## Failure mode transition of Zr-based bulk metallic glass

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### **Abstract**

 $Zr_{41.2}Ti_{13.8}Cu_{10}Ni_{12.5}Be_{22.5}$  (Vit 1) bulk metallic glass (BMGs) exhibits different failure modes under low strain rate ( $10^{-4}s^{-1}$ ) and high strain rate ( $10^{3}s^{-1}$ ) uniaxial compression at room temperature. Quasistatically deformed samples often fail along one dominant shear band and fracture into two large millimeter-scale blocks, whereas at impulsive loading, the samples usually break into many small scale fragments with rough fracture surfaces, such as non-uniformly distributed vein patterns and micro multiple shear bands (network-like shear bands). A theoretical model that takes into account the balance between the energy dissipation within shear band and the stored energy released in the vicinity of the shear band to fuel shear localization is developed. Furthermore, the underlying mechanisms of one dominant shear band and network-like multiple shear bands controlling the failure mode transition are revealed.

**Keywords:** Compression test; Bulk metallic glass; Failure mode; Shear bands.

### 1. Introduction

Because of their unique properties such as high room-temperature(RT) strength and large elastic limit, bulk metallic glasses (BMGs) as a potential engineering and structural material have triggered extensive scientific interest over the years [1-5]. However, the poor macroscopic plastic deformation ability of BMGs limits their application. Therefore, the need for a more fundamental understanding of the deformation and failure mechanisms in BMGs has motivated numerous experimental investigations, especially under high strain rate. It has been found that some tough amorphous metals, such as Zr- and Pd-based metallic glasses, often fail along a narrow shear band both under quasi-static and dynamics compressive loading[6-10]. But some authors reported that the dynamically BMG samples fractured into several fragment similar to the failure behavior of some brittle Mg-,Fe-,and Co-based metallic glasses subjected to quasi-static loading[11, 12]. In this paper, we find that the failure mode of Zr<sub>41.2</sub>Ti<sub>13.8</sub>Cu<sub>10</sub>Ni<sub>12.5</sub>Be<sub>22.5</sub> (Vit1) bulk metallic glass (BMGs) was dependent of the strain rate in compression at room temperature. And, we develop local evolution model of the shear band, as to why Zr-based metallic glass exhibit the different failure modes.

### 2. Experimental

The  $Zr_{41.2}Ti_{13.8}Cu_{10}Ni_{12.5}Be_{22.5}$  bulk metallic glass was prepared by arc melting high purity composition elements together in a Ti-gettered purified argon atmosphere. Each ingot was re-melted several times to ensure homogeneity and then prepared by suction-casting the molten alloy into a copper mold to form rods ( $\Phi$ 5×100mm). Quasi-static and dynamic compression tests were performed on a MTS-810 material testing machine and SHPB using cylinders 5 mm in diameter and 7.5 mm height. In quasi-static compressive test, the strain rate was fixed at  $1.0\times10^{-4}s^{-1}$ . In dynamic compression, the strain rate ranged from  $1.0\times10^{3}s^{-1}$  to  $2.5\times10^{3}s^{-1}$ . After testing, the scanning electron microscopy (SEM) was used to characterize the fracture morphology of all specimens.

### 3. Results

The material exhibits the maximum fracture strength~1.9GPa and less macroscopic plastic strain at a quasi-static strain rate. It is of interest to note that the fracture strength markedly decreases at high strain rates, which agree well with the previous observations for other Zr-based [8, 13] BMGs. Another interesting observation is that quasistatically deformed samples fractured into two large millimeter-scale blocks, whereas at impulsive loading, the samples broke into many small scale fragments. Fractured samples were examined to understand the failure behavior by SEM. The samples fracture along a single plane at low strain rates, indicating a major shear band dominates the final fracture process. And vein-like pattern spreads over the whole fracture surface and extends in a uniform direction, corresponding to the propagation direction of the primary shear band. On the other hand, the considerable randomly distributed vein-like patterns, corresponding to the different propagation directions of shear bands on surface of fragments formed in dynamic loaded case show that multiple shear bands occur and dominate failure process. The network-like multiple shear bands are observed in the surface of the small fragments. Therefore, the transition from one dominant shear band to network-like multiple shear bands results in the different failure modes. But the mechanisms of transition are unknown.

### 4. Discussion

#### 4.1 Local evolution model for shear band

Room-temperature plastic deformation of metallic glasses has been known to be accomplished through shear bands in which plastic flow driven mainly by shear stresses is localized within a nanoscale zone [14, 15]. As is known, the shear-banding process is a dissipation system [7, 16-20]. There are three types of diffusion, i.e. conventional momentum/viscous, thermal/energy and special free-volume dissipation within the propagation shear band. In our previous work, the coupled effect of free-volume softening and thermal softening upon shear-banding evolution in metallic glasses was discussed [6, 9, 21, 22]. Nanometer-scale defects[23], a density fluctuation[24] and then a viscosity fall[9, 10, 18, 25] usually are results of the shear band propagation, suggesting the coalescence of free volume in the band. When the shear stress  $\tau$  at the shear band vanishes (or the shear displacement  $\psi$  reaches a critical  $\psi_c$ ), the shear band is regarded as being fully mature, and a finite amount of energy is expended. Zhang et al [18] proposed a micromechanical model based on momentum diffusion controlling shear band spacing. Additionally, Lewandowski and Greer[26, 27] have experimentally shown a significant temperature rise within and around the shear bands using tin-coated specimens, and some authors [27-29] observed the heat-affected zone (HAZ) around the shear band due to heat conduction which may play an important role in shear-band propagation. As discussed above, momentum and thermal derived from shear band spread to the neighboring elastic medium. Thus shear stress release also occurs in the undisturbed medium and stored energy is released. Based on these analyzes, a theoretical model that takes into account the balance between the energy dissipation within shear band and the stored energy released in the vicinity of the shear band to fuel shear localization is developed.

