failure (Hays et al., 2000). To improve the ductility of BMGs effectively, it is necessary to make a thorough and systematic investigation on the failure process and mechanism in advance.

Lund and Schuh (2004) systematically analyzed and summarized the deformation behavior of BMGs, and thought that the macroscopic yielding and failure of BMGs consisted of many small-scale events including: (1) the nucleation of shear transformation zones, in which atoms rearrange to accommodate the applied shear strain (Argon, 1979); (2) the propagation of shear localization, or the growth of shear band (Donovan, 1988; Spaepen, 1977); (3) an adiabatic heating in localized deformed regions (Lewandowski and Greer, 2006); (4) the nucleation of nano-crystallites in or near shear bands (Jiang and Atzmon, 2003); (5) the nucleation of nano-voids in shear bands (Donovan and Stobbs, 1981); (6) the coalescence of voids leading to failure (Jiang et al., 2008; Zhang et al., 2003). Thus, the nucleation and coalescence of nano-voids in shear bands are key factors to clarify the failure mechanism of BMGs.

Some researchers observed and analyzed the deformed regions of BMGs by using transmission electron microscopy (Donovan and Stobbs, 1981), and found that the nano-voids about 0.3–0.8 nm in diameter mainly gathered in the regions where the concentration of the free volume was high; thus, they speculated that these voids formed from the coalescence of excessive free volume in the shear bands. Generally, the diameter of nano-voids is larger than that of the free volume. Unlike the free volume, the nano-void is the cavitation in the

* Corresponding author at: State Key Laboratory of Traction Power, Southwest Jiaotong University, Chengdu, Sichuan, China.
E-mail address: guozhengkang@home.swjtu.edu.cn (G. Kang).

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metallic glasses, and once the nano-void nucleate, the nano-void concentration would never decrease until the failure of the sample occurs or the rapidly quenched metallic glasses are annealed. Moreover, although the nucleation of nano-void is caused by the coalescence of excessive free volume, the intrinsic structural fluctuation related to the free volume has no effect on the evolution of nano-void. To further quantitatively investigate the nucleation of nano-void, Wright et al. (2003) supposed that the shear-band had the same structure as a solidified glass, and then put forward the concept of the fictive temperature; they further suggested that the nucleation of nano-void should be spontaneous and without any energetic barrier, and the shear band contained excessive free energy, which was taken as the driving force of free volume condensation.

With the increase of shear localization, there are some atomic clusters with an excessive concentration of free volume (these atomic clusters are called as the shear transformation zone) in the shear band of BMGs; and then the condensation of excessive free volume in the shear transformation zone would result in the nucleation of nano-voids; finally, the coalescence of nano-voids would induce the initiation of micro-cracks in the region near the shear transformation zone. Therefore, a shear transformation model is often used as a mechanism of direct breakage of local atomic clusters in the BMGs (Argon, 1979). Moreover, except for the shear transformation model, Jiang et al. (2008) suggested that the failure of BMGs might be resulted from the tensile stress in some specific cases, and then proposed a tensile transformation model so that both the ductile and brittle failure modes of BMGs can be explained well. From the view of Jiang et al. (2008), if there is no enough time to accomplish the viscoplastic flow of viscoplastic solid, the shear transformation mode will be constrained, and then the fracture occurs via the tensile transformation one. It means that the tensile transformation mode acts as a good complementary mechanism to the shear transformation one, and the combination of two modes can explain lots of experimental phenomena observed in the failure process of BMGs (Jiang et al., 2008). However, both two models treat the spatial correlation effects in a mean-field level, it is difficult to use them to describe the spatio-temporal evolution of inhomogeneous structure involved in the nucleation and propagation of shear bands and the onset of fracture (Jiang et al., 2008).

The further experimental investigation on the origin of failure in BMGs requires very careful technique and significant resources; and the microscopic theories also have some inherent shortages, for example, it is difficult to obtain the material parameters used in these theories, and the precise spatio-temporal evolution of inhomogeneous structure occurred in shear bands is difficult to be described. However, based on the finite element implementation of the constitutive model of BMGs considering the failure mechanisms, a systematic numerical simulation can be performed to investigate the failure process of BMGs and the nucleation and coalescence of nano-voids. Therefore, it is an important attempt to investigate the deformation and failure behaviors of BMGs by developing a failure mechanism based constitutive model. So far, many constitutive models have been constructed to describe the stress-strain response of BMGs at low homologous temperatures, such as the models done by Huang et al. (2002), Anand and Su (2005), Yang et al. (2006), Thamburaja et al. (2007) and Jiang and Dai (2009). However, the models proposed by Huang et al. (2002), Yang et al. (2006) and Jiang and Dai (2009) didn't take the failure of BMGs into account. Even if the concentration of free volume is regarded as the failure criteria in the models proposed by Anand and Su (2005) and Thamburaja and Ekambaram (2007), the failure of BMGs is not directly caused by the evolution of the free volume concentration in fact. Thus, the failure mechanism of BMGs cannot be well reflected in such models.

