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The intrinsic and extrinsic factors for brittle-to-ductile transition in bulk metallic glasses

Yujie Wei *

State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, PR China

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ABSTRACT

We propose the ratio of critical strain energy density by distortional deformation over that by volumetric deformation as a material parameter to quantify the ductile-to-brittle transition in bulk metallic glasses (BMG). A BMG is regarded to be ductile (with high fracture toughness) if the ratio is low, implying shear dominated deformation precedes cavitation failure. In contrast, the BMG is brittle (with low fracture toughness) when the ratio is large, suggesting that cavitation is prone to occur before energy being dissipated via massive shear bands. The theory naturally reflects the intrinsic and extrinsic factors which could influence the brittle-to-ductile transition in bulk metallic glasses.

1. Introduction

The Poisson's ratio is found to have strong connection with the fracture toughness of bulk metallic glasses, with a brittle-to-ductile transition occurring at a critical Poisson's ratio about 0.31–0.33 [1,2]. Beyond this critical point, further increasing in Poisson's ratio of BMGs gives rise to more diffusive shear bands and more uniform plastic deformation, as seen in the analysis by Wei et al. [3]. Similar to the brittle-to-ductile transition seen in crystalline metals as temperature rises, the transition at the critical Poisson's ratio has to connect with deformation mechanisms. Since the Poisson's ratio can be directly expressed by the ratio of shear modulus μ over bulk modulus κ, it is not surprising that μ/κ had also been suggested to be an index for brittle-to-ductile transition [4,2]. In addition, interfacial energy was also proposed for brittle-to-ductile transition in crystalline materials [5].

In crystalline solids, metals in particular, plastic dissipation is achieved through dislocation gliding. The fracture toughness could be influenced by the local microstructures and crystal orientations of individual grains at a crack tip. At low temperatures, dislocation activities are largely suppressed and grain boundary deformation or cleavage failure occur, and the yielding zone at the crack tip is small. In contrast, dislocation mechanisms dominate plastic deformation at high temperature and give rise to large yielding zone. The difference in the size of the yielding zone around the crack tip for those two scenarios results in the significant change in fracture toughness of such crystalline metals. Metallic glasses are regarded as homogeneous down to nanoscale and are considered to be isotropic, as the materials own no internal long-range order to facilitate preferential slips. Plasticity in BMGs is accommodated by massive shear bands due to local strength softening in shear bands [6,7]. The larger fracture toughness for BMGs with higher Poisson's ratio is associated with dense and uniform shear bands around crack tip regions of the materials [3,7]. As the formation of shear bands is directly related to distortional deformation, it is convenient to adopt the strain energy density as a measurement for brittle-to-ductile transition in BMGs.

So far, the strain energy density concept has been successfully applied to analyze material failure, in particularly for fracture behavior of brittle media, e.g. [8,10,9,11,12]. It is also recognized that contributions by distortional deformation and volumetric deformation in the strain energy density may attribute differently to trigger crack propagation [13]. Given that the two parts of the strain energy density not only are influenced by material properties of a BMG (e.g., the Poisson's ratio or μ/κ), but also depend on boundary conditions which may trigger different deformation modes, we expect that the proposed index could reflect both the intrinsic and the extrinsic factors which govern the brittle-to-ductile transition in bulk metallic glasses. In what follows, we give detailed formulae to obtain the index.

2. Distortional and volumetric parts of strain energy density

Following the steps given by Wei [13], we consider a material point with general stress state $(\sigma_x, \sigma_y, \sigma_z, \tau_{xy}, \tau_{yz}, \tau_{zx})$ in a Cartesian coordinate (x, y, z). The total strain energy per unit volume W can

* Tel.: +86 10 82544169.
E-mail address: yujie_wei@lnm.imech.ac.cn

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be decomposed into a distortional part W_d and a volumetric part W_v . They are respectively written as

$$W_d = \frac{1+v}{6E}\left[(\sigma_x-\sigma_y)^2+(\sigma_y-\sigma_z)^2+(\sigma_z-\sigma_x)^2 + 6\left(\tau_{xy}^2+\tau_{yz}^2+\tau_{zx}^2\right)\right] \tag{1}$$

and

$$W_v = \frac{1-2v}{6E}(\sigma_x+\sigma_y+\sigma_z)^2 \tag{2}$$

where E and v are the Young's modulus and Poisson's ratio of an isotropic material. These two terms, if written in the principal stress coordinate axes $(\sigma_1, \sigma_2, \sigma_3)$, are

$$W_d = \frac{3(1+v)}{2E}\tau_{oct}^2 = \frac{3}{4\mu}\tau_{oct}^2 \tag{3}$$

and

$$W_v = \frac{3(1-2v)}{2E}p^2 = \frac{p^2}{2\kappa} \tag{4}$$

respectively, with $\tau_{oct} = \frac{1}{3}\left[(\sigma_1-\sigma_2)^2+(\sigma_2-\sigma_3)^2+(\sigma_3-\sigma_1)^2\right]^{1/2}$, and $p \equiv (\sigma_1+\sigma_2+\sigma_3)/3$, and μ and κ are the shear modulus and the bulk modulus, respectively. We define the quantity J which is the ratio of distortional energy over volumetric energy

$$J = \frac{W_d}{W_v} = \frac{1+v}{1-2v}\left(\frac{\tau_{oct}}{p}\right)^2 = \frac{3\kappa}{2\mu}\left(\frac{\tau_{oct}}{p}\right)^2 \tag{5}$$

