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Compressive yielding of tungsten fiber reinforced bulk metallic glass composites

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Abstract

In-situ uniaxial compression tests were conducted on four tungsten fiber reinforced bulk metallic glass matrix composites using neutron diffraction. The results were interpreted with a finite element model. Both phases were seen to approximately obey the von Mises yield criterion. The fibers were observed to yield first and then transfer load to the matrix.

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1. Introduction

Recently developed bulk metallic glass (BMG) alloys [1] have attractive mechanical properties for structural applications [2,3]: yield strength around 2 GPa, fracture toughness above 20 MPa m^{1/2}, good corrosion resistance and high specific strength. Unfortunately, BMGs fail catastrophically by formation of macroscopic shear bands during unconstrained deformation at room temperature [2,3]. To avoid this failure mode, BMG

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matrix composites have been developed where the reinforcements appear to inhibit the formation of a single, catastrophic shear band [4]. This way, total strain to failure values of 10–16% in uniaxial compression have been obtained. Although Conner et al. speculated that multiple shear bands form in the matrix following the yielding of the tungsten (W) reinforcements [4], they presented no conclusive evidence about the in-situ deformation of each phase. Recently, Balch et al. studied the deformation of Ta particle reinforced BMG composites using high energy X-ray diffraction and confirmed that the yielding of the reinforcements precedes that of the matrix [5].

Another recent study by Dragoi et al. [6] determined the thermal residual stresses in W fiber reinforced BMG matrix composites with 20, 40, 60 and 80 vol.% fibers using neutron diffraction

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Table 1 Compressive yield behavior of four W/BMG composites (all stress data are in MPa)

The estimated error bar on stresses predicted in the present study is about ± 30 MPa.

measurements and finite element modeling (FEM). This study showed that the stresses are generated during cooldown starting near the glass transition temperature of the BMG and can exceed -500 MPa longitudinal (axial) compression in the W fibers (see Table 1). The present article describes the compressive yielding of the same composites. In this case, neutron diffraction and FEM were used to deduce the in-situ constitutive behavior of each phase under uniaxial compression.

2. Experimental procedure

Four composites of Vitreloy 1^{TM} (Zr_{41.2}Ti_{13.8}-Cu_{12.5}Ni_{10.0}Be_{22.5}) BMG alloy matrix containing (nominally) 20%, 40%, 60% and 80% volume fraction of continuous W fibers (250 µm diameter) were prepared by melt infiltration casting. The fibers were obtained from Thermionics Products Co., North Plainfield, NJ. After cleaning and straightening, they were inserted in a quartz-glass tube which was heated to about 1200 °C, infiltrated with molten BMG and then quenched in a brine solution. The total holding time at high temperature was estimated to be about 1 h. The actual fiber volume fractions were measured on scanning electron micrographs of the composites as: 21%, 42%, 62% and 84% (±2%). These values were used in all subsequent calculations. Neutron diffraction measurements were conducted at the Los Alamos Neutron Science Center (LANSCE) using the new SMARTS engineering diffractometer [7]. In-situ uniaxial compression experiments were carried out on cylindrical specimens as shown in Fig. 1. This geometry allowed the measurement of the longitudinal (scattering vector: Q_{\parallel}) and transverse (scattering vector: Q_{\perp}) lattice



Fig. 1. Schematic of compression loading set-up at SMARTS. Samples were about 8 mm in diameter and 19 mm long (aspect ratio = 2.4). The two scattering vectors, Q_{\parallel} and Q_{\perp} , are parallel and perpendicular to the loading direction, respectively. The diffraction data represent the bulk average from the highlighted sampling volume.

parameters simultaneously using the $2\theta = \pm 90^{\circ}$ detector banks. Elastic strain in the W was calculated from changes in its lattice parameter as a function of applied stress. Strains are reported relative to the initial strain state at a -5 MPa applied stress (which was needed to hold samples in a horizontal loading geometry). The W lattice parameter was determined using the entire diffraction pattern via the Rietveld method to within a 5×10^{-5} error [8,9]. Additional details about the Rietveld analysis can be found in [6]. Each composite was subjected to at least one load-unloadreload cycle (up to about -2000 MPa) while its longitudinal macroscopic strain was measured with an extensometer. Neutron data were collected under load control in 15-20 min runs at approximately 100 MPa stress intervals.

Complementary tensile tests to failure were conducted at Caltech (using an Instron 4100 load frame) on five as-received W fibers. Strain was

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measured at a strain rate of 10^{-3} /s with an extensioneter attached to the fibers.

3. Finite element modeling

The neutron diffraction measurements only recorded the elastic (lattice) strain in the W fibers, thus for a more comprehensive interpretation of the composite's deformation, a mechanics model is required. This model is especially essential here because no direct measurement of the response of the BMG matrix is possible as it cannot provide lattice strain data due to its amorphous nature. A finite element model was developed for this purpose using the commercial software ABAQUS[™] [10]. The present model is similar to that used in the previous thermal residual stress study [6], but to allow for loading along the fiber axes, the current model is three-dimensional where all planes perpendicular to the fibers remain plane. The FEM meshes used for the 20% and 80% W/BMG composites are shown in Fig. 2. Second order 20 node brick elements with reduced integration points were employed to model the cylindrical fibers. The fibers were placed on a hexagonal pattern for all composites (a square pattern would not allow an 80% volume fraction). The material pa-



Fig. 2. Meshes used in the FEM calculations: (a) the 20% fiber model, and (b) the 80% fiber model. The fibers occupy the lower left and upper right corners of each mesh. Consistent with the experiments, loading is applied parallel to the fiber axes.

rameters for both BMG and W as well as the thermal residual stresses were described in [6] since the same composites were used in both studies: for BMG, Young's modulus, $E_{BMG} = 96$ GPa [4], Poisson's ratio, $v_{BMG} = 0.36$ [4], and coefficient of thermal expansion (CTE), $\alpha_{BMG} = 9.0 \times 10^{-6}$ - 15×10^{-6} /K [11]; for W, $E_W = 410$ GPa [12], $v_W = 0.28$ [4], $\alpha_W = 4.5 \times 10^{-6}$ - 4.7×10^{-6} /K [13].

