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Shear fracture and fragmentation mechanisms of bulk metallic glasses

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Zr- and Co-based bulk metallic glasses display completely different failure modes under compressive loading. Zr-based metallic glasses always fail in a pure shear mode, whereas Co-based metallic glasses often break into small particles or powder, exhibiting a fragmentation mode. The difference in the failure modes for the two glassy alloys indicates that different mechanisms control the fracture processes, which can be described by a combined effect of surface energy γ, cleavage strength σ_0, fragmentation coefficient F_n and fracture mode factor $\alpha = \tau_0/\sigma_0$.

1. Introduction

Metallic glasses were first discovered in 1960 [1] and offer new opportunities to reveal the basic deformation and fracture mechanisms of matter [2–6]. Normally, bulk metallic glass (BMG) materials exhibit very high strength and hardness, a relatively low Young's modulus and poor ability for plastic deformation. The main limitation for their application as structural materials is their pronounced brittleness under external loading. Therefore, the need for a more fundamental understanding of the deformation and fracture mechanisms in various BMGs has motivated numerous experimental investigations [7–21]. However, most of these studies focused only on shear fracture behaviour [7–11]. It has been frequently found that some metallic glasses, for example Mg-, Co-, Fe- and Ti-based alloys [19–28], do not fail in a pure shear fracture mode, but sometimes break into several parts after compression. As is well known, BMGs have an amorphous structure with isotropic features and, consequently, there are no grain boundaries or crystallographic effects that have to be considered. This raises the interesting question as to why metallic glasses exhibit different failure modes. In this paper, we investigate the relationship between shear fracture and fragmentation failure modes for $Zr_{59}Cu_{20}Al_{10}Ni_8Ti_3$ and $Co_{43}Fe_{20}Ta_{5.5}B_{31.5}$ BMGs.

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2. Experimental procedure

Master ingots with compositions of $Zr_{59}Cu_{20}Al_{10}Ni_{8}Ti_{3}$ and $Co_{43}Fe_{20}Ta_{5.5}B_{31.5}$ were prepared by arc-melting elemental powders with a purity of at least 99.9%, as reported elsewhere [10, 25]. The master ingots were then re-melted in a quartz tube using induction melting and injected into a copper mould in a purified inert atmosphere to obtain rod samples 2 mm in diameter and 30 mm in length (Co-based glass) and 3 mm in diameter and 50 mm in length (Zr-based glass). Then, the cast alloys were cut into compressive specimens with different aspect ratios (H/D = 0.67–2.0). Compression tests were conducted at a constant strain rate of $10^{-4}\,s^{-1}$ with a MTS 810 testing machine at room temperature. After fracture, the specimens were observed with an optical microscope to reveal fracture features.

3. Results and discussion

Figure 1 shows the dependence of compressive fracture strength on the aspect ratio of the specimens for $Zr_{59}Cu_{20}Al_{10}Ni_{8}Ti_{3}$ and $Co_{43}Fe_{20}Ta_{5.5}B_{31.5}$ BMGs. The fracture strength of the Co-based BMG is extremely high (4–5 GPa) and reaches a maximum value of 5.2 GPa at an aspect ratio of 1.5. The extremely high strength agrees well with previous results [19], though the observed dependence of strength on aspect ratio is not clear at present. During compression tests, all Co-based BMG samples emitted a 'bomb-blast-like' sound on breaking into fine particles or powder, independent of the aspect ratio, as shown in figure 1a. The particles or powder are

