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Influence of thin-film metallic glass coating on fatigue behavior of bulk metallic glass: Experiments and finite element modeling

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ABSTRACT

A coating of the Zr-based thin-film metallic glass (TFMG) was deposited on the $Zr_{50}Cu_{30}Al_{10}Ni_{10}$ bulk metallic glass (BMG) to investigate shear-band evolution under four-point-bend fatigue testing. The fatigue endurance-limit of the TFMG-coated samples is ~ 33% higher than that of the BMG. The results of finite-element modeling (FEM) revealed a delay in the shear-band nucleation and propagation in TFMG-coated samples under applied cyclic-loading. The FEM study of spherical indentation showed that the redistribution of stress by the TFMG coating prevents localized shear-banding in the BMG substrate. The enhanced fatigue characteristics of the BMG substrates can be attributed to the TFMG coatings retarding shear-band initiation at defects on the surface of the BMG.

1. Introduction

Bulk metallic glasses (BMGs) have attracted considerable attention as structural materials, due to their high strength, superior elasticity, and high corrosion resistance [1]. However, the applicability of these materials is restricted by poor room-temperature plastic deformability and fatigue properties, which can lead to catastrophic failure under mechanical loading. Brittle fractures in BMGs are associated with the formation of highly-localized shear regions, referred to as shear bands. Crystalline materials are easily susceptible to crack propagation, which greatly undermines their resistance to fatigue [2–5]. Researchers have proposed two mechanisms to explain fatigue-crack initiation in BMGs [6,7]. The first involves the initiation of cracks when the stress is concentrated at casting defects, such as pre-existing pores and inclusions. The second involves the initiation of shear bands from the free surface of the BMGs under cyclic loading. Shear bands accommodate the release of elastic energy and heat, causing the shear regions to weaken into shear steps to produce microcracks under further cyclic loading [8]. Several methods have been proposed to improve the fatigue resistance of BMGs [9–11]. The fatigue mechanisms of BMGs differ considerably from those of crystalline materials, due to differences in their atomic and microscopic structures [7]. The method used to enhance the fatigue-endurance of crystalline materials (shot peening) is inapplicable to glassy alloys. Raghavan et al. [9] determined that during fatigue cycles, stress would concentrate in softened regions or shear bands induced by shot peening, thereby accelerating crack initiation and reducing fatigue resistance. Another approach to improving the fatigue endurance of BMGs involves the introduction of a second phase into the matrix in order to constrain the propagation of shear bands and cracking [10–12]. However, some BMG composites exhibit fatigue lifetime lower than that of monolithic BMGs in the low-cycle-fatigue region, due to the fact that crack propagation occurs more rapidly in the second phase than in the BMG matrix [10,12]. Furthermore, various microstructural characteristics of BMG composites, such as phase size and spacing, are difficult to control. In the current study, we conducted four-point-bend fatigue tests to determine whether a thin coating of metallic glass (~260 nm) could delay shear-band propagation and thereby improve the fatigue characteristics of BMGs.

We determined that the deformation behavior transits from the localized shear banding to homogeneous plastic flow when the sample size is reduced from the millimeter- to nanometer-scales [13–16]. According to Weibull statistics, the strength of small-scale MGs should be higher due to a smaller flaw-size distribution, requiring a higher stress (i.e., more energy) to initiate the formation of shear bands [17,18]. Thin-film metallic glasses (TFMGs) on the sub-micrometer

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scale provide strength and ductility superior to those of its bulk form [19]. TFMGs have been used to improve the fatigue properties of crystalline materials, including 316 L stainless steels [20], nickel-alloy [21], titanium-alloy [22], and aluminium-alloy [23]. The improved fatigue characteristics can be attributed to the high ductility and strength of the TFMG coatings, which retards fatigue-cracking-initiation in TFMG/substrate materials under cyclic loading. Few studies have reported on efforts to improve the fatigue properties of BMGs through the application of coatings. This is one of the first studies to extend the use of TFMG coatings as a protective layer on crystalline materials in order to improve the fatigue characteristics of BMGs. In this study, we investigated the effects of such coatings on shear-band initiation in BMG substrates during fatigue tests. We did not take into account the evolution of fatigue-crack propagation. We conducted a systematic investigation of shear-band evolution in film/substrate systems using experiments and numerical modeling. We conducted finite-element modeling (FEM) of film/substrate systems under the effects of fatigue and indentation to elucidate the means by which the coatings affect shear-band formation and evolution in BMG substrates.

2. Experimental methods

$Zr_{50}Cu_{30}Al_{10}Ni_{10}$ BMGs (in atomic percent, at%) were machined into rectangular slabs with sample dimensions of 3 mm×3 mm ×25 mm from as-cast ingots fabricated by arc melting under an argon atmosphere. Prior to thin-film deposition, the surfaces of the BMG samples were mechanically polished to a mirror finish. The 260 nm-thick MG films were deposited on the BMG substrates with a $Zr_{55}Cu_{29}Al_{11}Ni_5$ alloy target using radio frequency magnetron sputtering deposition at a base pressure of $<1\times10^{-6}$ Torr. Argon was introduced as a sputtering gas at a working pressure of 3 mTorr with an applied substrate bias of −50 V.

