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Micro-mechanical behavior of porous tungsten/Zr-based metallic glass composite under cyclic compression

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ABSTRACT

The micro-mechanical behavior of porous tungsten/Zr-based metallic glass composites with different tungsten volume fraction was investigated under cyclic compression by synchrotron-based *in-situ* high-energy X-ray diffraction (HEXRD) and finite element modeling (FEM). During cyclic compression, the dislocation in the tungsten phase tangled near the interfaces, indicating that the elastic metallic glass phase restricted dislocation motion and obstructed the deformation of the tungsten phase because of the heterogeneity in stress. After the metallic glass phase yielded, the dislocation tended to propagate away from the interfaces, showing the decrease of the interphase stress affected the direction of motion in the dislocations. The tungsten phase exhibited increased yield strength with the increase of cyclic loading number. Yield stress of the tungsten phase decreased with increasing the tungsten volume fraction during cyclic compression, which was influenced by the elastic strain mismatch between the two phases. The stress heterogeneity and the stress distribution difference between the two phases resulted in that the yield strength of the metallic glass phase decreased with the increase of tungsten volume fraction, and accelerated the formation of shear bands in the metallic glass phase as well as cracks in the tungsten phase. The heterogeneity in stress also excessed the interface bonding strength, inducing interface fracture near interfaces.

1. Introduction

Bulk metallic glasses (BMGs) have many superior mechanical properties, such as high yield strength, high hardness, and low Young's modulus [1–3]. However, the fracture mode of BMGs is highly localized by shear bands during deformation, leading to little macroscopic plasticity [4–6]. In order to improve the plasticity of BMGs, considerable efforts have been taken to develop BMG based composites (BMGCs) [7–10]. The second phases in BMGCs could obstruct the rapid propagation of one major shear band and induce the formation of multiple shear bands, which is demonstrated to be responsible for enhancing the plastic deformation of BMGCs.

There are two ways to add the second phase into the metallic glass matrix for preparing BMGCs. One is *in-situ* [11–13], which is performed by crystallizing the alloy partially upon cooling or subsequent heating; the other is *ex-situ* [14–17], which introduces the foreign crystalline phases into the metallic glass matrices. The majority of BMGCs exhibited work softening behavior, only several BMGCs had work hardening capability, which was mainly attributed to the volume fraction, microstructure, or reinforcing mode of the second phase [18–23]. The three factors referred above lead the second phase to suppress the work softening of BMGCs. Most of the BMGCs with work hardening behavior had large volume fraction of the second phase, exceeding nearly 50% [18–20,23]. The variation of microstructure, such as deformation-induced phase transformation, also has positive influence on the work hardening behavior of BMGCs [24]. Likewise, continuous and homogeneous distribution of the second phase, especially the porous reinforcement with completely interconnected network structure could obviously improve the work hardening behavior of BMGCs [25–27]. The porous tungsten/Zr-based metallic glass composite exhibits typical interconnected network structure, which could hinder the propagation of shear bands in three-dimensional (3D) directions, restricting the formation of mature shear bands and inducing abundant micro shear bands [28,29], leading the composite to exhibit work hardening behavior and excellent plasticity. To interpret the work hardening capability and large plasticity of the porous tungsten/Zr-based metallic glass composite, further micro-deformation behavior of the composite needs to be investigated in detail, such as stress distribution and load transferring between the two phases during deformation.

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In the present work, integration of *in-situ* synchrotron-based high-energy X-ray diffraction (HEXRD) method and finite element model (FEM) was used to investigate the stress evolution between the two phases in the porous tungsten/Zr-based metallic glass composites during cyclic compression. The effect of tungsten volume fraction on micro-deformation behavior of the composites was studied. The tungsten volume fraction related work hardening behavior of the composites was discussed in detail.

2. Experimental procedure

The porous tungsten with 3D interconnected network structure was prepared by powder metallurgy in hydrogen atmosphere. The porosity was controlled by adjusting the volume fraction of pore-creating agent. Five element metals (purity > 99.5%) were mixed and arc-melted to prepare ingots of $Zr_{38}Ti_{17}Cu_{10.5}Co_{12}Be_{22.5}$ alloy in Ti-gettered argon atmosphere. The porous tungsten/Zr-based metallic glass composites with 67, 72, and 80 vol% W were prepared by pressure infiltration. The preparing details were presented in Ref. [30]. The rectangular specimens with dimensions of $1.6 \times 1.6 \times 3.2$ mm^3 were machined for compression in synchrotron-based HEXRD experiment. The ends of the specimens were polished to ensure parallelism and all surfaces of the specimens were mirror polished to minimize scattering.