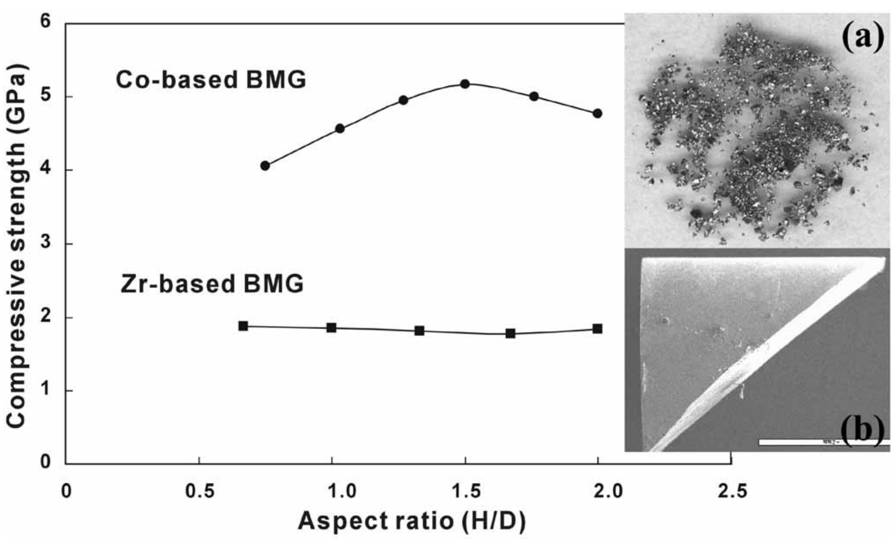

Figure 1. Dependence of compressive fracture strength on the aspect ratio H/D for Zr- and Co- based metallic glasses. (a) Fragmentation fracture morphology and (b) shear fracture feature.

very uniform and smaller than 50 μm. Hereafter, this behaviour is termed 'fragmentation fracture'. A similar fragmentation failure was also observed for some other BMGs [18–28], as will be discussed later.

The relationship between fracture strength and the aspect ratio for the Zr-based BMG is also plotted in figure 1. The fracture strength of these samples remains almost constant and varies only from 1.77 to 1.88 GPa, being independent of the aspect ratio of the tested specimens [29]. After compression, all the Zr-based BMG samples failed in a pure shear mode, with a shear fracture angle of 40–43°, as shown in figure 1b, which agrees well with the previous observations for other BMGs [2, 7–11]. This indicates that the shear fracture behaviour of the Zr-based BMG samples does not follow the Tresca criterion, but can be well described by the Mohr–Coulomb criterion [2, 7–11, 29]. The shear fracture surfaces of the Zr-based BMG samples display a typical vein-like structure, as shown in figure 2a. This vein-like structure often spreads over the whole fracture surface and extends in a uniform direction, corresponding to the propagation direction of the primary shear band, as illustrated in figures 4a and b. The vein-like pattern may be explained by local melting within the narrow, propagating shear band upon instantaneous fracture of the Zr-based BMG sample [11].

After failure of the Co-based BMG samples, some relatively larger particles were carefully observed by scanning electron microscopy (SEM) (figure 2b). There are

