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Tensile fracture of metallic glasses via shear band cavitation

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Abstract—Tensile fracture of metallic glasses due to shear-band-to-crack transition was studied by molecular dynamics. Such transition is difficult to characterize experimentally as it occurs within nanoseconds in the buried nanometer-thin shear band. We show that the sample fractures via shear band cavitation under high initial tensile stress, or with long sample length. The critical thermomechanical conditions for shear band cavitation, strongly influenced by shear, were identified. An analytical model was developed, leading to a length scale and a time scale for shear-band-to-crack transition.

Keywords: Metallic glasses; Tensile fracture; Shear band cavitation; Molecular dynamics

1. Introduction

Metallic glasses (MGs) have emerged as a promising candidate for the new generation of structural materials due to their high strength and corrosion resistance, among other merits [1–3]. However, bulk monolithic metallic glasses exhibit zero tensile ductility due to catastrophic failure along a primary shear band [4,5]. For instance, the recently developed Pd-based MG is among the strongest and toughest materials known, yet still fails catastrophically under uniaxial tension [6]. It is generally understood that a shear band initiates via structural softening (with negligible thermal softening [7–9]), then propagates and slips (accompanied with significant temperature rise [5,10]), until transits into a crack via cavitation. The involvement of cavitation in tensile fracture can be inferred from fractographs of MGs under tension [11,12], and is different from the scenario ahead of crack tips in bending tests of notched samples [13,14], or compressive fracture [9]. Quantitative understanding of shear band cavitation is currently lacking, yet is crucial to realize MG as a practical structural material.

Several models have been proposed to understand the failure modes of MGs, including the critical temperature rise [9,10,15–17] or thermal runaway [18,19] in the shear band, the critical shear band energy density [20,21] and the critical shear off distance [11,12,22]. However, there is no direct examination of the above failure criteria in the case of tensile fracture of MGs, as the thermomechanical state of the shear band at the onset of fracture is extremely difficult to characterize in experiments [23,24]. The shear band features a spatial scale of nanometers [25], evolves with a temporal scale of nanoseconds or shorter [10] and often propagates deep beneath the surface. As a result, the temperature rise in shear bands was only inferred indirectly in bending [10] or compression [26], not yet in tension. Moreover, there is no report on the local stress state of a shear band, let alone the stress state at the onset of failure. On the simulation side, a model MG sample under mode-III torsion has been studied, without fracture [15]. Simulations have also been conducted on fracture under hydrostatic tension or with a pre-existing crack [27–29] in MG systems. However, simulation on shear band-to-crack transition under uniaxial tension is still lacking. Such simulations are challenging as a large sample (estimated to be microns) in size is required for the shear band-to-crack transition. In addition, the experimental strain rates are orders of magnitude lower than those in typical molecular-level simulations.

In this study, we employed a uniaxial loading method termed perturbative static loading (PSL) to overcome the above spatial and temporal limitations in molecular dynamics (MD) simulations. This paper is organized as follows. Section 2 introduces the model glassy system, conventional uniaxial tension results and the PSL method for large-scale simulation. Next, Section 3.1 describes how PSL tests were employed to show size-induced brittle fracture under uniaxial tension. The shear band evolution and the critical cavitation states under uniaxial tension are described in Section 3.2. By comparison between large-scale uniaxial tension tests and small-scale simulations under more general loading conditions, the importance of shear flow to cavitation is demonstrated in Section 3.3. Based on the cavitation criterion observed in the large-scale

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simulations, an analytical model is introduced to understand shear band-to-crack transition (Section 4). Concluding remarks can be found in Section 5.

2. Simulation methodology

2.1. Interatomic force field

The MD simulations were carried out using the LAMMPS package [30] on a model metallic glass interacting with a customized force field. This force field is the modified binary Lennard–Jones (BLJ) glass-forming system with the original form devised by Wahnstrom [31]. Inspired by the Dzugutov potential [32] that mimics the electron interactions and Friedel's oscillations [32–37], we superimposed an energy penalty, between $r^s_{\alpha\beta}$ to $r^c_{\alpha\beta}$ with a height of ε_B, to the original Wahnstrom system, which can be described in the form:

$$\phi_{BLJ}(r) = \begin{cases} \phi_{LJ}(r), & r < r^s_{\alpha\beta} \\ \phi_{LJ}(r) + \varepsilon_B\varepsilon_{LL} \cdot sin^2\left(\pi \frac{r^c_{\alpha\beta} - r}{r^c_{\alpha\beta} - r^s_{\alpha\beta}}\right), & r \geqslant r^s_{\alpha\beta} \end{cases} \quad (1)$$

