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Macroscopic tensile plasticity of metallic glass matrix composites through gradient microstructures

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ABSTRACT

Effectively improving the tensile plasticity of metallic glasses (MGs) becomes more and more important in order to promote their wide application in the structural engineering. In this contribution, numerical designs were performed to explore the efficiency of gradient microstructure on the tensile plasticity of the resulting composites. The free volume theory was incorporated into the ABAQUS code via a user material subroutine UMAT, which is used to depict the shear banding evolution in the MGs. Ductile particles are dispersed in form of various gradient functions, and the composite samples were loaded under uniaxial tension. Numerical simulations demonstrated that some special gradient microstructures could effectively enhance the tensile plasticity of MGs. Based on this work, the derived conclusions are helpful in establishing the interaction between gradient morphology and mechanical behaviors, and will provide an alternative approach to design some novel MG matrix composites with special functions.

1. Introduction

As a type of advanced material, metallic glasses (MGs) possess a large amount of unique properties, e.g., exceptionally high strength, large elastic limit, high hardness, good corrosion resistance and reduced sliding friction coefficient etc., and are therefore regarded as the first choice in the structural engineering applications [1]. However, their wide application is seriously stymied by their limited plasticity, which is confined to a few narrow regions near shear bands at the ambient temperature, which is lower than glass transition temperature T_g [2]. It is well known that the mechanical performance of materials mainly relies on their inherent microstructures, and thus designing some novel microstructures is conducive to the improvement of tensile plasticity of MGs.

Many innovative researches have been conducted to explore the potential feasibility of improving the tensile plasticity of MGs. Based on the free volume theory, Jiang et al. [3–5] conducted the parameter analyses on the roles of particle volume fraction, particle shape, particle orientation and particle yielding strength in improving the tensile ductility for MGCs. Shete et al. [6–7] performed finite strain continuum finite element method (FEM) to reflect the role played by the volume fraction and strain hardening behavior of crystalline particles on the strength and ductility of the composites. Fan et al. [8] utilized short-peening (mechanical crystallization) to create a composite layer of 80 μm upon the MG sample surface, in which many isolated crystal islands are randomly generated, and acts as the obstacles to impede the highly localized deformation induced by shear bands/cracks, which contributes to the improvement of uniform plastic deformation. Sarac et al. [9] discussed the influence of pores on the mechanical properties of MGs, and found that the pore configuration, overall porosity and diameter to the spacing ratio of the pores all affect the resulting plasticity. Zhao et al. [10] introduced two symmetrical semi-circular notches in Zr-based MG samples, and confirmed that a steady shear deformation can be created by the large-scale stress gradient, and enhanced the plasticity of metallic glass to a high value of about 10% under compression. Sopu et al. [11] numerically studied pore density, distribution, size and number on the deformation behavior of nanoporous $Cu_{64}Zr_{36}$ glass by using both molecular dynamics and FEM. Varying the pore distribution leads to a clear transition from a localized deformation through one dominant shear band to a homogeneous plastic flow mediated by a pattern of multiple shear bands. In the real composite systems, many microstructure parameters are interplayed, and the individual effect of each factor should be well understood. However, such work is not easily realized by the experiment method, and some numerical methods are sought to solve this dilemma. Wang et al. [12] numerically analyzed the effect of initial free volume gradient distribution on the mechanical behaviors of MGs, and pointed out that the gradient degree greatly affects both the strength and ductility.

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Fan et al. [13] prepared a novel structural gradient MGCs by subjecting fully glassy alloy to surface mechanical attrition treatment. The structural gradient includes the submicron-scale crystallites on the top surface, followed by nano-scale crystallites and a fully amorphous glass matrix inside. Plasticity was greatly improved.

Inspired by Wang's innovative work [12,13], the effect of particles with gradient distribution on the tensile behaviors is deeply studied. The main emphasis was played on the toughening efficiency with gradient morphology, and compared with other no-gradient counterparts, such as random and regular cases. Numerical simulations illustrate that some special gradient microstructures will change the deformation mode of MGs from strain localization to necking. The present study could provide us some instructive guidance in the further designing of novel composites.

2. Constitutive relations of the constituents

2.1. The free volume model for MG matrix

The shear-band initiation, growth, and propagation form the fundamental deformation mechanism in MGs. At the microscopic scale, shear-band formation is believed to be associated with the evolution of the local structural order. One atomistic mechanism capturing shear-band formation and evolution in metallic glass is the free volume theory developed by Spaepen [14] and further extended by Steif [15]. From a continuum mechanics point of view, the shear-band is a result of strain softening and considered to be a strain localization phenomenon. The free volume model regards free volume as an internal state variable, which controls the structural evolution of MGs at the atomic level.

