



Full length article

Ductile fracture in notched bulk metallic glasses



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ABSTRACT

The deformation of bulk metallic glasses (BMGs) is generally driven by highly localized shear. Due to such inhomogeneous flow, failure occurs in a catastrophic **brittle** manner through rapid shear banding, often associated with very limited plastic strain macroscopically. Here, we demonstrate metal-like **ductile** fracture in Zr-based BMGs under tension, a completely opposite situation, by suppressing shear banding. In the absence of shear bands, nucleation of cavities/voids and subsequent void growth and coalescence dominate the initial plastic failure process, enabling BMGs to display the essential characteristics of ductile fracture, with deep dimples and *cup-and-cone* morphology. This ductile fracture only occurs in amorphous alloys, but not in the fully crystallized counterpart. Furthermore, the characteristic decohesion strength of the ductile fracture in Zr-based BMGs was found to be 1.75 GPa, one of the highest among engineering metals and alloys. These present findings reveal the previously hidden ductile behavior of BMGs, suggesting an alternative method to enhance the ductility of BMGs by removing shear banding.

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1. Introduction

Mechanical failure often causes to the great loss in property and human life, thus the study of fracture behavior and mechanism of materials are crucial in both engineering and materials science. In general, the tensile fracture of materials can be broadly classified into two categories: brittle fracture and ductile fracture. Brittle fracture is characterized by minimal macroscopic plastic deformation before fracture, driven by cleavage or brittle intergranular fracture, with cracks proceeding normal to the applied tension [1,2]. Tensile ductile fracture exhibits extensive plastic deformation (necking) before fracture. It occurs through slow tearing of the metal with the expenditure of considerable energy, resulting in a rough fracture surface, characterized by dimples and cracks [1,2]. The inherent bond characteristics and crystal structure are the reasons for different classes of materials exhibiting differing tendencies for brittle versus ductile fracture [3–5]. Due to metallic bonding, metals are relatively ductile compared to materials that are either ionically or covalently bonded, which are typically far more prone to brittle fracture.

Although the bonding nature in BMGs is primarily metallic in character, they exhibit extremely *brittle* behavior with no tensile

plasticity [6,7], even though their fracture toughness can be as high as $100 \text{ MPa m}^{1/2}$ [8,9]. Unlike their crystalline metallic counterparts, whose deformation is usually driven by the movement of dislocations, many previous studies on the fracture of metallic glasses showed that shear banding is the dominant plastic deformation mode [7,10–12]. The tendency of shear localization leads to the self-focusing concentration of plastic strain as well as rapid propagation of shear band causing premature fracture of BMGs. The fracture surface of BMGs is relatively flat, with vein patterns caused by microscopic plastic strain [13,14], similar to the cleavage brittle failure in crystalline metals.

Since shear banding is regarded as the root cause of the brittle failure in BMGs, it can be imagined that if the shearing nature of the deformation mode in BMGs can be suppressed or completely eliminated, then the deformation of metallic glass based on metallic bonding would occur through a completely different form [15–20], hinting at the manifestation of the ductile nature of BMGs. Previous experiments had shown that shear banding could be effectively suppressed when the sample size is comparable to the thickness of shear band [17–20], giving rise to significant homogeneous tensile plasticity, high strength, and ductile fracture. For example, Jang and Greer reported that the nano-scale samples produced by focus ion beam (FIB) show significant plasticity of ~25% true strain, work hardening behavior, and ductile fracture [18]. Ghidelli et al. studied $\text{Zr}_{65}\text{Ni}_{35}$ metallic glass films by on-chip tensile testing, and they also found large homogeneous

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deformation up to 15% and ductile fracture when the sample thickness is below 360 nm [20]. However, these were observed only when sample dimension is reduced to nanoscale. Homogeneous deformation and ductile fracture in the bulk specimens at room temperature is rarely reported.

Here, we reveal the metal-like ductile fracture in Zr-based BMGs when shear banding is suppressed using the notched specimens. Under this condition, several Zr-based BMGs not only display enhanced strength and obvious plasticity during tension, but also possess all the key characteristic signatures of ductile fracture, similar to those of crystalline metals and alloys. Void formation initiates from the center of the specimen, followed by crack propagation and finally shearing lips, leaving behind a “cup-and-cone” morphology. The fracture surface is characterized by deep dimples and micro-cracks, indicating that BMGs are capable of ductile fracture, similar to crystalline metals. Furthermore, this ductile fracture was analyzed using decohesion theory, and its characteristic strength was among the highest of all metals and alloys.

2. Experimental

The triaxial stress state can be achieved by introducing a circumferential notch in a cylindrical bar specimen. The level of stress triaxiality at the center of notched specimen can be calculated using the Bridgman's analysis [21]:

$$\frac{\sigma_m}{\sigma_{eq}} = \frac{1}{3} + \ln\left(1 + \frac{d}{2h}\right) \quad (1)$$

where σ_m is the hydrostatic stress, σ_{eq} the von Mises equivalent stress, d is the diameter of remaining cross sections of the notched rods and h is notch height (as illustrated in Fig. 1(a)), respectively. By varying d and/or h , the stress state may be varied from uniaxial ($d/2h \rightarrow 0$, $\sigma_m/\sigma_{eff} \rightarrow 1/3$) to nearly triaxial ($d/2h \rightarrow \infty$, $\sigma_m/\sigma_{eff} \rightarrow \infty$).