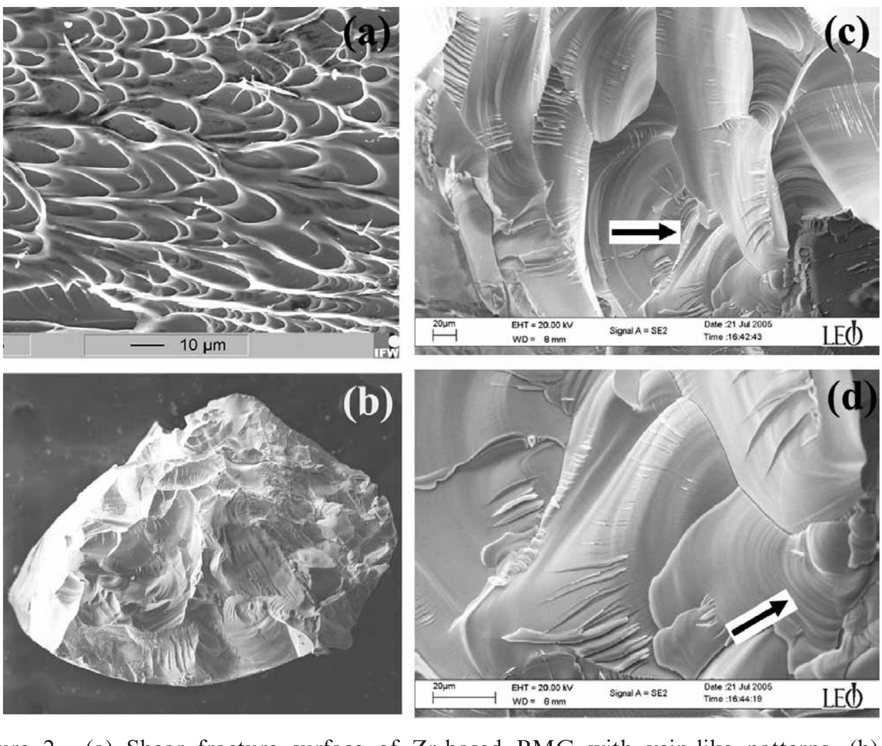

Figure 2. (a) Shear fracture surface of Zr-based BMG with vein-like patterns. (b)–(d) Fragmentation fracture morphology of Co-based BMG with many radiating cracks.

many small pits, corresponding to fracture sites, on the surfaces of the broken particles. At high magnification, these fracture sites display features radiating from the centre towards the outer edge, as shown in figures 2c and d. Some fracture sites interact with each other. However, no veins or traces of melting were observed on the fracture surfaces. In addition, there is a clear core in the centre of each fracture site, as indicated by the arrow in figure 2d. This indicates that the formation of the fracture sites in the Co-based BMG has gone through nucleation and rapid growth. It is deduced that there must be numerous such fracture sites nucleated almost instantaneously just prior to final fragmentation of the Co-based BMG, as illustrated in figures 3c and d. It can be concluded that the failure of the Co-based BNG samples follows a typical cleavage fracture during fragmentation. Therefore, the fragmentation failure of the Co-based BMG samples is distinctly different from the shear fracture mode found for Zr-based BMGs [2, 7–11, 29]. For some other BMGs, such as Mg-, Fe- and Ti-based alloys [19–28], it has been frequently observed that their failure occurs in the same fragmentation mode as for the present Co-based BMG samples. For example, Stoica *et al.* [23] found that the fracture surface of $Fe_{65.5}Cr_4Mo_4Ga_4P_{12}C_5B_{5.5}$ BMG consists of a high number of small fracture zones, leading to a breaking of the samples into many small parts. Inoue *et al.* [20] attributed the nearly simultaneous generation of a number of small fracture zones to an easy initiation of fracture at many sites induced by a shock wave at an extremely high stress level of 4000 MPa. Based on the above results, it is suggested that the fragmentation fracture can be regarded as a failure mode for BMGs additional to the conventional pure shear fracture mode.

Since some BMG samples can fail in a fragmentation mode rather than in a pure shear mode, one should consider this fragmentation process in detail. For a cubic sample of unit length, as shown in figure 3, the area A_0 of the original surfaces is equal to 6. If it is broken into eight equal cubic samples, the area A_n of the new surfaces should be equal to 6. In the same way, if the cube sample is broken into $N = 8^n$ equal cubic samples (see figure 3), the area sum A_n of the new surfaces would be:

$$A_n = 6(2^n - 1). \qquad (1)$$

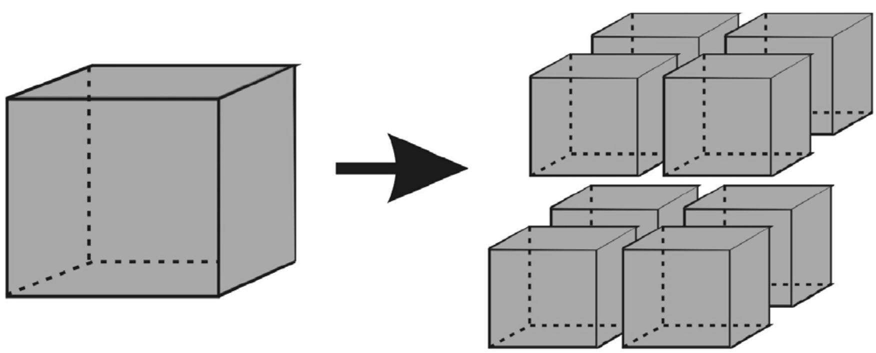

Figure 3. Illustration of fracture process for a unit cubic sample into eight equal cubic samples.