and propose it as an index for brittle-to-ductile transition. It is convenient to see that J depends not only on the Poisson's ratio, but also on the externally applied stress. By knowing that distortional deformation will promote shear deformation and dissipate more energy, we see that $J \to 0$ corresponding to high fracture toughness; while $J \to \infty$ implying the brittle side. When the material point reach von Mises yielding [14] first, and also recognize that we have $\tau_{oct} = \sqrt{2/3}\tau_y$ on the basis of yielding at pure shear, we have

$$J_s = \frac{1+v}{1-2v}\frac{2}{3}\left(\frac{\tau_y}{p}\right)^2 \tag{6}$$

In this scenario, current hydrostatic tension plays a central role to the fracture toughness of BMGs. Minimizing the hydrostatic tension could substantially increase the fracture toughness of BMGs, since the formation of shear band – while reduces the strength – still remains the integrity of the material [6,15]. The analysis shown here explains why mode II crack would exhibit higher fracture toughness than that of mode I crack in BMGs. Similarly, one may imagine the situation where hydrostatic tension is significant and reaches the critical value first,

$$J_t = \frac{1+v}{1-2v}\left(\frac{\tau_{oct}}{p_c}\right)^2 \tag{7}$$

In this case, the BMG will behavior like brittle materials. While reducing the distortional deformation could give rise to increase J_t and hence increasing ductility, we expect this change could be rather small as cavitation failure would directly break the material apart.

So far, we have demonstrated that the brittle-to-ductile index does not only depend on material properties, but also vary as the loading conditions change. By combining the two scenarios depicted by Eqs. (6) and (7), we may obtain a brittle-to-ductile transition index which is solely dependent on material parameters. In that limit case, the brittle-to-ductile index is given as:

$$J_c = \frac{2(1+v)}{3(1-2v)}\left(\frac{\tau_y}{p_c}\right)^2 \tag{8}$$

As discussed by Wei [13], τ_y and p_c are independent material parameters. There is a fundamental difference between the resistance to glide a dislocation in a crystallographic plane and the strength to separate an atomic plane into two free surfaces. An intuitive explanation on this see [13] is that the presence of dislocations in an atomic plane would dramatically change the resistance to relative gliding between the top and the bottom blocks separated by the plane, i.e., τ_y drops, but has minor impact to p_c.

3. Application to mode I crack

Now we demonstrate how we combine the intrinsic and extrinsic factors to understand the brittle-to-ductile transition in metallic glasses. For a crack under far-field mixed-mode loading k_1 and k_2, its stress components σ_r, σ_θ and $\tau_{r\theta}$ ahead of the crack tip are given by Williams [16]:

$$\sigma_r = \sqrt{\frac{2}{r}}\,[k_1(3-\cos\theta)\cos(\theta/2)+k_2(3\cos\theta-1)\sin(\theta/2)]+\ldots \tag{9a}$$

$$\sigma_\theta = \sqrt{\frac{2}{r}}\,[k_1(1+\cos\theta)\cos(\theta/2)-k_2(3\sin\theta)\cos(\theta/2)]+\ldots \tag{9b}$$

$$\tau_{r\theta} = \sqrt{\frac{2}{r}}\,[k_1\sin\theta\cos(\theta/2)+k_2(3\cos\theta-1)\cos(\theta/2)]+\ldots \tag{9c}$$

Note that the stresses ahead of the crack tip are expressed in the cylindrical polar coordinates (r, θ). When only k_1 is applied, it is convenient to obtain the maximum shear stress τ_{max} at any θ

$$\tau_{max}^{\theta} = \sqrt{\frac{2}{r}}\,k_1\cos(\theta/2)\sqrt{(3-\cos(\theta))(1-\cos(\theta))} \tag{10}$$

The maximum shear stress τ_{max} for all θ occurs when $\theta = \theta_m = 103.8^\circ$. The hydrostatic tension, for the plane strain crack, is given as

$$p = \frac{4}{3}\sqrt{\frac{2}{r}}\,k_1(1+v)\cos(\theta/2) \tag{11}$$

and its maximum p_{max} occurs at $\theta = 0$. Now the maximum shear stress over the maximum hydrostatic tension is given as

$$\frac{\tau_{max}}{p_{max}} = \frac{3\cos(\theta_m/2)\sqrt{(3-\cos(\theta_m))(1-\cos(\theta_m))}}{4(1+v)} \tag{12}$$

By taking $v = 0.33$, we find that $\tau_{max}/p_{max} = 0.7$. It suggests that if τ_c/p_c in Eq. (8) is smaller than τ_{max}/p_{max}, we expect shear dominated deformation and the tested material would be *dutile like*. while $\tau_c/p_c > \tau_{max}/p_{max}$, we may find the material is *brittle like*.

4. Discussion and concluding remarks

Since fracture toughness measures the energy dissipation while a crack propagates [17], the strain energy based index seems to be more appealing to quantify brittle-to-ductile transition in contrast to other material parameters like Poisson's ratio, the ratio of shear modulus μ over bulk modulus κ, or the surface energy. We also note that while the critical index given in Eq. (8) seems to be more universal, it is hard to reach both shearing yielding and cavitation failure simultaneously at a material point during experiments. So the fracture toughness measured in real experiments may be better captured by either Eq. (6) or (7), depending on whether the shear stress or the hydrostatic tension reaches their respective threshold first. In addition, more experimental validations are desired to test the predicability of the above brittle-to-ductile transition index.

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