Spiral fracture in metallic glasses and its correlation with failure criterion

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1. Introduction

The pressure sensitivity of failure in metallic glasses has been a topic of active research since the early experimental work of Davis and Kavesh [1] on ribbons, and more recent work by a number of authors [1–7]. This topic is tied to understanding the fundamental aspects of plastic deformation mechanisms which are still not fully understood [2,8]. Experimentally, the pressure sensitivity of failure can be directly examined by conducting experiments with superimposed hydrostatic pressure [1,3–7] in the manner of Bridgman [9], while any tension/compression asymmetry that exists at one atmosphere may also indicate some pressure sensitivity. For example, tension and compression tests conducted at one atmosphere by Donovan [10] found that the failure strength of Pd40Ni40P20 followed the Mohr–Coulomb failure (M–C) criterion. Various works by Lewandowski et al. [3–7] found only a moderate normal stress or pressure sensitivity for tests conducted with superimposed hydrostatic pressure [1,3–5] going from tension to compression at atmospheric pressure. This asymmetry in fracture angle [3–5] going from tension to compression at atmospheric pressure. This asymmetry in fracture angle was later shown to be influenced by stress concentrations at the sample/platen interface that biased the compression fracture angles, later rectified by the design of tapered grips [11,12]. Other recent work by Lu and Ravichandran [13] utilized confined compression tests on Zr41.2Ti13.8Cu12.5Ni10Be22.5 and found a more significant effect of confinement, although frictional restraint of the confining rings may have affected the magnitude of the pressure effect reported. Earlier work [14] utilized tension, compression, and torsion samples on a similar material and suggested that a von Mises criterion (i.e. pressure independent) might be appropriate. All of these previous works highlight the importance of continuing to examine the effects of changes in stress state and loading mode, as these have been observed to affect the deformation and fracture toughness, as shown by others [15–17].

In addition to experimental characterization, computational techniques were also employed to examine the validity of broadly used strength criteria including the Mohr–Coulomb criteria, Drucker–Prager criterion (D–P), and von Mises criteria. By using atomistic simulations, Lund and Schuh in 2004 [18] found that a pressure or normal stress dependence must be included in the failure criterion of metallic glasses, and they also suggested a range of Mohr–Coulomb internal friction coefficient of $\alpha = 0.12–0.4$ [19,20]. These atomistic simulations often produced much higher values for the friction coefficient than what was obtained experimentally, as well as what is found presently. Instrumented indentation and finite element simulations have also been employed to examine the pressure sensitivity of strength in BMGs [21–24] and they all suggested that pressure sensitive M–C or D–P [25] were better suited to capture deformation in structures with complex stress state. Finite-element modeling with embedded M–C criterion is able to capture typical features seen from systematic experimental characterizations of BMGs [26]. Later on simulations by Zhao and Li
Mechanical characterization of cylindrical metallic glass Zr41Ti14Cu12.5Ni10Be22.5 subjected to both normal and shear stress. (a) Sample layout. (b) Dimensions of Fig. 1.

[27] showed that taking consideration free volume dilatation [28] and the pressures sensitive D–P failure criterion are sufficient to explain the tension–compression fracture asymmetry in BMGs. Note that aforementioned experiments were typically performed at room temperature or temperature far below their respective glass transition temperatures of the tested materials. Recent work by Thamburaja et al. [29], guided by a series of molecular dynamics simulations conducted at low-homologous temperatures under homogeneous deformations, quantitatively prove that the continuum plastic behavior in metallic glasses could be described by the von Mises-type plastic yield criterion in that particular.

It is now generally accepted that criteria taking pressure sensitivity into account such as the M–C and the D–P are more appropriate to describe the strength of BMGs than pressure-independent ones like the Mises criterion when BMGs were tested at a temperature far below their glass transition temperature. However, regarding the exact formula to quantify the contribution of pressure to failure in BMGs, it remains an open question. For example, Zhang et al. suggested a modified M–C criterion where the internal friction parameters are different in tension and compression surface stress states [30]. Chen et al. [31] proposed an eccentric elliptical criterion on the basis of atomistic potential analysis. Later on, Wei [32,33] considered the different contributions of the distortional part and the volumetric part in total strain energy density to failure, and developed an energy based criterion where the shear strength and the normal strength are considered as two independent material parameters in BMGs. Recent experiments by Lei et al. [34] indeed found that distinct shear strength and normal strength are responsible for notch strengthening in BMGs: The tensile strength of the net section in circumferentially notched cylindrical BMGs increases with the constraint quantified by the ratio of notch depth over notch root radius. In summary, substantial understanding has been developed about the strength criterion of BMGs in the last two decades. Quantitatively, existing data about the material parameters of BMGs in different failure criteria are very scattered. There are compelling needs to critically examine the applicability of different failure criteria and to explore novel experimental strategies for calibration. In this work, we conducted combined torsion–tension experiments on Zr41Ti14Cu12.5Ni10Be22.5 bulk metallic glass rods, and we further validated the applicability of Mohr–Coulomb failure criterion on the tested metallic glasses from the spiral fracture angle aspect. In contrast to the classic torsion–tension tests to a polycrystalline thin-walled tube by Taylor and Quinney in 1931 [35], the metallic glass could be better suited for failure analysis because the onset of plastic flow in polycrystalline materials is very likely to be influenced by preferred orientations of individual grains [36].