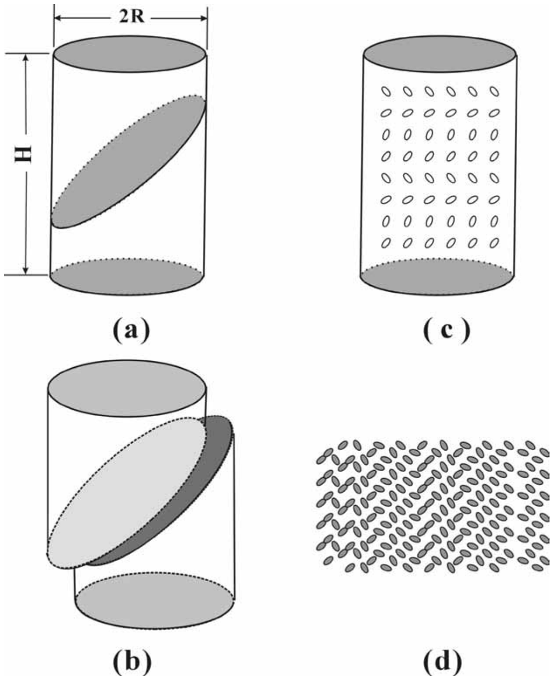

Figure 4. Schematic illustrations of the failure modes for different metallic glasses. (a) and (b) Shear fracture of Zr-based BMG; (c) and (d) fragmentation failure of Co-based BMG.

Therefore, we define a new parameter, i.e. the fragmentation coefficient F_n, which is the ratio of the area A_n of the new surfaces to the area ($A_0 = 6$) of the original surface:

$$F_n = \frac{A_n}{A_0} = 2^n - 1 \tag{2}$$

Normally, the fragmentation degree will increase if a sample breaks into more particles or even fine powder. Therefore, the fragmentation coefficient F_n represents the fragmentation degree of brittle fracture for a given sample. For two samples with different volumes, if they break into the same number (N) with homogeneous size, according to equation (2), their fragmentation coefficient F_n should be identical.

It is well known that BMGs can store larger elastic strain energy than conventional crystalline metallic materials [8]. The elastic energy density δ_E stored in a BMG sample upon failure can be expressed as:

$$\delta_E = \frac{\sigma_F^2}{2E} \tag{3}$$

where, E is Young's modulus and σ_F is the fracture strength of the BMG material. After fragmentation of the glass samples, assuming that the efficiency of the elastic energy density δ_E into new surfaces is equal to η, one finds:

$$A_n \gamma = \eta \delta_E V_0. \tag{4}$$

Here, V_0 is the volume of the sample, γ is the surface energy of the material. According to equations (2)–(4), the surface energy γ can be written as:

$$\gamma = \frac{\delta_E V_0}{F_n A_0} = \frac{\eta}{F_n}\frac{\sigma_F^2}{2E}\frac{V_0}{A_0}. \tag{5}$$

Equation (5) indicates that the surface energy γ is inversely proportional to the fragmentation coefficient F_n (or the number of broken particles) if the fracture strength σ_F of the BMG sample is constant. In other words, the material will have lower surface energy γ if the sample breaks into more particles upon compression.

