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Effects of geometric factors and shear band patterns on notch sensitivity in bulk metallic glasses☆

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ABSTRACT

Recent experiments in notched bulk metallic glasses have found reduced, or insensitive, or improved strengths, while in many of these cases the ductile strain prior to final failure is enhanced. First, although the inverse notch effect is explained by a shift from shear localization to cavitation failure, it is suggested in this work that the synergistic effect between cohesive fracture at the notched area and shear bands emanating from the notch roots may extend the parametric space for the notch insensitive behavior. Second, the dependence of shear band patterns on notch geometric factors is determined by the Rudnicki-Rice theory and the free-volume-based finite element simulations. These results suggest conditions for shear band multiplication to take place and for the shear-localization-induced failure to be delayed.

1. Introduction

In contrast to crystalline metals, bulk metallic glasses (BMGs) possess amorphous packing of the constituent metallic elements, and thus do not involve plasticity mechanisms arising from dislocations and grain boundaries. At temperatures lower than the glass transition temperature, BMGs deform by strain localization into narrow shear bands, which rapidly lead to catastrophic failure if these shear bands are not geometrically blocked. Consequently, BMGs are oftentimes brittle, and the lack of ductility prior to fracture failure prevents their wide applications as engineering structural materials.

The study of notches, cracks, and more generally flaws is of paramount importance in engineering applications, because failures are likely to take place at these geometric irregularities and stress risers. It appears from the linear elastic fracture mechanics (LEFM) that notches and flaws will reduce the strength of BMGs as in other brittle solids. However, recent studies have reported a diverse variety of observations on notched BMGs [1–8]. As summarized in Pan et al. [7] and shown in the geometric setup in Fig. 1(a), the notch shape can be described by a geometric ratio, $\lambda = (L - 2a)/w$. With the increase of λ, Flores and Dauskardt [1] found the reduction of the failure stress for notched cylindrical samples, termed as positive notch effect; Qu et al. [4] found notch sensitivity of the failure stress for notched plate samples; and Pan et al. [7] found the increase of the failure stress for notched cylindrical samples, termed as inverse notch effect. These results are rationalized in Pan et al. [7] by the competition between cavitation failure at the center of the notched area and shear bands adjacent to the notch roots. As these two mechanisms are dictated by the hydrostatic stress, σ_m, and Mises stress, σ_{eq}, respectively, their ratio for a notched sample is given by

$$\frac{\sigma_m}{\sigma_{eq}} = \frac{1}{3} + \ln\left(1 + \frac{\lambda}{2}\right) \tag{1}$$

Then they introduced a material parameter, σ_c/σ_s, where σ_c and σ_s are the critical stresses for cavitation and shear localization, respectively. If σ_c/σ_s is very large (e.g., >2), the increase of λ will

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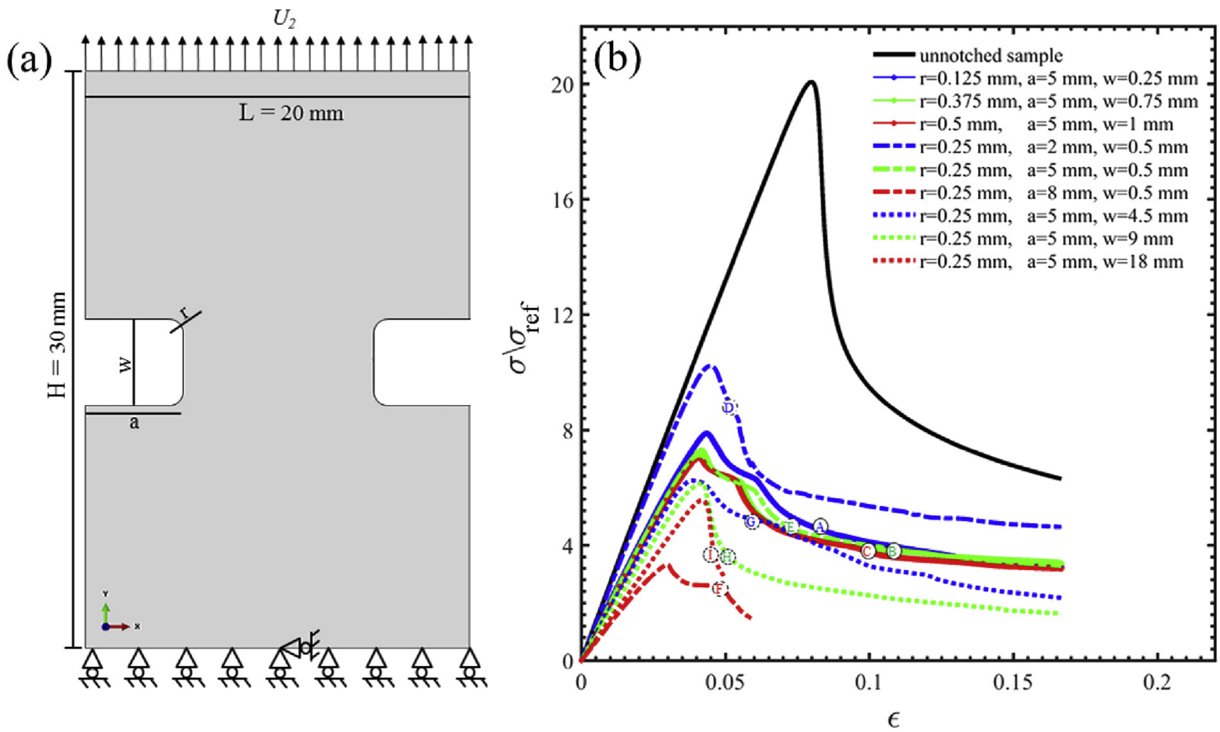