Four-point bending fatigue tests were conducted on bare and TFMG-coated samples. The experiments were carried out using a Materials Test System (MTS370). The spans of between upper pins and bottom lower pins were 10 mm and 20 mm, respectively. The fatigue tests were performed under in load-control mode on a hydraulic load frame, using sinusoidal waveforms at frequencies of 10 Hz with R =0.1, where R is the ratio of the minimum stress to the maximum stress. Testing was conducted until the sample failed or until a predefined run out of 1×10^7 cycles was attained. The calculations of the nominal maximum alternating stress was obtained, using the following equation: $\sigma=3\times P\times(l\text{-}d)/2wt^2$, where P is the applied load, l is the support span, and d is the upper span, and w and t are the width and thickness of the specimens, respectively. The crystallographic structures of the samples were characterized using an X-ray diffractometer (XRD, D8 Discover) with Cu Kα radiation at 40 kV and 200 mA. A low glancing angle was used for analysis of the thin films. The element compositions of the samples was determined employing the energy-dispersive spectrometry (EDS), The fracture surfaces of the specimens were examined using a scanning electron microscope (SEM) with a dual-beam focused ion-beam system (FIB, FEI Quanta 3D FEG). The transmission electron microscope (TEM) foil specimens were prepared with a 30- kV Ga^+ focused ion beam for the initial sectioning, and 5 kV for the final ion polishing. A TEM operated at 200 kV was used to examine the microstructure and to obtain the selected-area electron diffraction (SAED) patterns of the samples.

3. Numerical approaches

The experiments on the TFMG-substrate materials were designed to elucidate the structure and mechanical properties of the thin films as well as substrates. However, the extreme thinness of the films hampered the formulation of stress and strain plots. Furthermore, illustrating the shear-band initiation and propagation in metallic glasses is difficult using experimental methods. Thus, we employed FEM to derive this information.

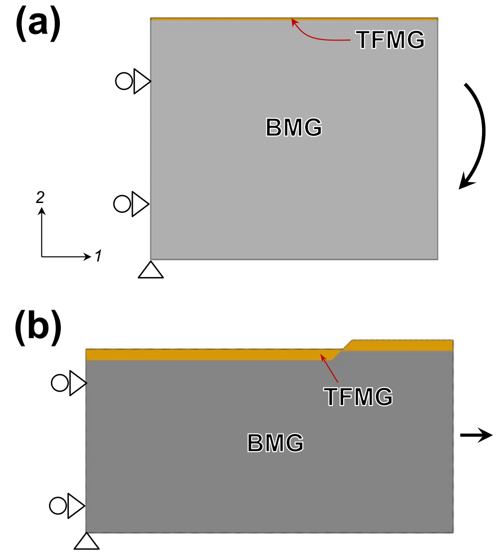

Fig. 1. Numerical models representing (a) the through-thickness segment of the TFMG-coated material under cyclic bending; and (b) the local top segment with the existing shear step under cyclic tension loading.

3.1. Fatigue Model

FEM of uncoated and TFMG-coated BMG substrates is performed, with an aim to rationalize the fatigue behavior observed experimentally. Fig. 1**(a)** illustrates the computational model and boundary conditions employed for the cyclic bending test. The thickness of the TFMG coating is identical to the experimental value, and the substrate thickness is taken as 20 µm. Another case involving only a bare BMG without any coating is also considered. Bending deformation is introduced by imposing displacements along the 1-direction, linearly graded through the thickness, to the right-hand boundary. The maximum bending tensile strain on the top side is set at 0.025. Cyclic deformation between zero strain and this peak value is then simulated. Along the left-hand boundary, displacement in the 1-direction is forbidden during deformation, but movement in the 2-direction is allowed except that the lower-left corner node remains fixed.

In a separate analysis, attention is directed to the effect of an existing shear offset (as observed in the experiment described below) on subsequent deformation. The model features a local region on the top (tensile) side of the fatigue specimen, as shown in Fig. 1**(b)**. The size of the shear step is taken to be 5/6 of the film thickness. Since the analysis is intended for the quantification of the local deformation field around the surface step, the uniform pulling displacement along the 1-direction on the right-hand boundary is imposed. Cyclic loading between the tensile strains of 0 and 0.025 is simulated. As in the bending fatigue model, a pure BMG counterpart of Fig. 1**(b)** is also included in the investigation.

The materials are treated as isotropic elastic-plastic solids. The Young's modulus and Poisson's ratio of BMGs are 108 GPa and 0.37, respectively. Plastic yielding follows the von Mises criterion and incremental flow theory. The choice of appropriate constitutive laws for amorphous alloys has been a topic of active research [1]. Within the continuum framework, plasticity in crystalline metals is generally controlled only by the deviatoric part of the stress tensor. For disordered materials, such as metallic glasses, hydrostatic pressure is expected to influence the yield behavior. Many experimental investigations have concluded that the pressure dependence of plastic deformation is relatively weak (see Ref [1]. for discussion). Some studies specifically showed that the von Mises criterion is adequate for describing the yield response [24,25]. Therefore, for simplicity purposes, the von Mises criterion with perfect plasticity upon yielding at a uniaxial stress of 2.2 GPa is chosen for this part of the modeling study.