For the shear fracture of the Zr-based BMG sample, there are only two new fragmentation surfaces, i.e. shear fracture planes, as illustrated in figures 4a and b. Therefore, the area A_n of the two new shear fracture surfaces is equal to:

$$A_n = \frac{2\pi R^2}{\sin\theta_C}. \tag{6}$$

Here, θ_C is the shear fracture angle between the stress axis and the shear fracture plane, as defined previously [10]. The original area A_0 of all the surfaces is equal to:

$$A_0 = 2\pi R^2 + (2\pi R)(4R) = 10\pi R^2. \tag{7}$$

Therefore, the fragmentation coefficient F_n of the shear fracture is almost a constant, i.e.

$$F_n = \frac{A_n}{A_0} = \frac{1}{5}\sin\theta_C \approx 0.28 \quad (\text{assuming } \theta_C \approx 45^\circ). \tag{8}$$

From the analysis above, it is suggested that shear fracture can be regarded as a special failure mode with a fragmentation coefficient of $F_n = 0.28$, which is the lowest value among all the fragmentation fracture modes. For most BMG materials, such as Zr-, Cu-, Ni-, and Pd-based alloys [2, 7–11, 14–18], shear fracture is the typical failure mode. Therefore, it is concluded that the surface energy γ of these BMGs is higher than those of Mg-, Fe- and Co-based BMGs. This might be the reason why some BMGs break into small particles under compression, as observed in Mg-, Cu-, Fe-, Ti- and Co-based BMGs, and even for some Zr-based BMGs [19–28]. In addition, there is another explanation in the literatures [30, 31]. These authors claimed that the brittleness of the BMGs strongly depends on the ratio μ/B of the elastic shear modulus μ to the bulk modulus B. The presence of ductility in Cu-, Zr-, Pd- and Pt- based BMGs can be attributed to the low value of the μ/B ratio [30, 31]. However, a high μ/B ratio makes BMGs brittle. In addition, annealing-induced embrittlement of intrinsically tough BMGs is often attributed to structural relaxation, which might result in a decrease in the surface energy γ in some Zr-based BMGs, for example [2, 27, 28].

On the other hand, it is well known that the theoretical strength (or cleavage strength) σ_0 of a material can be expressed as [32]:

$$\sigma_0 = \sqrt{\frac{(E\gamma)}{a_0}}. \tag{9}$$

Here, a_0 is the equilibrium distance of atomic pairs, and γ is the surface energy. Since the Co-based BMG samples always fail in a fragmentation mode, their surface energy γ should be distinctly lower than the value necessary for shear fracture. Therefore, the theoretical strength (or cleavage strength) $\sigma_0 = \sqrt{(E\gamma)/a_0}$ must be greatly reduced. Under compressive loading, the strength of a material should mainly depend on the critical shear fracture strength τ_0 rather than on the cleavage strength σ_0 [3]. The extremely high compressive fracture strength σ_F (~5 GPa) of the Co-based BMG demonstrates that their critical shear fracture strength τ_0 is also quite high. Therefore, the fracture mode factor $\alpha = \tau_0/\sigma_0$ of the Co-based BMG must be relatively higher than that for other BMGs, which fail in a pure shear mode. According to the unified failure criterion [3], a higher fracture mode factor $\alpha = \tau_0/\sigma_0$ should promote cleavage fracture rather than shear fracture. During compression, it is extremely difficult to nucleate a long primary shear band (or shear crack) because the critical shear fracture strength τ_0 is quite high. Consequently, numerous small fracture sites nucleate almost instantaneously just before final fragmentation of the Co-based BMG samples, as illustrated in figures 4c and d. Finally, the Co-based BMG samples locally fail in a cleavage fracture mode through rapid propagation of the numerous small fracture sites, leading to fragmentation fracture rather than pure shear fracture.

4. Conclusions

The compressive failure of a BMG material consists of typical shear fracture and fragmentation fracture, depending on the surface energy γ or bonding strength of the atomic pairs. Differences in the failure modes for Co- and Zr-based glasses indicate that different mechanisms control fracture. This can be explained by the combined effect of surface energy γ, cleavage strength σ_0, fragmentation coefficient F_n and fracture mode factor $\alpha = \tau_0/\sigma_0$. To some extent, shear fracture can be regarded as a special mode of fragmentation fracture with a minimum fragmentation coefficient of 0.28. It is suggested that the fragmentation coefficient F_n is a suitable parameter to describe the degree of brittleness for a given metallic glass.

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