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Progressive shear band propagation in metallic glasses under compression

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Abstract—Shear band plays a key role in dominating the strength and plasticity of metallic glasses, and exhibits two kinds of propagation modes under compression, i.e., progressive and simultaneous propagation. These two different propagation modes of shear bands lie in different stages of plastic deformation. Prior to macroscopic yielding, shear bands have already been initiated yet not penetrated through the sample. These inserting shear bands exhibit linearly decreasing plastic strain from the end to tip, demonstrating a progressive propagation mode. Once the macroscopic yielding occurs, the major shear band fully transects the sample and propagates in a simultaneous sliding manner. The progressive propagation of shear bands causes an apparent work-hardening behavior, which can be well explained by assuming a higher critical stress for shear band initiation than propagation. The results demonstrate that metallic glasses with a smaller difference between critical conditions for initiation and propagation of shear band should have better plastic deformability, which can be reflected by the plastic strain to macroscopic yielding read from stress–strain curves. © 2015 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

Keywords: Metallic glass; Shear band; Compression; Plastic deformation; Stress-strain response

1. Introduction

As emerging structural materials, metallic glasses (MGs) attract much attention owing to their impressive mechanical properties such as high strength, high elasticity and high toughness [1–3]. At room temperature, plastic strain in most MGs is usually localized into a narrow region that is termed as shear band. The shear banding behavior is believed to be a main mechanism dominating the mechanical properties of MGs. For instance, the critical stress for initiating a shear band determines the upper limit of yield stress, while the density of shear band and the critical failure condition of shear band control the global plasticity of MGs. However, the formation mechanism of shear band still remains unclear so far, although great strides have been made over the past decade in understanding the inherent mechanism of shear banding behavior in MGs (e.g., [4–22]).

Recently, Greer et al. [4] have summarized the possible mechanisms for shear band formation into three scenarios. (1) Homogeneous nucleation mechanism of shear band. In this model, MGs are assumed to have an ideally defect-free structure. Shear band could be initiated from the percolation of homogeneously activated shear transformation zones (STZs) [4]. (2) Aged-rejuvenation-glue-liquid (ARGL) model of heterogeneous nucleation of shear band [14]. In this scenario, a propagating shear band could be divided into three zones that include shear-rejuvenated glass near the shear band tip, glue zone, and liquid or near-liquid tail. Ahead of the shear front, the glass is well-aged and elastically deformed. (3) Two-stage model of heterogeneous nucleation of shear band [5]. In this model, the two stages include: (a) the creation of a viable band for shearing by structural disordering (rejuvenation) that propagates at a velocity of the order of the shear-wave speed ($\sim 1000 \text{ m/s}$), and (b) the synchronized sliding and shear-off along the rejuvenated plane. One major difference between the ARGL model and the two-stage model lies in the propagation mode of the shear band. The ARGL model assumes a progressive propagation mode, while in the two-stage model the shear band slides simultaneously along a rejuvenated shear plane.

Then how does a shear band propagate in MGs? To deal with this question, substantial researches have been conducted recently, including the investigations on the propagation dynamics of an individual shear band and/or the interactions between shear bands [23–25], effects of extrinsic factors like sample size, machine stiffness, testing temperatures and strain rates on shear banding behaviors [26–31], and *in situ* or quasi-*in situ* observations on shear band evolution [14,32,33], and so on. Theoretical models such as the stick–slip model [5,25,31,34], the shear instability model [26–28] and the quasi-phase transition model [11] have also been proposed and applied to account for the inherent mechanisms behind experimental observations. However,

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concerning the propagation mode of shear band, although two modes of progressive shearing and simultaneous propagation have been assumed [4,35], only the simultaneous propagation mode has been experimentally confirmed so far. Through the observation using high-speed camera, localized shear banding was confirmed to occur in a simultaneous fashion, i.e., the shear band operates simultaneously across the entire shear plane, rather than in a progressive manner [36,37]. However, the spatial resolution of high-speed camera imaging, which is at the scale of $\sim 1 \,\mu m$ [36,37], is not high enough compared with the characteristic size of a shear band (~10 nm in thickness [38,39]). Hence the initial stages of shear banding (during which the shear amount should be at nano-scale [22]) may not be well captured by the current high-speed imaging system. In particular, it should be also worth noting that current experimental studies on shear band propagation mainly focus on plastic deformation after macroscopic vielding; whereas prior to macroscopic vielding, despite that it has been proved that plastic deformation could occur, how shear band originates has rarely been investigated.

