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# Micromechanics constitutive model for predicting the stress–strain relations of particle toughened bulk metallic glass matrix composites

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A B S T R A C T

Based on the secant modulus and extended Mori-Tanaka method for dual ductile phases, a micromechanics model is proposed to predict the monotonic mechanical behaviors of bulk metallic glass matrix composites (BMGCs) toughened by particles. In this model, the deformation behaviors of the BMG matrix and particles are described by the use of the free volume model and the simple Ludwik flow equation, respectively, and Weng's homogenization frame is adopted to bridge the constituents and the composites. As compared to the existing relevant models, the present model is much more convenient for applying, and more readily to be extended. The developed model is applied with stain-controlled loading, and is verified by modeling the monotonic stress-–strain relations of particle toughened BMGCs. The predictions were in good agreement with the experiments from the literature, which confirms that the developed analytical model is capable of successfully describing the mechanical properties, such as yield strength, stress hardening and strain softening elongation, of composites.

## 1. Introduction

Bulk metallic glass matrix composites (BMGCs) are commonly utilized to effectively circumvent the poor damage tolerance of the pure BMGs. Up to now, the drastic changes in the production method and material form also lead to a significant extension of application fields of glassy alloys. Despite the fact that a large number of researches have already been performed and many qualitative conclusions were reached, we, however, are far away from a complete and thorough understanding of the fundamental synergic mechanisms governing the compatible deformations between the soft and ductile second phase reinforcements and the hard and brittle matrix in BMGCs.

Analytical models are more efficient than those numerical methods, but lag far behind the experiments and simulations. Based on the principle of thermodynamics and free energy, Marandi et al. [1] developed an elastic-viscoplastic, three-dimensional, finite deformation constitutive model to describe the large deformation behavior of BMGCs, but their model is fairly complicated and short of the micromechanics significance. Marandi et al. [2] established an elastic–viscoplastic, three-dimensional, finite deformation constitutive model to describe the behavior of La-based *in-situ* BMGC (*In-situ* composites are multiphase materials where the reinforcing phase is synthesized within the matrix during composite fabrication), within the super-cooled liquid region, at ambient pressure and a range of strain rates. Yang et al. [3] developed a constitutive model of BMG plasticity which accounts for finite deformation kinematics, the kinetics of free volume, strain hardening, thermal softening, rate-dependency and non-Newtonian viscosity. The model has been validated against uniaxial compression test data; and against plate bending experiments. Qiao et al. [4] firstly gave a micromechanics based model to elucidate the work-hardening behavior of ductile dendrites and softening of the amorphous matrix, and could fatherly simulate the tensile response of BMGCs, yet the interaction between two phases was not well considered. Only quantitative relations can further greatly improve the ductility/toughness of BMGs via efficiently tailoring the microstructures in an optimized manner. It is impeding to establish quantitative relations between microstructure parameters and material properties at the mesoscopic scale. Recently, Sun et al. [5] improved their previous micromechanics model to better predict the tensile behaviors of *in-situ* BMGCs based the *in-situ* measured data by the nanoindentation test.

Doghri et al. [6] once proposed a general formulation for the mean-field method of elasto-viscoplastic composites. The evolution equations for inelastic strain and internal variables at the very beginning of each time interval are linearized with the ending time of the same interval, and then numerically integrated through a fully implicit backward Euler scheme, which results in thermoelastic-like relations directly in the time domain, and not in the Laplace-Carson one. Their method can be readily applied to sophisticated elasto-viscoplastic models with an arbitrary set of scalar or tensor internal variables, and is valid for multi-axial, non-monotonic and non-proportional loading histories. Guo et al. [7] further extended this method to describe the stress–strain responses