4. Results and discussion

The experimental data (Figs. 3 and 4) were combined with model calculations to deduce the in-situ constitutive behavior of each phase (Fig. 5). The calculations assumed the von Mises yield criterion for both phases and literature values were used for their yield points: 1300 MPa for W [14] and 1900 MPa for BMG [15]. As seen in Figs. 3 and 4, these values appear to be good estimates of the yield points of W and BMG in all four composites. The in-situ hardening behavior of each phase was regarded as variable and the FEM predictions were systematically fit to the experimental data (both lattice strain in W and macroscopic strain in the composite) until a satisfactory agreement was obtained for all four composites. The estimated error bars for this fit are about 5%.

The comparisons between experimental data and FEM predictions are quite favorable (Figs. 3 and 4). The model is able to closely follow the loading-unloading behavior of the fibers (Fig. 4) as well as the composite (Fig. 3) in the elastic and early yield regions. It is clear that the model predictions improve significantly when the deduced in-situ stress-strain plot (Fig. 5) of W is used. There is a pronounced difference between the inferred and measured (as-received) versions of fiber stress-strain plots likely due to annealing during the casting of the composites as well as the constraint imposed by the BMG matrix. This result proves the need to perform an in-situ investigation of the constitutive behavior of phases in a composite and not rely entirely on data obtained from monolithic specimens.

Table 1 summarizes the results of this investigation in comparison with literature data. It is seen that while the fibers and matrix yield at 1300 and



Fig. 3. Comparison of the FEM calculations ("as-received" and "in-situ") with the longitudinal macroscopic stress–strain curves for all four composites obtained from the extensometer: (a) 20%; (b) 40%; (c) 60% and (d) 80% W/BMG. The FEM employed two versions of the W constitutive behavior: (i) data from tests on free (as-received) fibers, and (ii) in-situ stress–strain plot inferred from neutron experiments on composites (see Fig. 5).

1900 MPa von Mises stress, respectively, the composite yield strength is dictated by the thermal residual stresses. Namely, the 20% W composite yields first since the fibers are under largest thermal residual stress (-520 MPa axial). This also indicates that the fibers enter the plastic regime first while the BMG matrix remains elastic until about -1900 to -2000 MPa applied uniaxial (composite) stress. The reader should also note the significant discrepancy between the literature data [4] for the composite axial yield stress and that obtained in this study (Table 1). Not surprisingly, the yielding in the matrix is seen to initiate in the

highly constrained regions between fibers where the FEM predicts the highest von Mises stress concentrations (not shown). It is also worth noting that in order to obtain a good fit with the experimental data, the FEM included strain hardening in the BMG (Fig. 5). The physical explanation of this behavior is the likely generation of multiple shear bands in the matrix as was also observed elsewhere [4]. This "plastic" behavior of the BMG accelerates at higher applied stresses where increasingly large plateaus are observed in the macroscopic stress–strain curves (Fig. 3). Noting that the neutron data were collected under constant load and



Fig. 4. Comparison of FEM calculations ("as-received" and "in-situ") to the longitudinal lattice strains in W fibers obtained from neutron diffraction data for all four composites: (a) 20%; (b) 40%; (c) 60% and (d) 80% W/BMG.

for a fixed period at each stress level, this behavior of the composite at high stresses suggests an inelastic, time-dependent relaxation mechanism the details of which are currently lacking. The current model does not include shear banding in the matrix; therefore, its predictions were terminated at about 2% total strain. Nevertheless, the model is able to successfully depict the early yielding behavior of the composites. Current work includes an upgrade of the finite element model to describe shear banding in the matrix.

5. Conclusions

A combined neutron diffraction and finite element modeling investigation was performed on four W fiber reinforced bulk metallic glass matrix composites to study their response to uniaxial compression. The conclusions can be summarized as follows:

- Fibers yield first (at about 1300 MPa von Mises stress) and then transfer load to the matrix.
- Matrix yields later (at about 1900 MPa von Mises stress) likely by multiple shear band formation.
- Overall composite yield point is dictated by thermal residual stresses. For instance, the 20% W composite yields first due to the largest thermal residual stress in its fibers.
- The deduced (in-situ) constitutive behavior of W is found to be different than that obtained from single fiber tests. This is probably due to



Fig. 5. Stress-strain curves for the W fibers and the BMG matrix. The in-situ curves are the ones deduced by and used in the FEM calculations, and they were determined from the neutron measurements on all four composites. The "as-received" W curve is an average of five single fiber tensile tests on loose fibers. The dashed lines on each side of this curve indicate the envelope of the data from these tests. The literature curve for BMG is based on published data for monolithic Vitreloy 1 [4].

the annealing it experienced during composite fabrication.

• The FEM developed in this study is capable of successfully describing the early compressive yielding of these composites.

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