Comparison of compressive deformation and fracture behaviors of Zr- and Ti-based metallic glasses with notches

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A R T I C L E   I N F O

Article history:
Received 29 November 2010
Accepted 5 December 2010
Available online 10 December 2010

Keywords:
Metallic glass
Notches
Plasticity
Shear band
Fracture

A B S T R A C T

Compressive tests on the Zr- and Ti-based metallic glasses with different notches were investigated to compare their shear fracture mechanism and plastic deformation abilities. It is found that the plasticity of the two metallic glasses can be improved by installing two semicircular symmetrical notches even for the Ti-based metallic glass which has nearly zero compressive plasticity. The enhanced plasticity may be ascribed to the easy initiation of shear bands (SBs) around the notches, and the consequent blocking effect of notches on the propagation of shear bands according to the large-scale stress gradient. Additionally, based on a theoretical model originated from the concept of critical steady shear displacement (CSSD), compared with the sizes of smooth regions on the fracture surface, the plasticity difference of the two different metallic glasses was analyzed quantitatively. The current findings might provide an approach to understand and estimate the difference in the plastic deformation abilities on diverse metallic glasses, as well as the ones with large-scale stress gradient.

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1. Introduction

Metallic glasses, due to the high strength and hardness, have been regarded as a potential material in engineering fields [1–5]. Unfortunately, the vital fault, low plasticity has confined its applications as structural materials since the samples may fail in short time [6–12]. However, these brittle materials could display relatively high fracture toughness sometimes. For example, it was reported that the fracture toughness of metallic glasses Vitreloy-1 (Zr41.25Ti13.75Cu12.5Ni10Be22.5) varied from 16 to 55 MPa [6–12]. However, these brittle materials could display steady shear behavior up to a plasticity of 10% [12]. The Zr- and Ti-based metallic glasses with nominal chemical compositions of Zr52.5Ni14.6Al10Cu17.9Ti5 and Ti40Zr25Ni3Cu12Be20 have been regarded as a potential material in engineering fields [1–5]. Therefore, this significant character in fracture toughness has been attracted many attentions. Afterwards, some scholars had tried different ways to investigate the shear deformation mechanisms of metallic glasses by installing the notches [16–24]. For instance, Henann and Anand [19] approached the fracture of metallic glasses at notches. They demonstrated that the fracture initiated ahead of the notch root where the mean normal stress reached a maximum value [19]. Besides, by systematical investigation on the metallic glasses with different notches, Zhao et al. [24] pointed out that the proper notches in specimens could improve the global plasticity of metallic glasses in a large extent, in which the sample with two symmetrical notches could display steady shear behavior up to a plasticity of ~10%. All the above researches testify that the metallic glass specimens with notches exhibit different deformation features from the unnotched samples [6], which should be studied deeply through various means.

Above all, the previous references supplied several ways to understand the shear deformation mechanism of metallic glasses with different settings of notches [16–24]. Then, one assumption could be aroused: can all the metallic glasses display enhanced plasticity by installing notches? What is the difference in deformation mechanism of diverse metallic glasses and how to understand this discrepancy? Therefore, for revealing the difference in the plastic deformation abilities between different metallic glasses induced by stress gradient, we explored a series of compression experiments on the Zr- and Ti-based metallic glasses with different notches which could induce diverse stress gradients. The experimental results showed that the large-scale stress gradient might make the SBs extend steadily and enhance the plasticity of the metallic glass specimens. However, for the Ti-based metallic glass, the improved plasticity is obviously smaller than that of the Zr-based metallic glass. Moreover, to understand the differences in the plastic deformation abilities of different metallic glasses with stress gradient, a theoretical model based on the concept of the critical steady shear displacement (CSSD) is proposed to analyze the essential factors of plasticity diversity. It is expected that the current results may be beneficial to understand the difference of plastic deformation abilities for different metallic glasses quantificationally.

2. Experimental procedures

The Zr- and Ti-based metallic glasses with nominal chemical compositions of Zr52.5Ni14.6Al10Cu17.9Ti5 and Ti40Zr25Ni3Cu12Be20
were prepared by arc-melting method. The final metallic glass plate has a rectangular shape, with dimensions of 60 mm × 30 mm × 3 mm. The microstructure of the as-cast specimens was characterized by using a Leo Supra 35 scanning electron microscope (SEM), as well as a Rigaku X-ray diffractometer (XRD) with Cu Kα radiation. XRD patterns show that the as-cast Zr- and Ti-based metallic glasses have fully glassy structure. As displayed in Fig. 1, the two metallic glass plates were cut into four kinds of specimens defined as A, B, C, D with the dimensions of 3.0 mm × 3.0 mm × 6.0 mm and some semi-circular notches have a radius of 0.5 mm. The lengths between the center of the semi-circular notches and the end of specimen are also indicated in Fig. 1. Conventional compression tests were carried out to measure the mechanical properties of the metallic glass specimens with an MTS810 testing machine at room temperature in air. All the tests were applied by using a constant strain rate of $10^{-4} \text{s}^{-1}$. After the experiments, all the specimens were observed by SEM to observe the deformation and fracture features.