2. Experimental

We use probably the most well investigated BMG Zr41Ti14Cu12.5Ni10Be22.5 (at.%). It represents a substantial amount of existing BMGs which offer almost no tensile ductility but exhibit intermediate-to-high resistance to fracture. The material is made in a water-cooled arc-melting hearth under a titanium-gathered argon atmosphere. Elemental metals (>99.9% purity) are used to form the master alloy and suction-casted into a $\odot 9$ × 100 mm cylinders. Those cylinders are then lathed using carbide tool into dog-bone samples with dimensions shown as Fig. 1a and b. The gauged sections of the samples are then mirror-polished to smooth the surface. A servo-hydraulic MTS 809 test system is used to do the torsion–tension tests. We first exerted prescribed axial normal load within 20 s. This loading condition corresponds to a strain rate on the order of 10^{-3}/s since Zr41Ti14Cu12.5Ni10Be22.5 breaks after an elastic strain limit about 0.02. We then twist the samples to failure. The torsion is applied at an angular velocity of 5°/min (corresponding to a maximum shear strain rate of about 2.5 × 10^{-4}/s). We also conducted contrast experiments with torsion loaded first (4 Nm/min, corresponding to a maximum shear strain rate about 1.2 × 10^{-3}/s), then axial load next (0.2 mm/min, corresponding to a strain rate about 2.5 × 10^{-4}/s), to character the normal–shear failure stresses combination’s dependence on loading path. The range of the axial normal stress $\sigma_0$ (see Fig. 1c) for the tested samples is from $\sigma_0 = 1.98$ GPa (uniaxial tension) to $\sigma_0 = -1.84$ GPa, and is listed in detail in Table 1.

3. Results and discussion

As a BMG sample (see layout and dimensions in Fig. 1a and b) is subjected to mechanical twist while an exact axial load is applied, any material point in the sample is subjected to two stress components: the axial normal stress $\sigma_0$ and the shear stress (as illustrated in Fig. 1c). The shear deformation along the radial direction in a crosssection perpendicular to the cylinder axis is linear in nature (as seen in Fig. 1d), resulting in a linear variation in shear stress...
along the radius. We show in Fig. 1d three typical torque-twisting angle curves for an arbitrary material point in the outer-most surface of the sample under different axial normal stress $\sigma_n = -1.8$ GPa (black), $\sigma_n = -0.4$ GPa (blue) and $\sigma_n = 1.76$ GPa (purple), and we reach a stiffness of $47.9 \pm 2.0$ Nm/rad basing on all the test samples (see listed in detail in Table 1); and we show in Fig. 1f the three typical maximum shear stress versus its respect maximum shear strain curves with respect to Fig. 1e. The failure points supply information about the critical combination of shear stress and normal stress which lead to failure.

A set of tension–torsion data are obtained as we gradually change the pre-applied normal stress from tension to compression. We show in Fig. 2 the critical combinations of maximum shear stress $\sigma_{1\text{max}}$, and axial normal stress $\sigma_2$, which lead to failure in the principal stress coordinate. Theoretical predictions by the M–C criterion, the Mises criterion, and the D–P criterion, by using the least square fittings, are also shown. For the metallic glass $\text{Zr}_{41}\text{Ti}_{14}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5}$ tested here, the yielding point, where the strength maximizes, is also where fracture occurs. There is no perceivably macroscopic yielding before failure, as seen in the torque-twist angle curves in Fig. 1e. We hence use the term “failure” instead of “yielding” to describe the critical combinations of shear and normal stress which trigger fracture in $\text{Zr}_{41}\text{Ti}_{14}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5}$. It is noted that there could be possibilities when shear banding does not lead to catastrophic failure, for example in bending tests [37] and in indentation experiments [21–24]. In those states of stress, “yielding” apparently differs from “failure”. In the M–C criterion,

