Acta Materialia 103 (2016) 587–594

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

A model metallic glass exhibits size-independent tensile ductility

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ARTICLE INFO

Article history:
Received 30 July 2015
Received in revised form 8 October 2015
Accepted 19 October 2015
Available online 21 November 2015

Keywords:
Tensile ductility
Cavitation
Shear band
Metallic glasses
MD simulation
Multiscale simulation

ABSTRACT

Metallic glasses (MGs) usually suffer brittle fracture under uniaxial tension due to size-dependent shear band cavitation. Here we developed a concurrent multi-scale simulation method to describe the uniaxial tension of a binary Lennard-Jones (BLJ) model glass up to 88 microns in length. No cavitation or brittle fracture was found even for the longest BLJ sample. As the length increases, the shear band temperature increases, then saturates, while the elastic unloading from shear-off diminishes. We conjecture that the shear band of a BLJ sample, even with a macroscopic length, cannot reach the herein estimated critical cavitation conditions. Thus, BLJ samples appear to be free of size-induced tensile brittleness. Based on the shear band evolution and the critical cavitation conditions, we propose three classes of MGs in terms of tensile ductility: brittle-MGs (brittle for all lengths), normal-MGs (ductile for short samples, brittle for long samples), cohesive-MGs (ductile for all lengths). Our simulation results illustrate limitations of existing molecular models, and suggest that certain experimental metallic glasses may be free of size-induced tensile brittleness.

1. Introduction

Metallic glasses (MGs) can exhibit high toughness [1], high strength [2–4] and excellent formability [5,6]. Although certain amount of ductility can be achieved under both compression and bending [2,3,7,8], monolithic metallic glasses lack tensile ductility, constituting the major drawback for load bearing applications. To achieve tensile ductility, various microstructural engineering approaches have been investigated, including the introduction of crystalline phases [9,10], regular pores [11], notches [12,13], or structural gradient [14]. Aside from microstructural engineering, it is generally believed that the tensile brittleness of metallic glasses is size-dependent, which has been demonstrated experimentally [4,15–17]. Thus, an alternative approach to achieve tensile ductility is to reduce the MG sample length.

However, the size-dependent tensile ductility in MG system has not been fully understood [4,16–23]. The brittle tensile fracture of macroscopic MG sample generally results from the development of a run-away shear band, which transits to a crack via shear band cavitation, causing catastrophic failure. The critical shear band cavitation process occurs within nano-second in a shear band of nano-meter thickness, on which direct quantitative experimental characterization is extremely challenging [24]. To this end, atomic-scale simulations [25–29] with high temporal and spatial resolution become increasingly important to understand the fracture process of metallic glasses. However, there are only few atomic-scale simulations on size-dependency of MG systems. We have previously shown ductile-to-brittle transition as sample length increases in a model modified binary Lennard-Jones (mBLJ) system using full-atomic molecular dynamics (MD) simulations [30]. To our best knowledge, there is no report on other model glass forming system that exhibits such size-dependent behavior in uniaxial tension. One possibility is that the critical length for the ductile-to-brittle transition is too long to simulate with full MD simulations. Alternatively, such size-dependent tensile ductility may not be universal among all glass formers.

To address this issue, we selected a well-studied Wahnstrom binary Lennard-Jones (BLJ) system to examine whether it exhibits size-dependent tensile ductility. To simulate long samples, we designed a concurrent multi-scale simulation technique to model uniaxial tension test on metallic glass samples with a length up to 88 microns. The multi-scale scheme combines an atomic region containing the shear band and the vicinity, while the rest of the sample is modeled at the continuum level. This scheme takes advantage of the fact that plasticity and possible cavitation only occur in a highly localized region, i.e., the shear band, while the rest of the material serves merely as heat-conducting elastic medium. Based on the estimated critical shear band cavitation conditions and the thermomechanical evolution of the shear band under uniaxial tension, we conjecture that BLJ system does not exhibit shear band cavitation at infinite length. Therefore, BLJ system does not exhibit size-dependent tensile ductility, instead, exhibits size-independent ductility under uniaxial tension. We further propose a classification of metallic glasses in terms of the tensile ductility.

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http://dx.doi.org/10.1016/j.actamat.2015.10.029

2. Multi-scale simulation setup

The brittle fracture of a typical MG sample under uniaxial tension proceeds as follows. The sample first elastically deforms, usually followed by the development of a dominant shear band. The shear band then glides, and may transit to crack via cavitation within the shear band. Therefore, the shear banding region (typically nm-in-thickness) plastically flows and cavitates, while the rest of sample only deforms elastically and conducts heat, as shown in Fig. 1. Such situation is well suited for a concurrent multi-scale simulation: the atomic-level details in the shear band and its vicinity (very small region of the sample, shown in the right pane of Fig. 1) will be captured by MD simulations; the elastic response and thermal conduction of the rest of the sample will be described at the continuum-level. Note that periodic boundary conditions are present in all three directions in the MD region. This multi-scale simulation strategy allows significant speed-up compared to the full-MD simulations, thus permitting simulations of samples up to 88 microns.

Similar to our previous work on shear band cavitation [30], we considered a thin-slab sample under plane strain conditions (corresponding to a thick sample in experiments). The mechanical and thermal coupling between the MD simulation and the continuum-level modeling will be described in details below.