Therefore, based on the free volume theory (Spaepen, 1977) and the failure mechanism of BMGs (i.e., the nucleation and coalescence of nano-voids induce the initiation of micro-cracks in shear bands), a 3-D finite deformation constitutive model is developed within the framework of continuum mechanics so that the deformation and failure behaviors of BMGs can be well described. The free volume concentration (defined as the atomic gap related to the overall volume of the system) and the nano-void concentration (defined as the volume of all the nano-voids in per unit volume of BMGs) are regarded as two internal state variables in the proposed model. The concentration of free volume is used to characterize the evolution of shear bands caused by the structure relaxation in BMGs, and the formation and evolution of shear bands is regarded as a primary mechanism of inelastic deformation in BMGs; the concentration of nano-voids is used to measure the nucleation and coalescence of nano-voids caused by the coalescence of the free volume, and the nucleation and coalescence of nano-voids are regarded as a primary nucleation mechanism of micro-cracks. To describe the macroscopic failure and tension-compression asymmetry of BMGs, a new failure criterion is proposed based on the ductile-brittle transition mechanism established by Jiang et al. (2008). With the help of the finite element implementation of newly proposed constitutive model, both the failure process of BMGs and the formation and evolution of nano-voids in shear bands are predicted by using the finite element method. The comparison of the predicted results and experimental ones demonstrates the reasonability and validity of the proposed model.

2. Failure mechanism based constitutive model of BMGs

2.1. Kinematics

Considering a deformable body identified with the region $\mathbf{B}$, and assuming that $\mathbf{X}$ is an arbitrary position vector of a material point in the fixed reference configuration and $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$ is the corresponding space position vector at current time, the deformation gradient tensor $\mathbf{F}$, velocity vector $\mathbf{v}$ and velocity gradient tensor $\mathbf{L}$ can be written, respectively, as

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}, \quad \mathbf{v} = \dot{\mathbf{x}}, \quad \mathbf{L} = \mathrm{grad}(\mathbf{v}) = \dot{\mathbf{F}}\mathbf{F}^{-1} \tag{1}$$

Hereafter, the symbol $\dot{(\cdot)}$ denotes the material time derivative of scalar or tensor fields.

The deformation gradient tensor $\mathbf{F}$ would be multiplicatively decomposed as

$$\mathbf{F} = \mathbf{F}^e\mathbf{F}^p \tag{2}$$

where, the tensor $\mathbf{F}^e$ denotes the elastic distortion and $\mathbf{F}^p$ is the inelastic distortion.

The well-known right polar decomposition of elastic deformation gradient tensor $\mathbf{F}^e$ is given by

$$\mathbf{F}^e = \mathbf{R}^e\mathbf{U}^e, \quad \mathbf{R}^{e\mathrm{T}} = \mathbf{R}^{e-1}, \quad \mathbf{C}^e = \mathbf{U}^{e2} = \mathbf{F}^{e\mathrm{T}}\mathbf{F}^e \tag{3}$$

where, the orthogonal tensor $\mathbf{R}^e$ is an elastic rotation tensor, and the symmetric positive definite tensors $\mathbf{U}^e$ and $\mathbf{C}^e$ are the right elastic stretch and right elastic Cauchy-Green deformation tensors, respectively.

Combining Eqs. (1) and (2), it yields

$$\mathbf{L} = \mathbf{L}^e + \mathbf{F}^e\mathbf{L}^p\mathbf{F}^{e-1} \tag{4}$$

where, $\mathbf{L}^e = \dot{\mathbf{F}}^e\mathbf{F}^{e-1}$ and $\mathbf{L}^p = \dot{\mathbf{F}}^p\mathbf{F}^{p-1}$ are the elastic and plastic velocity gradient tensors, respectively.

Standardly, the symmetric parts of $\mathbf{L}^e$ and $\mathbf{L}^p$ are defined as the elastic stretching tensor $\mathbf{D}^e$ and plastic stretching tensor $\mathbf{D}^p$, and the skew parts are called as the elastic spin tensor $\mathbf{W}^e$ and plastic spin tensor $\mathbf{W}^p$. They yield

$$\mathbf{D}^e = \frac{1}{2}(\mathbf{L}^e + \mathbf{L}^{e\mathrm{T}}), \quad \mathbf{W}^e = \frac{1}{2}(\mathbf{L}^e - \mathbf{L}^{e\mathrm{T}}) \tag{5a}$$

$$\mathbf{D}^p = \frac{1}{2}(\mathbf{L}^p + \mathbf{L}^{p\mathrm{T}}), \quad \mathbf{W}^p = \frac{1}{2}(\mathbf{L}^p - \mathbf{L}^{p\mathrm{T}}) \tag{5b}$$