$$\Gamma_0 = c - \sigma_2 \tan \phi$$  \hspace{1cm} (1)

where material parameters $c$ and $\phi$ are respectively the cohesion of a material and the angle of the internal friction. For a given stress state leading to failure, $\Gamma_0$ is the shear strength along the failure surface, and $\sigma_n$ is the normal stress at the failure surface. By convention, we let $\sigma_n > 0$ correspond to a tensile stress and $\sigma_n < 0$ a compressive stress. We may express $\Gamma_n$ in terms of the principal stresses $\sigma_1$, $\sigma_2$ and $\sigma_3$ (with $\sigma_1 \geq \sigma_2 \geq \sigma_3$ and $\sigma_2 < 0$ in this work):

$$\tau_\theta = \frac{\sigma_1 - \sigma_3}{2} \cos \phi, \quad \sigma_n = \frac{\sigma_1 + \sigma_3}{2} + \frac{\sigma_1 - \sigma_3}{2} \sin \phi$$  \hspace{1cm} (2)

In that manner, Eq. (1) can be reformulated as:

$$\sigma_1 - \sigma_3 = 2c \cos \phi - (\sigma_1 + \sigma_3) \sin \phi$$  \hspace{1cm} (3)

From Eq. (3), it is convenient to obtain $c$ and $\phi$ for any two independent critical combinations of shear stress and normal stress.
Normally, $c$ and $\phi$ are derived by employing data from uniaxial tension ($\sigma_1 = \sigma'_1$, $\sigma_3 = 0$) and compression ($\sigma_1 = 0$, $\sigma_3 = -\sigma'_3$) tests, where $\sigma'_1$ and $\sigma'_3$ are respectively the tensile strength and the compressive strength. In that case, one may write the internal friction coefficient $\alpha$ and the cohesion $c$ as

$$\alpha = \tan \phi = \tan \left[ \sin^{-1} \left( \frac{\sigma'_1 - \sigma'_3}{\sigma'_1 + \sigma'_3} \right) \right], \quad 2c = \sqrt{\sigma'_1 \sigma'_3}$$  

(4)

Given the fluctuation of measured strengths [38,39], the internal friction coefficient $\alpha$ determined by Eq. (4) may vary significantly, which could be evidently seen from the scattering of $\alpha$ from literature. Part of this variation in $\alpha$ obtained from compression tests could arise from stress concentrations that occur in compression that bias the fracture angle, as well as defects in the material [11,12]. To circumvent the sensitivity of $\alpha$ to strength fluctuation, we use the least square fitting to obtain $\alpha$ and $c$. As shown in Fig. 2, the least square fitting to Eq. (3) yields $\alpha = 0.058 \pm 0.012$ and $c = 1.026 \pm 0.014$ GPa.

In the same manner, the strength $\sigma'_1$ in the Mises criterion is obtained by the least square fitting of the equation

$$\sqrt{\frac{1}{2} \left( (\sigma_1 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2 + (\sigma_2 - \sigma_3)^2 \right)} = \sigma_f$$  

(5)

to experimental data in Fig. 2, with $\sigma_3 = 0$ in this work. The least square fitting leads to $\sigma_f = 1.857 \pm 0.117$ GPa. The conventional D–P [25] criterion can be expressed in terms of principal stresses $\sigma_1$, $\sigma_2$ and $\sigma_3$ (with $\sigma_1 \geq \sigma_2 \geq \sigma_3$ and $\sigma_2 = 0$ in this work) as well:

$$\sqrt{\frac{1}{6} \left( (\sigma_1 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2 + (\sigma_2 - \sigma_3)^2 \right)} = A + B(\sigma_1 + \sigma_2 + \sigma_3)$$  

(6)

The parameter $A$ reflects the role of the equivalent stress (or von Mises stress) while $B$ is a dimensionless coefficient which quantifies the contribution of the hydrostatic (or mean) stress. In the absence of pressure sensitivity, $A$ is exactly the shear strength used in the von Mises criterion. Both parameters could be determined from experiments. As D–P criterion was also applied to the deformation experiments, we presented torsion induced failure when a constant compressive normal stress is applied. Alternatively, when we maintain the shear stress to be constant $\tau_{\text{max}} = 0.814$ GPa, the critical normal compressive stress is $\sigma_0 = -1.605$ GPa. While there are small difference between the combination of normal–shear stress due to the load-control difficulty in experiments, our contrast experiments shown in Fig. 3 suggest that the critical combination of stresses shown in Fig. 2 is independent on loading path.