### 3. Experimental results

#### 3.1. Compressive stress–strain responses

Fig. 2(a) illustrates the nominal compressive stress–strain curves of Zr- and Ti-based metallic glasses for the 8 kinds of specimens with the settings displayed in Fig. 1. In order to compare the stress–strain curves of the notched together with the un-notched specimens and obtain the global plasticity on these samples, we defined nominal stress to represent the global stress in specimen by selecting the area of the both un-notched and notched specimen ends as the nominal areas [24]. In this case, the area is about 3.0 mm × 3.0 mm. Herein, for convenience, we applied $Z_A$–$Z_D$ and $T_A$–$T_D$ to stand for the different specimens of Zr- and Ti-based metallic glasses, respectively. Wherein, the letters A–D represent for the corresponding specimens designed as Fig. 1. For the Zr-based metallic glass ($Z_A$–$Z_D$), the sample without notches $Z_A$ only manifests a little plasticity (about 0.5%) with the yield strength of $\sim 1.80 \text{GPa}$ [6,24]. Besides, the specimens $Z_B$ and $Z_C$ also display a little plasticity (0.3% and 0.7%) with reduced nominal yield strengths (1.50 GPa, 1.25 GPa for samples $Z_B$ and $Z_C$). The down-trend of yield strength can be attributed to the stress concentration around the notches [24]. However, about the specimen $Z_D$ with two symmetrical notches, a relatively high plasticity (9.2%) was found, accompanying with the maximum value $\sim 1.50 \text{GPa}$ [24]. Obviously, the large plasticity in the curve $Z_D$ was caused by the intersection of two major SBs, which initiated from the notches [24]. Similarly, the Ti-based specimens $T_A$–$T_D$ also displayed the same features. Wherein, the plastic strains of samples $T_A$–$T_C$ are nearly zero while the one with two symmetrical notches (sample $T_D$) shows a larger plasticity (1.7%). Complementally, the detailed experimental results are summarized in Table 1.

Additionally, Fig. 2(b) displays the compressive engineering stress–strain curves of Zr- and Ti-based metallic glass for the different samples. The compressive engineering stress [25] is given by $\sigma = F/A_0$ according to the real area as shown in Fig. 1, we can settle down the results of the area $A_0$: specimen A, $A_0 = 3 \text{mm} \times 3 \text{mm}$; specimen B, $A_0 = 3 \text{mm} \times 2.5 \text{mm}$; specimen C, $A_0 = 3 \text{mm} \times 2.0 \text{mm}$; specimen D, $A_0 = 3 \text{mm} \times 2.5 \text{mm}$. It is obviously shown that the strength values of Zr- and Ti-based metallic glasses are identical with the un-notched ones, separately [6,24]. It implies that the real strength of metallic glassy could not be influenced by the notches obviously, instead, the plastic deformation abilities would

### Fig. 2. Nominal and engineering compressive stress–strain curves for the eight kinds of specimens on the Zr- and Ti-based metallic glass. (a) Nominal stress–strain curves; (b) engineering stress–strain curves.
Table 1
The experimental and numerical results for different specimens.

<table>
<thead>
<tr>
<th></th>
<th>Zr52.5Ni14.6Al10Cu17.9Ti5</th>
<th>Ti46Zr25Ni12Cu12Be20</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ZA</td>
<td>ZB</td>
</tr>
<tr>
<td>θ</td>
<td>41°</td>
<td>41°</td>
</tr>
<tr>
<td>ε&lt;sub&gt;p&lt;/sub&gt;</td>
<td>0.5</td>
<td>0.3</td>
</tr>
<tr>
<td>CSSD (μm)</td>
<td>40</td>
<td>32</td>
</tr>
<tr>
<td>Size of smooth regions (μm)</td>
<td>41.4</td>
<td>32.6</td>
</tr>
</tbody>
</table>

* The sample ZD had not been broken when the plastic strain ε<sub>p</sub> reached 9.2%. Then, the sizes of smooth regions on the fracture surface and CSSD value for the specimen ZD are omitted.

be changed by setting different notches. For instance, the specimens with two symmetrical notches could display a larger plastic strain than the unnotched ones [24]. Furthermore, with the same geometry settings, the Zr-based ones exhibit a larger plasticity than the Ti-based ones.