with $\phi_{LJ}(r) = 4\varepsilon_{\alpha\beta}(\frac{\sigma^{12}_{\alpha\beta}}{r^{12}} - \frac{\sigma^6_{\alpha\beta}}{r^6}) - \varepsilon_{cutoff}$. Here $\varepsilon_{\alpha\beta}$ and $\sigma_{\alpha\beta}$ provide the energy and length scales, respectively, and $r^s_{\alpha\beta}$ is taken as $1.5\sigma_{\alpha\beta}$, which is outside the first neighbor shell. Here the cutoff is chosen to be species-dependent, such that all pair interactions are precisely 0.0163 ε_{LL} at the cutoffs of $r^c_{LL} = 2.5\sigma_{LL}, r^c_{LS} = 2.2917\sigma_{LL}, r^c_{SS} = 2.0833\sigma_{LL}$. The alloy consists of two species, which will be referred to as S and L for small and large atoms. The SS and LL bond energies are equal to that of the SL bond energy so that $\varepsilon_{SS} = \varepsilon_{SL} = \varepsilon_{LL}$. The SS and LL length scales are related to the SL length scale by

$$\sigma_{SS} = \frac{5}{6}\sigma_{LL}, \quad \sigma_{SL} = \frac{11}{12}\sigma_{LL}, \quad (2)$$

The two types of atoms have different masses such that $m_L = 2m_0, m_s = m_0$, where m_0 is the mass unit. In our simulations, the system is made of a 50:50 mixture of the two types of atoms. The reference time scale is $t_0 = \sigma_{LL}\sqrt{\frac{m_0}{\varepsilon_{LL}}}$. All physical quantities will be expressed in SI units following the conversion in a previous report [38]: $\sigma_{LL} \approx 2.7$ Å, $m_0 \approx 46$ amu, $\varepsilon_{LL} \approx 0.151$ eV and $t_0 \approx 0.5$ ps. There has been a systematical study on the tensile ductility of small sized (<100 nm) samples described by this modified LJ force field [39] with bump heights from 0 to 0.375. It was found that glasses with $\varepsilon_B < 0.25$ are intrinsically ductile, which is also shown in Fig. 1 (next section). In this study, $\varepsilon_B = 0.2$ is used for all samples. The timestep used is 5 fs.

2.2. Conventional uniaxial tension test

A conventional displacement-controlled uniaxial tension test was first carried out on a slab-shaped sample with a dimension of $22(X) \times 2.7(Y) \times 90(Z)$ nm^3. The glassy sample was cooled from a liquid isochorically from 2000 to 10 K in 23 ns. The sample was subjected to displacement-controlled loading, with a strain rate of 2×10^7 s^{-1}, by moving the two ends of the sample (serving as grips, 1.3 nm in length) in the loading direction, while allowing unrestricted motion along transverse directions. The sample was under plane-strain conditions. It is apparent in Fig. 1 that a dominant shear band first forms, and then glides until the sample shear fractures. One can further measure the shear band angle, with respect to the loading direction, to be 51°, and the thickness of the shear band to be ~6 nm. Both of these measurements will be used as input parameters for the following large-scale PSL simulations.

2.3. Perturbative static loading test

It should be noted that a conventional incremental loading test, as in the preceding section, usually leads to the formation of multiple shear bands in large samples, probably due to the extremely high strain rates. The presence of multiple shear bands undermines the sample length (the effective sample length per shear band), thus preventing the shear-band-to-crack transition. In the PSL test, only one dominant shear band will form under zero strain rate loading, enabling the modeling of the shear band-to-crack transition in MG samples (up to 1 μm).

The essence of the PSL test is to facilitate the formation of a single cross-sample shear band under tensile loading, which subsequently glides under zero strain rate loading.

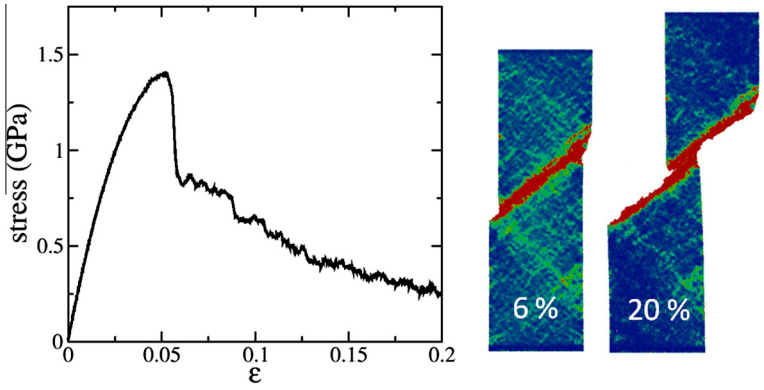

Fig. 1. Conventional uniaxial tension tests of an amorphous slab. The left pane shows the stress–strain curve. The right pane shows the atomic configurations at 6% and 20% strain. The atoms are colored according to the local shear strain from blue (0% strain) to red (20% strain). A dominant shear band is apparent, which is similar to the experiment [41]. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)