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of composites under a stress-controlled cyclic loading. With the help of this homogenization formulation, Rao et al. [8] proposed a new meso-mechanical constitutive model to predict the monotonic tensile or compressive deformation of BMGCs with toughening phases. Since both algorithmic tangent operator and the affine strain increment should be firstly given, their analytical model appears very complicated in the form. Jiang et al. [9–11] regarded the shear bands as micro-cracks, and established their equivalence relation, finally developed two micro-mechanics models based on the incremental tangent stiffness and secant modulus, respectively. Their results demonstrate that these analytical models are capable of successfully capturing the main features, such as yield strength, strain hardening and stress softening elongation, of ductile particles filled BMGs. However, these models cannot involve the inherent essence in the deformation features of the BMG matrix. Recently, Ge et al. [12] embedded Mg nanocrystalline cores in amorphous glassy shells, and proposed a constitutive model to reflect the block effect by the crystalline phase on the propagation of localized shear bands. It is expected that only quantitative relations can further greatly improve the ductility/toughness of BMGs via efficiently tailoring the microstructures in an optimized manner. Therefore, establishing a quantitative relation between microstructure parameters and material properties is impeding and necessary.

Although many theoretical studies have been performed and shed insight into the mechanical behaviors of BMGCs, a simple micro-mechanics model is still needed to describe their intriguing experimental results. In this work, the deformation behaviors of the BMG matrix and particles are described by the use of the free volume model and simple Ludwik flow equation, respectively, and Weng's homogenization frame is adopted to establish the interaction between the constituents and the composites. Against the other models, the present model is much more convenient for applying, and more readily to be extended. The developed model is applied with stain-controlled loading, and is verified by modeling the monotonic stress–strain relations of particle toughened BMGCs.

## 2. Micromechanics model of BMGCs

The BMGCs consist of BMG matrix and ductile particle phase, and the stress–strain relations of the two constituents should be described by using suitable constitutive models. For such dual-phase composites, where both phases are able to undergo plastic flow, Weng [13] developed a elegant theoretical model to estimate the stress–strain relations of the composites, and later modified by Zhu [14]. Their formulas will be used as the basis of a new homogenization method for BMGC, a perfect interfacial bonding between two phases is assumed. For the dual-phase composites, the particle phase will be referred as phase 1 and BMG matrix as phase 0, and those of the composite are denoted by symbols without any script. All the tensors and vectors are written in boldface letters. The volume fractions of the particles and matrix are denoted by $c_1$ and $c_0$, respectively, and satisfy the relation $c_1 + c_0 = 1$.

### 2.1. Constitutive model of BMG matrix

The shear band formation and evolution leads to the fundamental deformation mechanisms in BMGs. At the microscopic level, 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 BMGs is the free volume model proposed by Spaepen [15] and later extended by Steif [16]. From the continuum mechanics point of view, the shear band is a result of strain softening and regarded as a strain-localization phenomenon. This model treats the free volume as an internal state variable to characterize the structural evolution at the atomic level in BMGs.

According to a $J_2$-type, small strain visco-plasticity framework, the free volume model can be generalized into multi-axial stress states. The total strain rate in the BMG is expressed by

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^{e} + \dot{\varepsilon}_{ij}^{p} \tag{1}$$

which includes the elastic part, $\dot{\varepsilon}_{ij}^{e} = \frac{1+\nu}{E}\left(\dot{\sigma}_{ij} - \frac{\nu}{1+\nu}\dot{\sigma}_{kk}\delta_{ij}\right)$, and the plastic part, $\dot{\varepsilon}_{ij}^{p}$. For the BMG phase, the plastic strain rate, i.e., the flow equation can be described as

$$\dot{\varepsilon}_{ij}^{p} = f\sigma_{ij}'/\sigma_{eq} \tag{2}$$

where $\sigma_{ij}' = \sigma_{ij} - \sigma_{kk}\delta_{ij}/3$ is the deviatoric stress tensor and $\sigma_{eq} = (\sigma_{ij}'\sigma_{ij}')^{1/2}$ is the von Mises' stress. $f$ is the flow stress, defined by

$$f = f_0\exp\left(-\frac{\Delta G^m}{k_B T}\right)\exp\left(-\frac{1}{\xi}\right)\sinh\left(\frac{\sigma_{eq}\Omega}{2k_B T}\right) \tag{3}$$