2.1. Mechanical coupling

2.1.1. Elastic regime

First we will establish the relations for both stress and strain between the MD region and the entire sample. As shown in Fig. 1, the stresses in the MD region (the shear band and its vicinity) are denoted as σ_{xx}, σ_{zz} and σ_{zx}, in the Cartesian system of *xyz*. *x*-, *y*-, *z*-axes point along the shear band direction, the paper normal direction (or the thickness direction of the slab), and the direction normal to the shear band, respectively. The tensile stress of the entire sample is denoted as σ_L. Resolving the tensile stress of the sample, it is straightforward to have,

$$\sigma_{xx} = \sigma_L \cos^2\theta \tag{1}$$

$$\sigma_{zx} = \sigma_L \sin\theta\cos\theta \tag{2}$$

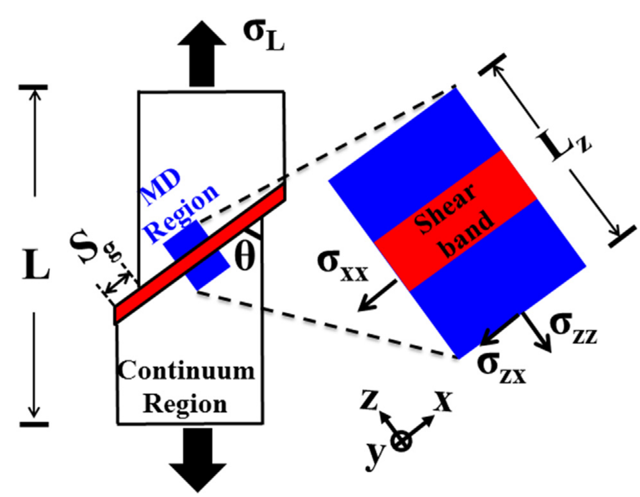

Fig. 1. Illustration of the multi-scale simulation strategy on a uniaxial tensile test of a metallic glass sample, which exhibits a single dominant shear band (colored red). The MD region describes part of the shear band and its vicinity (zoomed-in view on the right), while the rest of the sample is treated at the continuum level. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

$$\sigma_{zz} = \sigma_L \sin^2\theta \tag{3}$$

θ is the angle between the soon-to-be-formed shear band and the loading direction. Here θ is taken as 45°. Similarly, one can also relate the loading strain ε_L of the whole sample to the tensile strain ε_{zz} of the MD region. As shown in Fig. 1, the horizontal contraction strain of the whole sample is $\frac{v}{1-v}\varepsilon_L$ given plane strain conditions (v is the Poisson's ratio). Through strain tensor rotation, one can obtain,

$$\varepsilon_{zz} = \left(sin^2\theta - \frac{v}{1-v}cos^2\theta\right)\varepsilon_L \tag{4}$$

The elastic deformation of the continuum regime is trivial as the elastic constants of the model MG system are known. Nonetheless, one needs to elastically load the MD region that is consistent with the shear band angle. Here, the MD region is subjected to a constant strain rate tension in the direction normal to the shear band (*z*-direction, as shown in Fig. 1), with two barostats that control the normal stresses in the transverse direction (σ_{xx}) and the shear stress (σ_{xz}) as follows,

$$\dot{\varepsilon}_{zz} = \left(sin^2\theta - \frac{v}{1-v}cos^2\theta\right)\dot{\varepsilon}_L \tag{5}$$

$$\sigma_{xx} = \sigma_{zz}\cot^2\theta \tag{6}$$

$$\sigma_{zx} = \sigma_{zz}\cot\theta \tag{7}$$

Here σ_{zz} is the instantaneously measured normal stress in the z-direction. In this way, within the elastic loading regime, mechanical equilibrium between the continuum regime and the MD regime (i.e., Eqs. (1)–(3)) is guaranteed. Furthermore, the stress–strain response of the whole sample can be obtained from the MD simulation: the tensile stress of the whole sample σ_L can be obtained according to Eq. (3) from σ_{zz}, and the strain of the whole sample ε_L can be obtained according to Eq. (4) from ε_{zz}.

2.1.2. Plastic regime

During plastic deformation, mechanical equilibrium, guaranteed in the elastic regime, can be violated due to localized shear banding. Fig. 2 shows the driving resolved shear stress $\sigma_{zz}cot\theta$ and the resisting shear stress σ_{zx} using the elastic coupling scheme described above. It is apparent that as shear band forms (the visible drops in both stresses due to structural softening [25,31]), mechanical equilibrium can no longer be maintained. Here we identify the system configuration just prior to shear band formation, as σ_{zx}

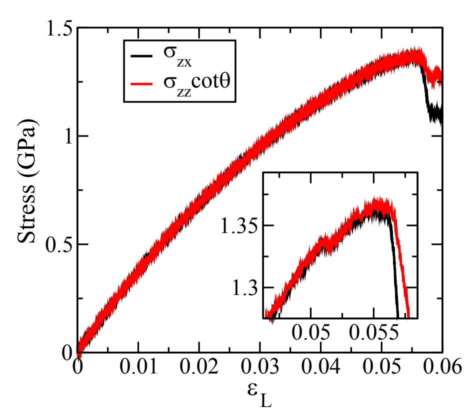

Fig. 2. The driving shear stress $\sigma_{zz}cot\theta$ and the resisting shear stress σ_{zx} as a function of the tensile strain. The elastic deformation ends approximately around 5.5% strain, at which the driving shear stress becomes higher than the resisting shear stress. The inset shows a zoomed-in view of the same plot.