Fig. 3. Independence of loading paths for the critical combination of shear–normal stress. (a) Torsion failure under a tensile normal stress state ($\sigma_0 = 1.070$ GPa, $\tau_{\text{max}} = 0.854$ GPa). (b) Tensile failure under a shear stress state ($\sigma_0 = 1.078$ GPa, $\tau_{\text{max}} = 0.819$ GPa). (c) Torsion failure under a compressive normal stress state ($\sigma_0 = -1.660$ GPa, $\tau_{\text{max}} = 0.770$ GPa). (d) Compress to failure under a shear stress state ($\sigma_0 = -1.605$ GPa, $\tau_{\text{max}} = 0.814$ GPa).
We further check the fractographies of the failed samples under mixing loading. Typically, the fractured samples subjected to tension and concurrent torsion show spiral fracture, as evidently seen in the scanning electron microscope images shown in Fig. 4. For completeness, we also show the fractographies of the metallic glass Zr$_{41}$Ti$_{14}$Cu$_{12.5}$Ni$_{10}$Be$_{22.5}$ under simple tension (Fig. 4a) and simple compression (Fig. 4i). The fractured angle in tension is about 58°, and that in compression is about 180° - 136.8° = 43.2°, in excellent agreement with previous report [40]. In Fig. 4b–h, we show failed samples at different critical shear–normal stress combinations while the normal stress decreases from $\sigma_0 = 1.28$ GPa to $\sigma_0 = 0.58$ GPa, respectively. It is interesting to see when a sample fails under shear (induced by clockwise torsion) and compressive normal stress, the fractured surface and the cylindrical surface form a right-hand spiral (Fig. 4f–h). In contrast, a left-hand spiral forms as the normal stress is tensile (Fig. 4b–d).

In Fig. 4j, we show how we define a characteristic spiral angle $\theta + \beta$, which is the angle between the fracture surface and the axial stress direction. Here $\theta$ is the angle between the fracture surface and the max principal stress $\sigma_1$ and $\beta$ is the angle between the axial stress $\sigma_0$ and $\sigma_1$ directions, as demonstrated in Fig. 4k.

Under classical Mohr–Coloumb strength criterion, the angle $\theta$ is constant, as illustrated in Fig. 5a. In this work, the equivalent internal friction angle $\phi = 3.3^\circ$, which leads to $\theta = 46.65^\circ$. As $\beta$ is the angle between the normal stress $\sigma_0$ and the max principal stress $\sigma_1$, as demonstrated in Fig. 4k, we may write $\beta$ in terms of $\alpha$ and $c$ in the Mohr–Coulomb strength criterion:

$$\beta = \tan^{-1} \left( \frac{\tau_{\text{max}}}{\sigma_1} \right)$$

with

$$\tau_{\text{max}} = \frac{2c \cos \phi - \sigma_0 (1 - \sin \phi)}{2}$$

$$\sigma_1 = \sqrt{\frac{2c \cos \phi - \sigma_0 \sin \phi^2 - \tau_{\text{max}}}{2}}$$

We may now apply Eq. (8), with $\alpha = 0.058$ and $c = 1.026$ GPa from Fig. 2 to calibrate the applicability of the M–C strength criterion. We show in Fig. 5b the measured spiral fracture angle $\theta + \beta$ (symbols) as a function of the normal stress $\sigma_0$. The solid purple line is the theoretical predictions by using Eq. (8), and it can be seen that the difference between the predictions from Eq. (8) and those from experiments is marginally small. When a sample is subjected to simple tension and the normal stress $\sigma_0$ being the maximum principal stress $\sigma_1$, we $\beta = 0$ and $\theta = \pm \left( \frac{\pi}{4} + \frac{\alpha}{2} \right)$.