where $f_0$ is the frequency of atomic vibration; $\Delta G^m$ is the activation energy; $k_B$ is the Boltzmann constant; $T$ is the absolute temperature; $\Omega$ is the atomic volume and $\xi$ is the concentration of free volume. The free volume evolution equation under multi-axial stress states is rewritten as

$$\dot{\xi} = \frac{1}{\alpha_0}f_0\exp\left(-\frac{\Delta G^m}{k_B T}\right)\exp\left(-\frac{1}{\xi}\right)\left\{\frac{2k_B T}{\xi v^* S}\left(\cosh\left(\frac{\sigma_{eq}\Omega}{2k_B T}\right) - 1\right) - \frac{1}{n_D}\right\} \tag{4}$$

where $\alpha_0$ is a geometrical factor of order unity; $\nu^*$ is a critical volume; $S$ is the Eshelby modulus, given by $S = 2(1 + \nu)\mu/3(1-\nu)$; $\nu$ is Poisson's ratio; $\mu$ is the shear modulus; and $n_D$ is the number of atomic jumps needed to annihilate a free volume equal to $\nu^*$ and is usually taken to be 3–10.

### 2.2. Constitutive model of ductile particles

The Ludwik equation is adopted for the ductile particles in terms of von Mises' effective stress and plastic strain

$$\sigma_{eq} = \sigma_y + h(\varepsilon_{eq}^{p})^n \tag{5}$$

in which $\varepsilon_{eq}^{p} = (2\varepsilon_{ij}^{p}\varepsilon_{ij}^{p}/3)^{1/2}$, $\sigma_y$, $h$ and $n$ are the initial yield stress, strength coefficient and the work-hardening exponent, in turn, and these three constants can be determined by fitting with a tensile stress–strain curve. In addition Hencky's flow rule is adopted here,

$$\varepsilon_{ij}^{p} = \frac{3}{2}\frac{\varepsilon_{eq}^{p}}{\sigma_{eq}}\sigma'_{ij} \tag{6}$$

### 2.3. Homogenization method for BMGCs

For the dual-phase composites, Weng's model is adopted here to establish the relationship among ductile particles, matrix and the resulting composites under monotonic uniaxial loading. The detailed deviation is very lengthy, and can be found in the original work [13]. The relationship between the hydrostatic and deviatoric strains of BMGCs are expressed as follows:

$$\bar{\sigma}_{kk} = 3\kappa_0\left[1 + \frac{c_1(\kappa_1 - \kappa_0)}{c_0\alpha_0^s(\kappa_1 - \kappa_0) + \kappa_0}\right]\bar{\varepsilon}_{kk} \tag{7}$$

$$\bar{\sigma}_{ij}' = 2\mu_0^s\left\{\left[1 + \frac{c_1(\mu_1 - \mu_0^s)}{c_0\beta_0^s(\mu_1 - \mu_0^s) + \mu_0^s}\right]\bar{\varepsilon}'_{ij} - \frac{c_1\mu_1}{c_0\beta_0^s(\mu_1 - \mu_0^s) + \mu_0^s}\varepsilon_{ij}^{p(1)}\right\} \tag{8}$$

where $\alpha_0^s$, $\beta_0^s$ are the components of Eshelby's tensor for spherical inclusions, and defined as

$$\alpha_0^s = \frac{1 + \nu_0^s}{3(1 - \nu_0^s)},\quad \beta_0^s = \frac{2(4 - 5\nu_0^s)}{15(1 - \nu_0^s)} \tag{9}$$

and $\kappa$, $\mu$ denote the bulk and shear moduli, and are written as follows to meet the isotropic relations,

$$\kappa_r = \frac{E_r}{3(1 - 2\nu_r)},\quad \mu_r^s = \frac{E_r^s}{2(1 + \nu_r^s)},\quad (\text{r}= 0 \text{ or } 1) \tag{10}$$