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Microstructure-sensitive investigation on the plastic deformation and damage initiation of amorphous particles reinforced composites

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In this paper, new analytical modeling and simulation methodology based on finite element method are proposed to study microstructure sensitivity of damage initiation and plastic deformation in amorphous particles reinforced Mg-composites. In this simulation methodology, composite microstructure has been discussed based on the real morphology considering the inclusions with their actual size, shape, spatial positioning, and in the exact amount. The main purpose of this study is to develop an in-depth understanding of relationship between the microstructure, plastic deformation and damage initiation of these novel light metal composites. Results indicate that when particles are closely associated in the cluster, the plastic flow of the matrix inside the cluster is constrained and would initiate only after plastic flow begins in the regions without clusters. The constraint of deformation will promote early the void formation in the matrix and interface debonding in the clustering region. Experimental findings show that there is a strong relationship between damage formation and the local volume fraction of the reinforcement. Moreover, the results of tensile testing and microstructural characterization clearly reveal that the distribution of reinforcement particles controls the extrusion load which obviously reflects the 0.2%YS of the composite samples.

1. Introduction

Recently, a new class of metallic materials, amorphous alloys/bulk metallic glasses (BMG), which is different from conventional crystalline metals/alloys, attracted attentions of material scientists as a potentially promising reinforcement for metal-matrix composites (MMCs) [1–3]. Due to their unique structure, amorphous alloys/BMG possesses extremely high strength (1–2 GPa), large elastic strain limit of $\sim$2% (conventional crystalline metals have elastic strain limit of 0.2%) and superior corrosion resistance [4,5]. Looking at the unique properties of the amorphous alloys/BMG, it is advantageous to use them as reinforcements for making light metal composites.

Spatial distribution of particles determines, or at least influences significantly, several important mechanical properties such as the yield strength [6], the onset of damage [7,8], the ductility [9], and the threshold of fatigue crack growth [10,11]. Although these behaviors are not quite well understood, there is general agreement that the microstructures with particle clustering tend to result in poorer mechanical properties. Therefore further understanding of the relationship between the processing, the structure and the properties of particulate reinforced MMCs is considerably important. In most particulate reinforced composite, the particles are not uniformly distributed. Instead, these materials contain local regions where the particles are clustered. Often there is a tendency for particle clustering in the fabrication processes for real materials, so the common assumption that the particles are uniformly spaced in theoretical modeling and simulation is generally more easily visualized than realized in reality (particularly in the field of MMC).

Mechanical properties of particulate reinforced composites are highly dependent on the real microstructure of the composite and particle distribution and volume fraction. There have been some attempts in recent years to take account of effects of the randomness of the particle in the matrix [12–16]. It has been shown that the mechanical behavior of these composites is greatly influenced by the spatial distribution of the reinforcement particles. It is well established experimentally that damage nucleation in polymer- and metal-matrix composites occurs in regions of the microstructure that contain high local volume fraction of reinforcements [17,18]. Thus, the accurate simulation of deformation and damage initiation in composites requires new simulation techniques which can include inhomogeneous reinforcement distributions. Due to the limitations of the traditional analytical

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approaches to account for the particle distribution, the distribution of the particles cannot be explicitly taken into account and finite element strategies have been employed to obtain insight into particle distribution effects on mechanical properties of particulate reinforced composites by many researchers [19–22]. In these analyses, clustering has been discussed considering randomly generated artificial microstructure, however; the particle microstructure is quite complex and normally differs from reality.

An analysis of the effect of the microstructure of materials on strength and failure mechanism of materials can be a basis for the improvement of the microstructure of the composite. The optimization of the mechanical properties of composites is based on the knowledge of the relationship between the microstructure and the macroscopic response. Thus, in-depth understanding of the relationship between particle distribution, deformation pattern and damage mechanisms in BMG reinforced MMCs based on real morphology is of major importance for their engineering applications.

In this paper, a new micromechanical modeling based on Eshelby's equivalence principle incorporated with the Mori–Tanaka's mean field concept is proposed to study effects of particle clustering on damage initiation and plastic deformation to advance the understanding of this defect. This micromechanical modeling not only can be used for metal–amorphous alloy composite, but also can be considered for all particulate reinforced composites. Moreover, a simulation methodology based on FEM model is presented that can consider microstructure variables, such as particle morphology and distribution. This simulation has studied influences of particle clustering on deformation and failure mechanism of particulate reinforced composites. To validate the predictions of the proposed model, the results are compared to those obtained from the experiment for novel amorphous particle reinforced composites. In this work, $Ni_{60}Nb_{40}$ mechanically alloyed amorphous powders were used to reinforce pure Mg metal, to produce Mg–amorphous alloy composite.