![Fig. 4. Spiral fracture of the metallic glass Zr$_{41}$Ti$_{14}$Cu$_{12.5}$Ni$_{10}$Be$_{22.5}$ subjected to shear and normal stresses. (a) Fracture angle under uniaxial tension. (b)–(h) Variation of spiral fracture angles at different critical maximum shear stress $\tau_{\text{max}}$ and axial normal stress $\sigma_0$. (b) $\sigma_0 = 1.28$, $\tau_{\text{max}} = 0.77$; (c) $\sigma_0 = 0.73$, $\tau_{\text{max}} = 0.89$; (d) $\sigma_0 = 0.63$, $\tau_{\text{max}} = 1.00$; (e) $\sigma_0 = 0$, $\tau_{\text{max}} = 0.99$; (f) $\sigma_0 = -0.17$, $\tau_{\text{max}} = 0.96$; (g) $\sigma_0 = -0.42$, $\tau_{\text{max}} = 1.05$; (h) $\sigma_0 = -0.58$, $\tau_{\text{max}} = 1.00$ (unit, GPa). (i) Fracture angle under uniaxial compression, and the angle value agree well with Jiang et al.’s report [40]. (j) Illustration to show the definition of angle $\theta + \beta$ to characterize the spiral fracture. (k) Stress components in different coordinates and the relationship between the angles and the stress: $\theta$ is the angle between the fracture fracture edge and the maximum principal stress $\sigma_1$, and $\beta$ is the angle between the normal stress $\sigma_0$ and the maximum principal stress $\sigma_1$; $\sigma_0$ is normal stress, e.g. the normal stress at the fracture surface, and $\tau_{\text{max}}$ is the relative shear stress.](image-url)
While the M–C failure criterion captures the fracture behavior in Zr41Ti14Cu12.5Ni10Be22.5 metallic glass, we neglect that dilatancy effect during the plastic flow of the metallic glass. As pointed out by Anand and Su [26], shear induced dilatancy could be crucial in governing shear-band formation and propagation, which has long been recognized in the deformation of granular materials [41–43]. Indeed, free-volume generation or shear induced dilatation was regarded to influence the plastic flow of metallic glasses [28], in particular during confined deformation [26]. By considering the shear induced dilatancy, Anand and spitzig showed that the inclination angle of the shear band with respect the max principal stress direction $\theta$ is determined by the internal friction parameter $\alpha$ and the dilatancy parameter $\eta$, and predicts that [43]

$$\theta = \arctan \left[ \sqrt{\frac{(1 + \alpha)(1 + \eta)}{(1 - \alpha)(1 - \eta)}} \right]$$

Here $\eta$ quantifies the difference between the averaged atomic cage volume in a metallic glass during deformation and the cage volume in a state of dense random packing, and is on the order of one hundredth. We apply $\alpha = 0.058$ and $\eta = 0$ and $\eta = 0.05$ to Eq. (9) to examine the dependence of the inclination angle $\theta$ on $\eta$, and we get $\theta = 45.83^\circ$ and $\theta = 46.55^\circ$ respectively. The values of $\eta$, as long as it is on the order of one hundredth, has negligible influence on the fracture angle. The small dependence of fracture angle on $\eta$ is apparently seen in Eq. (9) as $[(1 + \eta)(1 - \eta)]^{0.25}$ would be rather small if $\eta$ is on the order of one hundredth.

We note that spiral fracture can be utilized to reveal the deformation mechanisms of other materials like ductile metals and brittle ceramics. In Fig. 6, we show the mechanical response of ductile Al 6061 and brittle ceramic Al2O3 under combined shear and normal stresses. The plastic deformation and failure in Al 6061 is consistent with typical failure mode in materials governed by Mises type of plastic flow. Detailed analysis about the deformation pattern induced by Mises type of plastic flow or the maximum shear stress flow (also known as Mohr criterion where the frictional part is determined by the internal friction parameter $\alpha$) and the dilatancy parameter $\eta$, and predicts that [43]

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4. Conclusion

To conclude, we performed comprehensive experimental investigation on the failure of BMGs subjected to both shear and normal stress. Our work leads to the finding of spiral fracture in Vitreloy 1 subjected to both shear and normal stresses. The M–C criterion, using an internal friction coefficient of $\alpha = 0.058 \pm 0.012$ and a cohesion of $c = 1.026 \pm 0.014$ GPa, predicts the experimental stress envelope well at all range of normal stress. This value of $\alpha = 0.058 \pm 0.012$ is very consistent with other tests conducted with superimposed hydrostatic pressure [1,3–7]. In contrast, predictions by the other criteria deviate apparently from experiments, in particular when the normal stress approaches the compressive strength of Vitreloy 1. We further validate self-consistently the M–C criterion, by examining its predictability to the spiral fracture angles as a function of the applied normal stress. Our contrast experiments suggest that the critical combination of normal–shear stresses leading to failure is independent on loading path. While dilatation might have played an important role for the formation of localized deformation, we see that it exhibits negligible influence on the fracture angle as long as it is on the order of one hundredth. Our results showed here lead to a novel experimental strategy to examine critically the applicability of different strength criteria to metallic glass and other materials.

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