According to the J_2-type, small strain visco-plasticity framework [16], the free volume theory is extended to a multi-axial stress state. The strain rate is decomposed into the elastic and plastic parts: $\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^e + \dot{\varepsilon}_{ij}^p$, and the above elastic part is expressed by the general Hooke's law as

$$\dot{\varepsilon}_{ij}^e = \frac{1+\nu}{E}\left(\dot{\sigma}_{ij} - \frac{\nu}{1+\nu}\dot{\sigma}_{kk}\delta_{ij}\right) \quad (1)$$

where E is elastic modulus, ν is Poisson's ratio, and the plastic part is rewritten as [17]:

$$\dot{\varepsilon}_{ij}^p = \exp\left(-\frac{1}{\nu_f}\right)\sinh\left(\frac{\sigma_{eq}}{\sigma_0}\right)\frac{S_{ij}}{\sigma_{eq}} \quad (2)$$

where ν_f denotes the average free volume per atom, σ_0 is the reference stress, $S_{ij} = \sigma_{ij} - \sigma_{kk}\delta_{ij}/3$ is the deviatoric stress tensor, and $\sigma_{eq} = (3/2S_{ij}S_{ij})^{1/2}$ is the von Mises' stress. The free volume evolution equation in the multi-axial stress state is given by:

$$\dot{\nu}_f = \frac{1}{\alpha}\exp\left(-\frac{1}{\nu_f}\right)\left\{\frac{3(1-\nu)}{E}\left(\frac{\sigma_0}{\beta\nu_f}\right)\left(\cosh\left(\frac{\sigma_{eq}}{\sigma_0}\right)-1\right)-\frac{1}{n_D}\right\} \quad (3)$$

where α and β stand for the geometric factors of order 1, respectively, and n_D is the number of atomic jumps needed to annihilate a free volume equal to ν^* (ν^* is the hard-sphere volume of an atom), which is usually taken to be 3–10.

2.2. Elasto-plastic relation for particle phase

The ductile particles is supposed to be isotropic and deform elasto-plastically according to the following yielding principle with isotropic hardening,

$$\frac{\varepsilon_{eq}}{\varepsilon_y} = \left(\frac{\sigma_{eq}}{\sigma_y}\right)^{\frac{1}{N}} - 1,\ \sigma_{eq} \geq \sigma_y \quad (4)$$

where σ_y, σ_{eq}, ε_y and ε_{eq} are the yielding stress, von Mises's stress, yielding strain and equivalent strain, respectively. N is the strain hardening coefficient, and its effect was fully discussed in the previous study. The material properties for the MG matrix are [3]: $E_m = 130$Gpa, $\nu = 0.36$, $n_D = 3$, $\alpha = 0.35$, $\beta = 0.9$ and $\sigma_0 = 100$Mpa. It should be noted that σ_0 is very different from the strength of MGs, and generally $\sigma_0 = 100$Mpa corresponds to the fracture strength of 2.2Gpa for the pure MG. Those properties for the particle phase are [3]: $E_p = 150$Gpa, $\nu = 0.35$, $\varepsilon_y = 0.0067$, $\sigma_y = 1.2$Gpa and $N = 0.2$.

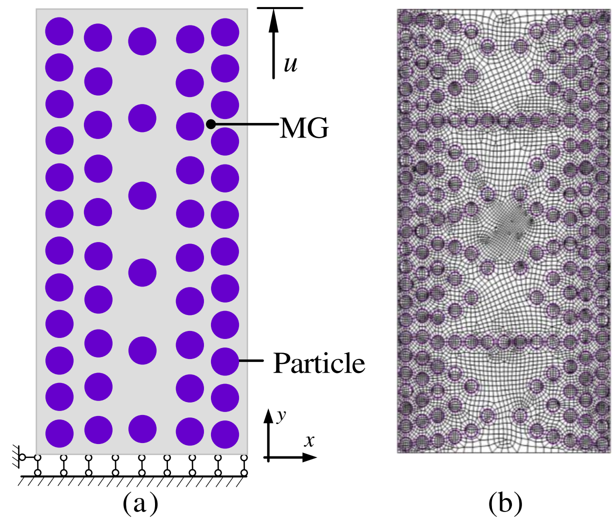

Fig. 1. Computational model adopted in the computation for 2D simulation of plane-strain tension and the corresponding boundary conditions exerted for particle filled composite in (a), and FEM meshed model in (b).

3. Numerical simulation

3.1. FEM model

The above free volume theory is implemented into the ABAQUS code through a user-defined material subroutine UMAT [18]. In this simulation, the shear band evolution is described by an *internal state variable*, i.e. the normalized free volume ν_f in Eq. (3). The computational model of this sample is shown in Fig. 1 (a) for particle filled composites, and the dimensions in directions of x and y are 50 μm × 100 μm, respectively. In order to accurately describe the stress transition field in such gradient microstructure, about 20,000 eight node plane strain elements are meshed, and one representative FEM model is shown in Fig. 1 (b). During the computation, all the nodes in the bottom node set are prevented from motion along axis-y. A positive displacement along axis-y is exerted to the single node located at the top-right corner with the desired test strain rate. The multi-point constraint (MPC) equation is applied to the rest of the nodes along the top surface in order to keep their deformation coordinate with the top-right corner node. To suppress rigid-body motions of the sample, the node located at the bottom-left corner is also prevented from moving along axis-x. The remaining nodes in the bottom and top nodes are free to move along axis-x. It should be noted that the periodical representative microstructures are absent in the real gradient composites, and then the present model cannot be regarded as representative volume element. From this point of view, the periodical boundary conditions should not be applied.

The particles are distributed in the MG matrix by obeying a certain gradient function, which is only assigned in the x-direction across the two dimensional plane under plane strain conditions. The specific gradient function is reflected by the variation of particle numbers along the sample width from the periphery to the center, whereby the gradient effect can be well embodied. Some typical gradient functions are imposed and the corresponding stress–strain relations are compared. Additionally, in order to better reflect the shear localization in the