BMG specimens with nominal compositions of $Zr_{64.13}Cu_{15.75}Ni_{10.12}Al_{10}$ were prepared by arc-melting mixtures of high-purity metals (above 99.9%) in a Ti-gettered high-purity argon atmosphere. Cylindrical samples with a diameter of 5 mm and a length of 75 mm were fabricated by tilt-casting into a copper mold. Notched tensile samples with different notch dimensions $d/h = 1, 1.5, 3, 4$ and 6, i.e., $d \times h$ of 2.10 mm \times 2.08 mm, 1.10 mm \times 0.73 mm,

1.40 mm \times 0.55 mm, 2.1 mm \times 0.50 mm, and 2.42 mm \times 0.4 mm, respectively, were produced by gentle grinding in a custom-made machine, followed by fine polishing. A typical sample with $d/h = 6$ was shown in Fig. 1(b). For comparison, the annealed and fully crystallized $Zr_{64.13}Cu_{15.75}Ni_{10.12}Al_{10}$ samples, which were prepared by heat treatment of as-cast samples at 620 K for 3 h and 793 K for 1 h, respectively, were also studied. The notch dimension of the annealed and crystallized samples was $d/h = 6$. The microstructure of as-cast, annealed, and deformed samples is examined by X-ray diffraction (XRD) employing a Bruker AXS (D8 ADVANCE) instrument with Cu-K α radiation at 40 kV. The microstructure of annealed sample was further examined by transmission electron microscopy (TEM, JEM, 2010F) with a field-emission gun.

Quasi-static tensile tests were conducted at room temperature using an Instron 5982 instrument at a cross head speed of 0.02 mm/min. An extensometer was attached across the notch to calibrate and measure the elongation during the test. Fracture morphology was examined by SEM (Philips XL30 FEG instrument).

3. Results

3.1. Stress-strain curves of BMGs with various notch dimensions

Fig. 2(a) shows the nominal stress-strain curves of $Zr_{64.13}Cu_{15.75}Ni_{10.12}Al_{10}$ BMG samples with notch dimensions d/h of 1, 1.5, 3, 4 and 6, respectively, as well as the un-notched sample. The fracture strength and tensile plasticity as a function of d/h are summarized in Fig. 2(b). The sample with $d/h = 1$ has a fracture stress of approximately 1.6 GPa at 2% elastic strain and then fails with little plasticity in a brittle manner due to shear banding [6,7], which is similar to those of un-notched specimen. As d/h increases from 1.5 to 6, the fracture strength increases gradually from 2.0 to 2.9 GPa, exhibiting an inverse notch effect [22,23]. Moreover, the plasticity is also significantly enhanced with increasing d/h , and the stress-strain curves reveal a considerable amount of plasticity (amounting to ~10% elongation of the notch region in the sample with $d/h = 6$). It should be mentioned that since the size of notch region falls into a narrow range from 1.1 to 2.4 mm, therefore the previous reported size effect [24,25] on the transition from brittle to ductile fracture could be negligible. The introducing of triaxial stress state should be the main reason for this transition in the

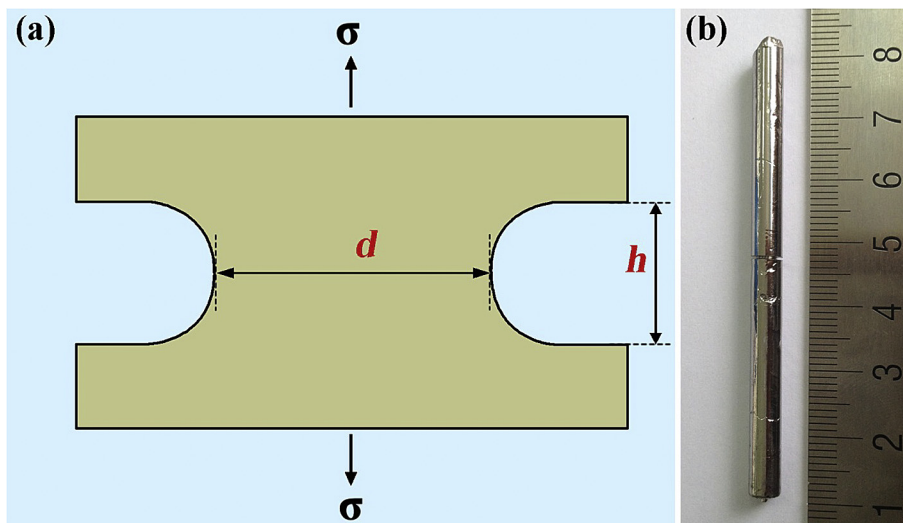


Fig. 1. (a) Schematic diagram of a deeply notched metallic glass tensile specimen used in this study. The stress state of notch region can be varied by adjusting d and/or h . (b) A typical notched Zr-based BMG specimen with notch dimension of $d/h = 6$.

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