Fig. 1. (a) Geometric illustration of the double-edge notched sample, from which the stress state is given in Eq. (1). (b) The engineering stress-strain curves from the free-volume-based finite element simulations, corresponding to the results in Figs. 5–7. The loading and boundary conditions used in the finite element simulations are also prescribed. The nine curves marked by "A"-"I" have different notch radius r, length a, and height w, as given in the legend. Also these letters are placed at certain strain levels that correspond to the contour plots in Figs. 5–7.

never result into a hydrostatic stress that reaches σ_c, since the shear localization condition will be first reached. This corresponds to the positive notch effect. For a small σ_c/σ_s (e.g., 1.4 in Pan et al. [7]), the increase of λ leads to a transition from shear localization to cavitation failure, corresponding to the inverse notch effect.

One important experimental observation that may not be rationalized by the above model is the size effect or flaw insensitivity at small dimensions in BMGs [9–11]. Consider a central crack with the length of $2a$ subjected to a faraway tensile stress of σ_{appl}. The LEFM analysis predicts that the tensile strength scales inversely to the square root of the crack size by

$$\sigma_{crt} = K_{Ic}/\sqrt{\pi a}. \tag{2}$$

Stress singularity cannot be reached in reality, and the flaw insensitivity observed in small dimensions apparently violates this prediction. Prior efforts in nonlinear fracture mechanics and composites have revealed the critical role played by the inelastic process zone in interpreting the observation of flaw insensitivity. For an example, the plastic zone near the crack tip has a size of $r_p \approx \frac{1}{3\pi}\left(\frac{K_{appl}}{\sigma_Y}\right)^2$ with the yield strength σ_Y and the applied stress intensity factor K_{appl}. The LEFM analysis is limited to the condition of $r_p << a$. When r_p is comparable to the crack size, the nonlinear fracture mechanics should be employed. When r_p is larger than the crack, a stress-based ductile failure criterion, such as the Gurson-Tvergaard model, should be used [12]. In the last case, the scaling in Eq. (2) is invalid and these flaws, since they are smaller than the plastic zone, will not reduce the tensile strength noticeably. For the other example, the inelastic process zone can be a bridging zone arising from atomic cohesion in brittle solids or fiber pull-out in composites [13–15]. As shown in Fig. 2, the singular stress field predicted by LEFM is now replaced by the solution from a cohesive interface in the crack advancing direction. A representative cohesive law is given in Fig. 2(b) with the interface strength σ_0 and the characteristic length δ_0. The flaw insensitivity is thus dictated by the comparison between the crack size and the cohesive zone size, given by $E\delta_0/\sigma_0$. For brittle solids, σ_0 and δ_0 derive from interatomic interactions, and the ratio of $E\delta_0/\sigma_0$ is on the order of nanometer. Therefore, except for vacancies or small vacancy clusters, flaws are usually detrimental in brittle solids. The classic Dugdale strip-yield model is mathematically equivalent to this cohesive interface model, so that the Dugdale plastic zone size can also be given by the above length when σ_0 is interpreted as yield stress. For fiber-reinforced composites, σ_0 and δ_0 are governed by the fiber pull-out process and the fiber volume fraction, and the cohesive zone size can extend to millimeters. In this case, microscopic flaws have virtually no effects on the composite strength. For a third example, we note that the long-chain molecular bonds in biological materials govern the interface adhesion [15]. For applications like cell adhesion, the cohesive zone size can indeed be very large, so the use of LEFM should be cautious.

The concept of crack bridging can certainly be applied to the BMG study, where the cohesive interface law in Fig. 2(b) can be used as a simplified description of the normal fracture process. Molecular simulations of small-sized BMGs in Refs. [9,10] resemble the large-scale-bridging characteristics (i.e., $E\delta_0/\sigma_0 >> a$), so that the failure strength is not governed by the flaw size as predicted by the LEFM. In addition, He et al. [14] found out that a localized band with reduced strength or stiffness, if emanating from a crack tip, will relax the stress concentration and effectively extend the cohesive zone length. It is thus anticipated that the synergy between the cohesive fracture and shear localization can extend the parametric space for the notch-insensitivity behavior. Along this line, the proposed governing boundary value problem in Fig. 2 will