2. Material and experimental procedure

Amorphous alloy powder with composition $Ni_{60}Nb_{40}$ (in atomic percent, at.%) was prepared by mechanically alloying powder mixtures of elemental Ni and Nb metals. The powder mixture was milled at room temperature in air for 87 h, using a Retsch PM400 planetary ball mill with a ball-to-powder ratio of 3:1 and milling speed of 200 rpm. To produce Mg-composites, elemental Mg-powder (99.6% purity) was blended with varying volume fractions (5% and 10%) of $Ni_{60}Nb_{40}$ powder for a duration of 1 h and consolidated at room temperature at 450 MPa for 1 min. The compacted cylindrical billets of 36 mm diameter were microwave sintered at 100% power level for 12.30 min so as to achieve a temperature of 550 °C (based on prior calibration). The sintered billets were soaked at 400 °C for 1 h, and hot extruded at 350 °C to produce rods of 8 mm diameter. The extruded rods were used for further testing.

The microstructure of 5 vol.% $Ni_{60}Nb_{40}$/Mg composites is shown in Fig. 1a. This image is fragmented into different parts with dark and light colors indicating the reinforcements and matrix respectively. The fragmentation was performed using image processing and the obtained digital image is shown in Fig. 1b. The particle clustering regions are clearly observed in the microstructure as depicted in Fig. 1c.

3. Methods

3.1. Micromechanical modeling

In this section, first, two parameters are defined to describe particle clustering and then a micromechanical modeling based on Eshelby's equivalence principle incorporated with the Mori–Tanaka's mean field concept is used to calculate the macroscopic stress which leads to initial yielding in the matrix while particle clustering is considered with those parameters. The spatial distribution of particles in the matrix is nonuniform such that some local regions have a higher concentration of particles than the average volume fraction in the material. These regions with concentrated particles are considered as "cluster" with different elastic properties from the surrounding material. The total volume V_f of particles can be divided into the two following parts:

$$V_f = V_f^c + V_f^m \tag{1}$$

where V_f is the volume of particles inside a cluster, and V_f^m is the volume of particles in the matrix outside the cluster. Two parameters are introduced to describe the particle clustering as follows:

$$\gamma = \frac{V_c}{V}, \quad \zeta = \frac{V_f^c}{V_f}, \quad (0 \leqslant \gamma, \zeta \leqslant 1) \tag{2}$$

where V is volume of composite, V_c volume of clusters, γ volume fraction of clusters, ζ volume ratio of the particles inside the clusters over the total particles inside the matrix. These two parameters, γ and ζ, can be used to describe the microstructural inhomogeneity of the particulate reinforced composite.

For a composite, the volume fraction of particles f_1 is defined by:

$$f_1 = \frac{V_f}{V} \tag{3}$$

Denote f_1^c as volume fraction of particles in the cluster and f_1^m volume fraction of particles in the matrix outside the clusters. We can give the relationships of f_1, f_1^c and f_1^m versus the clustering parameters, γ and ζ, as below:

$$f_1^c = \frac{\zeta f_1}{\gamma}, \quad f_1^m = \frac{f_1(1-\zeta)}{1-\gamma} \tag{4}$$

After defining clustering parameters, a stepping scheme is applied to calculate the effective properties of constituents of composite [23]. The cluster is homogenized to obtain an equivalent inclusion, and the same homogenization for the medium containing particles outside the clusters forms an equivalent matrix. Hence, the bulk and the shear modulus of equivalent matrix can be written as below:

$$\begin{aligned} \kappa_{0,eq} &= \kappa_0\left[1 + \frac{f_1(1-\zeta)(\kappa_1/\kappa_0 - 1)}{1-\gamma+\alpha[1-\gamma-f_1(1-\zeta)](\kappa_1/\kappa_0 - 1)}\right] \\ \mu_{0,eq} &= \mu_0\left[1 + \frac{f_1(1-\zeta)(\mu_1/\mu_0 - 1)}{1-\gamma+\beta[1-\gamma-f_1(1-\zeta)](\mu_1/\mu_0 - 1)}\right] \end{aligned} \tag{5}$$

and for equivalent inclusion as

$$\begin{aligned} \kappa_{1,eq} &= \kappa_0\left[1 + \frac{f_1\zeta(\kappa_1/\kappa_0 - 1)}{\gamma+\alpha(\gamma-f_1\zeta)(\kappa_1/\kappa_0 - 1)}\right] \\ \mu_{1,eq} &= \mu_0\left[1 + \frac{f_1\zeta(\mu_1/\mu_0 - 1)}{\gamma+\beta(\gamma-f_1\zeta)(\mu_1/\mu_0 - 1)}\right] \end{aligned} \tag{6}$$

where, for spherical inclusions

$$\alpha = \frac{1+\nu_0}{3(1-\nu_0)}, \quad \beta = \frac{2(4-5\nu_0)}{15(1-\nu_0)} \tag{7}$$

κ_r and μ_r are the bulk and the shear modulus of the matrix and inclusion ($r = 0, 1$).

The Poisson's ratio of the equivalent matrix is given as:

$$\nu_{0,eq} = \frac{3\kappa_{0,eq} - 2\mu_{0,eq}}{6\kappa_{0,eq} + 2\mu_{0,eq}} \tag{8}$$

The micromechanical modeling based on Eshelby's equivalence principle incorporated with the Mori–Tanaka's mean field concept is used to calculate the macroscopic stress which leads to initial