The synchrotron-based HEXRD experiment was performed on 11-ID-C beam line of Advanced Photon Source, Argonne National Laboratory, USA. A monochromatic X-ray beam with energy of 115 keV (wavelength 0.107980 Å) was used to study the lattice strain of the specimens under uniaxial cyclic compression at room temperature. Fig. 1 shows the *in-situ* HEXRD experimental set-up. The maximum applied stress in the first loading was lower than the yield strength of the composites, the maximum second loading stress was just exceeding the yield strength of the composites, and the maximum applied stress in the third loading was higher than that in the second loading. Different diffraction patterns of the tungsten phase were collected by the two-dimensional (2D) detector placed ~1.4 m behind the specimens during loading. Lattice strain ε_{hkl} of the $\{hkl\}$ plane during loading could be determined by the following equation:

$$\varepsilon_{hkl} = (d_{hkl} - d_0)/d_0 \tag{1}$$

where d is the interplanar spacing of the $\{hkl\}$ plane, d_0 is the interplanar spacing in stress-free material. In the present experiment, d_0 was determined to be the initial interplanar spacing of the specimen without loading.

The interplanar spacing of the $\{hkl\}$ plane is obtained by means of Bragg's law:

$$d_{hkl} = \lambda/2 \sin\theta_{hkl} \tag{2}$$

where λ is the wavelength and $2\theta_{hkl}$ is the diffraction angle from the Debye cone. $2\theta_{hkl}$ is obtained by the individual uniaxial peak fitting.

In order to understand the detailed deformation behavior of the tungsten phase, the variation of the principal stress in the tungsten phase with the increase of applied stress was obtained. The yielding situation in the crystalline tungsten phase could be analyzed by von Mises criterion [31]. The principal strains ε_1, ε_2, and ε_3 were measured by HEXRD, respectively. ε_1 is the lattice strain parallel to the loading axis, ε_2 and ε_3 are the lattice strain perpendicular to the loading axis, respectively. ε_2 is equal to ε_3. The principal stresses are obtained by constitutive equations:

$$\sigma_1 = \frac{E}{1+\upsilon}\varepsilon_1 + \frac{\upsilon E}{(1+\upsilon)(1-2\upsilon)}(\varepsilon_1+\varepsilon_2+\varepsilon_3) \tag{3}$$

$$\sigma_2 = \sigma_3 = \frac{E}{1+\upsilon}\varepsilon_2 + \frac{\upsilon E}{(1+\upsilon)(1-2\upsilon)}(\varepsilon_1+\varepsilon_2+\varepsilon_3) \tag{4}$$

where σ_1 is the principal stress in longitudinal direction, σ_2 and σ_3 are the principal stresses in transverse direction. von Mises stress is calculated as following:

$$\sigma = \frac{1}{\sqrt{2}}\left[(\sigma_1-\sigma_2)^2 + (\sigma_2-\sigma_3)^2 + (\sigma_3-\sigma_1)^2\right]^{1/2} \tag{5}$$

To guarantee the accuracy of peak fitting by Gaussian, lattice strain was calculated from the tungsten {211} reflection, because {211} is a strong peak, which has little recollection of plastic deformation history, so it is the best choice to serve as the internal probe for microscopic stress and strain in texture-free materials [32].

To investigate the micro-deformation behavior of the metallic glass phase, FEM was used to analyze the stress–strain behavior of the metallic glass phase under cyclic compression. Microstructure morphologies of the present composites with tungsten volume fraction of 67%, 72%, and 80% in longitudinal section by scanning electron microscope (SEM) are shown in Fig. 2(a), (b), and (c), respectively. The gray area is the tungsten phase and the dark area is the metallic glass phase. The model was built by a mesh-generated program under an independent development to capture the microstructure of the present composites, as shown in Fig. 2(d)–(f), respectively. The model details and parameters could be found in Ref. [29]. The typical flow stress of the tungsten phase and the metallic glass phase could be determined by the following equations:

$$\sigma_t = \sigma_{t0} + Kd^{1/2} \tag{6}$$

$$\sigma_m = \sigma_{m0} \tag{7}$$

where σ_t and σ_m are the flow stress of the tungsten phase and the metallic glass phase, respectively. σ_{t0} and σ_{m0} are yield strength of the tungsten phase and the metallic glass phase, respectively. From Eqs. (6) and (7), it could be seen that the deformation of the tungsten phase obeyed Hall–Petch equation, and the metallic glass phase exhibited no work hardening behavior. Based on the deformation behavior of the two phases, the Bilinear Kinematic (BKIN) Hardening Plasticity modeling was chosen in FEM, where the work hardening exponents of the tungsten phase were determined by HEXRD, and the exponents of the metallic glass phase were determined to zero [33].

To analyze the deformation characteristics of the composites during cyclic compression, the tungsten phase, the metallic glass phase, and the interfaces between the two phases were examined by SEM and transmission electron microscopy (TEM) when the composites were loaded to the selected applied stress. The selected applied stress in the second loading was 1300 MPa (close to the greatest applied stress in the second loading) and 1700 MPa in the third loading (close to the greatest applied stress in the third loading).

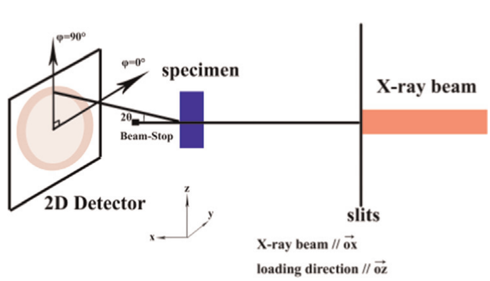

Fig. 1. Experimental set-up of high-energy X-ray diffraction.