3.2. Shear deformation features

Then, the SEM images of deformation features are expressed in Figs. 3 and 4. Hereby, Fig. 3(a)–(f) show the macroscopic fracture patterns of specimens ZA–ZC and TA–TC. It can be seen that all of them were compressed into two parts along one major SB traditionally [6,24,26,27]. In Fig. 3(a)–(c), for Zr-based specimens, the shear angles are almost 41°, this value is accordant with the previous results of the identical metallic glass [6,24,27]. Additionally, for Ti-based metallic glass specimens TA–TC, the traditional shear fracture character could be also found just like the former investigations [23,26,28], meanwhile, the specimens yielded along one SB with the inclined angle of 40°. It can be concluded that the settings like samples B and C cannot change the shear fracture behaviors visibly, the notches could only decrease the global yield strength to some extent [24].

Furthermore, as shown in Fig. 4(a), an obvious V-shaped structure caused by the intersection of two major SBs is formed in specimen ZD [24], the current plasticity enhancement could be ascribed to this intersection. About sample TD, as illustrated in

![Fig. 3. SEM images on the deformation and fracture morphologies of the specimens ZA–ZC, TA–TC. Additionally, the related shear angles are displayed in figures.](image-url)
Fig. 4. Deformation and fracture features of the samples ZD and TD. For specimen TD, two magnified regions are selected for further analysis. Also, the shear angles are marked in the pictures.

Fig. 4(b), although the specimen ruptured along one SB finally, the intersection of SBs could also be found according to the magnified images, as displayed in circular dashed line regions I and II. The amplified regions demonstrated that the SBs could initiate from the notched regions and intersected with each other, such behavior is similar to the specimen ZD [24]. However, because of the intrinsic brittleness of Ti-based metallic glass, the whole sample ruptured along one SB finally [26].

In a short summary, by installing notches in the different positions, the Zr- and Ti-based metallic glasses displayed various plasticity and deformation behaviors. Moreover, for the same settings, the two kinds of metallic glasses exhibited unlike plastic deformation abilities. Therefore, this finding needs the detailed analysis to reveal the plasticity discrepancy of different metallic glass specimens, as well as the ones with different stress gradients induced by notches.

3.3. Fracture morphologies

It is well known that the tensile fracture morphologies displayed smooth regions and vein structures [27,29,30]. Moreover, the smooth regions could be regarded as the result of steady shear process while the vein features might be caused by the fast propagation of SBs before the entire fracture [30]. Then, Fig. 5(a)–(h) illustrate the compressive fracture morphologies for each specimen, expect for sample ZD, since the specimen ZD had not been broken when the global plasticity reached 9.2%. As shown in Fig. 5(a) and (b), for the unnotched samples ZA and TA, the obvious smooth regions were also found at the beginning part of fracture surfaces. Similar to the tensile fracture features, along the shear banding direction (marked as arrows), the vein patterns appeared on the fracture surfaces, suggesting a fast shear fracture behavior [27]. Fig. 5(c) shows the shear mode of specimen with notches. Because of stress concentration around the notches, the SBs are formed on the notched region and strengthened with the increasing loadings. For observing the initial fracture surface, we selected the upper part for SEM observations, as shown in Fig. 5(c). Then, Fig. 5(d)–(h) displays the morphologies for the initial regions of the fracture surface. For notched specimens, smooth regions were also found at the beginning part of shear fracture. Furthermore, along the shear banding directions (show as arrows), the vein-like structures [27] were observed on the fracture surface, which were similar to the patterns for the unnotched samples [27].

As a complement, the average sizes of smooth regions are summarized in Table 1, for obtaining the reasonable numerical results, we selected five different smooth regions and averaged the corresponding five values. Then, Fig. 6 shows the size values of smooth regions for each specimen except for sample ZD. It is concluded that the size of smooth region for Zr-based metallic glass specimen is larger than that of the Ti-based one, with the same setting. Also, for the specimen TD, the size of smooth region is much larger than the values of samples TA–TC, suggesting that the sample TD could display a longer steady shear process, compared with the other Ti-based specimens. Therefore, the above findings for fracture morphologies are needed to be further understood by a depth analysis.

4. Discussions

4.1. The critical steady shear displacement (CSSD)

At room temperature, it is concluded that the plastic strain of metallic glasses is caused by the shear offset of the two undeveloped parts separated by the localized SB [28,31]. Once the yielding begins, the SBs initiate and expend until the length of SB reaches a critical value [28,31], then the metallic glass may fracture along one major SB [28,31]. As a whole, the deformation process of metallic glasses under compressive loadings could be divided into three stages I–III [31]. As shown in Fig. 7, at the first stage (stage I), multiplication and coalescence of the free volume take place at the elastic deformation process, then, some tiny SBs could be caused under loadings. With the increasing stress, the whole specimen will enter into the plastic deformation process (stage II). At this time, the stress retains constant while the strain increases, this deformation stage corresponds to the loop of accumulation and release of energy. According to the fracture morphologies, the smooth shear...
regions [28,30,31] would be observed at this stage. Therefore, the sample may shear along one SB steadily. Then, in stage III, when the shear displacement reached one critical value, the whole specimen would fracture along one SB instantly. Corresponding to the fracture surface, the vein patterns would be found because of fast fracture behaviors [28,30,31].