### 4.2 Shear-band dissipation energy

It has been demonstrated that the following equations properly govern the shear banding in BMGs [1, 9, 30]:

$$\rho \frac{\partial \mathcal{R}}{\partial t} = \frac{\partial^2 \tau_b}{\partial y^2} \tag{1}$$

$$\tau_b \frac{\partial \gamma_b}{\partial t} = \rho c \frac{\partial \theta_b}{\partial t} - \lambda \frac{\partial^2 \theta_b}{\partial y^2} \tag{2}$$

$$G = \frac{\partial \xi_b}{\partial t} - D \frac{\partial^2 \xi_b}{\partial y^2} \tag{3}$$

where  $\gamma_b$  is the shear strain,  $\gamma_b^{\mathcal{R}} = \partial \gamma / \partial t$  is the strain rate,  $\theta_b$  the temperature,  $\xi_b$  the concentration of free volume and G the net generation rate of free volume.

In order to capture free-volume and thermal softening nature, the elementary constitutive relation,

$$\tau_b = \tau_v (1 - \alpha \upsilon - \beta \theta) \tag{4}$$

in terms of flow stress  $\tau_y$ , free-volume softening coefficient  $\alpha$ , thermal softening coefficient  $\beta$ , free-volume concentration increment  $\upsilon=\xi-\xi_0$  from initial value  $\xi_0$  and temperature rise  $\theta=T-T_0$  with an initial temperature  $T_0$ .

The critical dissipated energy  $\Gamma_c$  within shear band as the deformation proceeds to a critical displacement  $\psi_c$ , is introduced as:

$$\Gamma_c = \left(\tau_y \psi_c\right) / 2 \tag{5}$$

Consistent with concepts of fracture mechanics,  $\Gamma_c$  is the energy per unit area within one-half of the shear band.

Combining Eqs. (1) — (5) results in an specific expression of the critical dissipation energy  $\Gamma_c$  omitted here.

### 4.3 Stored energy in the heat-affected zone and momentum diffusion zone

As we mentioned above, during the propagation process of the shear band, thermal diffusion and momentum diffusion out of the band and into neighboring medium both lead to stress relaxation and then energy residing in the material release to fuel the shear-band process [31]. Energy near the shear band resides as both kinetic energy and elastic strain energy. The cumulative energies of each contribution as a function of width of thermal or momentum diffusion region. The shear-banding event in BMGs is different from ASBs in crystalline alloys. Both low and high strain rate process can produce significant localization of plastic flow. And heat would not be trapped in the shear band. Now the question is in what situation, the shear-band is fueled predominantly by the momentum diffusion or the thermal diffusion region. As a result of thermal diffusion, energy residing in the material near the shear-band would be release. We discover that stored energy almost all releases due to the momentum diffusion at high strain rates; nevertheless, it doesn't reduce at low strain rates, considering the momentum equation (1) of the material near the shear band. Some investigators have attributed shear bands spacing to the momentum diffusion [18, 32-34]. Since the momentum diffusion is much faster than thermal diffusion, momentum diffusion region is much wider than thermal diffusion region. For the high strain rate process, the shear-band is fueled predominantly by the energy  $E_{\nu}$  of the momentum diffusion region. On the other hand, energy  $E_{\nu}$  within thermal diffusion region would be the principle energy fueling growth of the shear-band respect to the low strain rate process.

At quasi-static compression loading, the supplied energy, only from elastic strain energy residing in thermal diffusion region, is so smaller than the critical dissipated energy, i.e.,  $\Gamma_{sc} > E_h$ , that a single nucleated and propagated shear band would dominate and cause a catastrophic shear fracture of the material.

But under the dynamics loading, the strain and kinetic energy together drive the process of the shear-band evolution. Similarly, when one shear band is not sufficient to dissipate the supplied

energy, i.e.,  $\Gamma_{dc} < E_{\nu}$ , so that additional shear bands form and subsequently formation of a network of shear-bands induces the fragmentation failure mode of the material.

### 4.4 Fracture strength

Considering the intrinsic heterogeneity and preexisting flaw resulted from casting, the shear band generates via the cascade of a number of individual atomic jumps around free-volume sites[15] or shear transformation zones[14, 35] under the action of a stress smaller than macro yielding stress [2, 36]. Under dynamic compression, the formation and accumulation of damage resulted from network-like multiple shear bands events, causes the materials would loose bearing load earlier, however, the materials could not bear load until the stress level achieves macroscopic yield situation under quasistatic compression.

### 5 Conclusion

The mechanical properties of the Zr<sub>41.2</sub>Ti<sub>13.8</sub>Cu<sub>10</sub>Ni<sub>12.5</sub>Be<sub>22.5</sub> bulk metallic glass were investigated under uniaxial compression at strain rates from 10<sup>-4</sup>s<sup>-1</sup> to 10<sup>3</sup>s<sup>-1</sup>. The compressive failure process consists of typical shear fracture and fragmentation fracture, depending on the loading strain rate. The failure mode changes dramatically as loading strain rate is increased into high strain rate range. The different modes indicate that different mechanisms control fracture. Considering the balance between the energy dissipation within shear band and the energy residing within the vicinity of the shear band released to fuel shear localization, one dominant shear band controls the failure process at low strain rate, however, that is controlled by network-like multiple shear bands at high strain rate. The relationship between the failure mode and fracture strength is briefly discussed.

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