Atomistic simulations, which could break the limitation of spatial resolution in experiments, can provide some important insights into shear banding mechanism at initial stages. A detailed examination on the formation of shear bands in several simulation studies [18,22,40] revealed that the plastic shear offset of a growing shear band always exhibits the maximum value at the origin site of a shear band (usually at the sample edge) and vanishes at the shear band tip (e.g., see Fig. 2 in Ref. [18] or Fig. 2 in Ref. [22]). These results implied that the growth of shear bands should be in a progressive way rather than a simultaneous manner. Therefore, although the progressive propagation of shear band has not been experimentally confirmed, we cannot claim that this mode does not occur.

In this work, we focus not only on shear band propagation after the macroscopic yielding of two MGs, but emphatically on the shear banding behavior prior to macroscopic yielding. We conducted interrupted compression experiments and employed the shear-offs of surface scratches as rulers to quantitatively characterize the shear band propagation of two MGs with different plastic deformabilities. The experimental results provide compelling evidence to confirm that both progressive and simultaneous shear modes do exist but perform different dominative roles in different stages of shear banding. Before macroscopic yielding, the major shear band grows in a linearly progressive manner, while after yielding it slides simultaneously. The progressive shear banding exhibits an apparent "work-hardening" behavior in its stressstrain response, the mechanism for which will be discussed. Especially, the plastic deformation of MGs prior to macroscopic yielding, which is often neglected previously, will be elucidated.

2. Methods

Two bulk MGs (BMGs) of $Ti_{40}Zr_{25}Ni_3Cu_{12}Be_{20}$ (at.%) (Ti-BMG) and $Pd_{30}Ni_{50}P_{20}$ (at.%) (Pd-BMG) with different plastic deformabilities were selected for investigations. The amorphous structure of the alloys was confirmed by a Rigaku X-ray diffractometer (XRD) with Cu K α radiation. The compressive samples were cut from the as-cast Ti-BMG plate and Pd-BMG rod and subsequently ground and polished. To ensure the simplicity of the observation of shear bands, all the samples were fabricated to be of rectangular shape with a relatively low aspect ratio (height/width) of ~1.5. Uniaxial compression tests were conducted using an MTS 810 testing machine at a quasistatic strain rate of 10^{-4} s⁻¹ at room temperature. The deformation features were observed with a Quanta 600 scanning electron microscope (SEM).

Interrupted compression technique was used to investigate the shear band evolution process. The samples were unloaded at different stages of compressive deformation, and then the deformation features were observed by SEM. During the initial stages of shear banding, the two adjacent faces of a rectangular sample were observed to avoid missing useful information. Because of the rectangular shape of the sample, the shear plane intersects with the sample surface to form shear step along a straight line, which makes the observation of shear band propagation much easier. Some scratches introduced during the grinding process were used to measure the local shear offset of a propagating shear band, which is of importance for determining the shear band propagation mode.

3. Results

3.1. Compressive stress-strain responses

Fig. 1 presents the typical engineering stress–strain curves for the two MGs under compression. Although the curves for the brittle Ti-BMG (the plastic strain to failure, ε_{pf} , is ~1.6%) and the ductile Pd-BMG ($\varepsilon_{pf} = 16.7\%$) are different, they are practically similar to those of other brittle and ductile MGs [6,41,42]. Both of the two stress–strain curves have two important points, i.e., the elastic limit point and the macroscopic yield point (MYP). The elastic limit point corresponds to the first pop-in on the curve. The MYP is defined as the point at which a stress plateau appears, representing the onset of steady plastic flow.



Fig. 1. Typical engineering stress–strain curves for the Ti-BMG and the Pd-BMG samples under compression. Noting that the curve-end for the Ti-BMG corresponds to fracture, while at the curve-end for the Pd-BMG the stress rapidly drops as increasing strain, corresponding to the onset of the fake stress–strain response due to the contact of platform and sheared-off part of the sample [44]. For the Pd-BMG, the test was stopped without fracture.

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