Herein, we defined one concept of critical steady shear displacement (CSSD) to describe the critical value. Therefore, the larger CSSD value corresponds to the larger plasticity. By means of this concept, the plasticity difference of Zr- and Ti-based metallic glasses can be understood and compared quantitatively.

4.2. Solutions on the CSSD of different samples

For obtaining the CSSD values of the different metallic glasses, Fig. 8 proposes the simplified theoretical model for the specimens without notches and notched samples. As shown in Fig. 8(a) and (b), the specimen without notches, the original and final lengths of specimens are \( l_0 \) and \( l \). According to the CSSD concept, the specimen should pass a steady shear process with the critical value (CSSD) and then fracture along one major SB [6,27,28,30,31], as shown in Fig. 8(b). Similarly, assuming that the original length of sample is \( l_0 \), after being compressed to a plastic strain \( \varepsilon_p \), in view of the geometric relation, the variation along the loading direction \( \Delta l \) may be estimated as [32]:

\[
\Delta l = \varepsilon_p \cdot l_0
\]
Additionally, considering the shear angle $\theta_A$, we can get the following relationship:

$$w_A = \frac{(\varepsilon_p \cdot l_0)}{\cos \theta_A} \quad (2)$$

Then, the value $w_A$ is the CSSD value for sample without notches. The corresponding values about $\varepsilon_p, \theta$ for all the samples were calculated and illustrated in Table 1. Therefore, with the same procedure, as shown in Fig. 8(c)-(e), the CSSD values for the notched samples could be settled down. The related results are summarized in Table 1.

In the following, Fig. 9 illustrates the plasticity and CSSD values with different specimens. Wherein, Fig. 9(a) displays the plasticity values of each specimen. In Fig. 9(b), the comparison illustration of the size results of smooth regions and the CSSD values computed by the present models are displayed. It is found that the computed results of CSSD employed by the current model are close to the measured values about the smooth regions. Therefore, based on the experimental numerical results, three conclusions can be summarized as follows.

1. The plasticity of metallic glasses can be improved by installing two symmetrical notches as shown in Figs. 2 and 8(a). The plasticity of Zr-based metallic glass could be improved from 0.5% to 9.2% by installing two symmetrical notches [24]. Similarly, about the more brittle Ti-based metallic glass, the global plasticity could be also enhanced to 1.7%, as shown in Fig. 9(a). The enhanced plasticity could be ascribed to the intersection of major SBs due to the stress gradients.

2. By employing the CSSD concept, the size of smooth regions on the fracture surface could be interpreted suitably. As shown in Fig. 9(b), the computed results are identical with the measured values.

![Fig. 8. The analytical model for computing the CSSD values of different samples.](image1)

![Fig. 9. (a) The graph of plasticity values with Zr- and Ti-based specimens. (b) The comparison illustration of the size results of smooth regions and the CSSD values computed by the present models.](image2)
sured values on the whole, suggesting that the present model is reasonable.

(3) The plasticity differences between the Zr- and Ti-based metallic glasses can be explained by the difference in the values of CSSD. As shown in Fig. 9(b), with the same geometry design, the CSSD values of Zr-based specimens are obviously larger than the ones for Ti-based samples. It is indicated that the Zr-based metallic glass can sustain a larger plasticity compared with the Ti-based one, under the same large-scale stress gradient situation. Therefore, by the CSSD concept, the essential character of different metallic glasses could be described quantitatively.

5. Conclusions

This work investigated the shear deformation mechanisms of Zr- and Ti-based metallic glasses with diverse stress gradients induced by notches. Based on the experimental results, it was found that the specimens with two symmetrical notches could display a larger plasticity compared with the other situations, even for the Ti-based metallic glass. The results demonstrate that the plasticity of metallic glasses can be improved by installing large-scale stress gradient by all means. For revealing the plasticity differences between the Zr- and Ti-based metallic glasses, we proposed the concept of CSSD for discussions. Combined with the size results of smooth regions on the fracture surfaces, the CSSD model could interpret the sizes of the smooth regions suitably. Also, the plasticity differences of various metallic glasses could be interpreted by the present model. The discussions imply that the analytical results can interpret the experimental results suitably.

Acknowledgements

The authors would like to thank Prof. J. Shen for the metallic glass sample preparation, as well as the stimulating discussion with Prof. A.L. Greer and Prof. L.Z. Sun. The work was financially supported by the National Natural Science Foundation of China (NSFC) under Grant Nos. 50625103, 50871117, 50890173 and 50931005, and the National Basic Research Program of China under Grant No. 2010CB631006.

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