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Shear band evolution during large plastic deformation of brittle and ductile metallic glasses

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Four monolithic metallic glasses (MMGs) with different plasticities varying from brittle to ductile behavior under unconstrained loading were subjected to small punch testing. All specimens undergo large plastic deformation with multiple cobweb-like shear bands under these conditions. The process of shear band evolution was carefully controlled and investigated. Plasticity of MMGs is characterized by equivalent plastic strain ε^* (product of shear band density and critical shear offset). Thus, this article provides an experimental basis for a better understanding of the shear band evolution during plastic deformation of MMGs.

Keywords: metallic glasses; plastic deformation; shear bands

The metallic glasses with high elasticity, strength, and hardness are promising candidates for future high-performance structural and functional materials [1–4]. However, due to their amorphous structure, plastic deformation of monolithic metallic glasses (MMGs) is closely linked with initiation and propagation of shear bands, which is associated with lack of work-hardening capability and strain localization [5]. Hence, MMGs generally exhibit lower plasticity as compared to crystalline materials, and fail along a single shear band [3,4] or even split into pieces [6]. Thus, wide-spread applications are impeded by limited plasticity (<2%) and catastrophic failure. However, recently, some MMGs with large plasticity have been found [7–9] and much of the latest works have focused on the shear bands evolution differences between brittle and ductile MMGs [10–13].

Previous studies of the plastic deformation mechanisms of MMGs were mainly carried under uniaxial compression, bending or indentation, and macroscopic observations on the evolution of shear bands have been performed [4].

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These investigations attempt to find structural explanations for the plastic deformation and fracture of MMGs. For example, it was reported that strain localization caused by work softening can be effectively prevented by *in situ* nanocrystallization within the shear bands during plastic deformation, leading to large plasticity [10]. Microscopic heterogeneity is also regarded as a major means of toughening MMGs [11]. Another viewpoint considers B/G (B and G are the bulk and shear modulus, respectively) or Poisson's ratio as controlling factors for the brittle-to-ductile transition of MMGs in terms of atomic bonding and connectivity [12,13]. It is widely accepted that the initiation and propagation of shear bands are essential for the plastic deformation of MMGs [3], and further studies need to systematically and quantitatively compare the microscopic observations on the initiation and evolution of shear bands for both brittle and ductile MMGs. In this study, small punch testing (SPT) was successfully introduced to observe and characterize the evolution processes of shear bands during plastic deformation of MMGs [14–16].

For the experiments, four typical Fe-, Zr-, Cu-, and Pd-based MMGs with compositions of $Fe_{65.5}Cr_4Mo_4Ga_4P_{12}C_5B_{5.5}$, $Zr_{59}Cu_{20}Al_{10}Ni_8Ti_3$, $Cu_{60}Zr_{30}Ti_{10}$, and $Pd_{30}Ni_{50}P_{20}$ with compressive plasticities ε_c of 0%, 0.5%, 1.6%, and 11% were selected [3,17–19]. Alloy ingots of the Zr-, Cu-, and Pd-based metallic glasses fabricated by arc melting were machined and polished to circular plates with dimension of 3 mm in diameter and 100 µm in thickness; the Fe-based metallic glass produced by melt spinning was machined and polished to circular plates with the dimension of 3 mm in diameter and 40 µm in thickness. The diameters of the upper and lower die used for SPT were 0.5 mm and 1 mm, respectively [14–16]. All SPT experiments were performed in an Instron E1000 testing machine with a punching rate of 0.001 mm/s. The tests were interrupted deliberately at different deflections, and the morphologies of the shear bands were observed by a LEO Super 35 scanning electron microscope (SEM).

Uniform multiple shear bands were observed not only for the ductile Zr-, Cu-, and Pd-based MMG specimens (Figure 1a), but also for the brittle Fe-based MMG specimens (Figure 1b), which can hardly be observed for other testing methods. The cobweb-like shear bands are classified as circumferential and radial according to their shear directions [14–16]. The morphology of the shear bands on the crosssectional plane is shown in Figure 1c via the bonded interface method [20]. Different from the observations in bending or indentation, shear bands propagate through the whole specimen comparatively freely without significant suppression. The specimens display a membrane-stretching manner with tensile stress on the shear plane.

A schematic illustration of the shear band evolution in comparison with crystalline material is shown in Figure 2. Both of the crystal materials and MMGs obey similar geometrical necessities though the physical mechanisms of shear process are completely different. Crystalline materials and MMGs microscopically shear during plastic deformation with differences in slip/shear plane, and slip/shear direction. For crystalline alloys [21] with inherent slip planes, which become the preferential slip direction for the simultaneous movement of dislocations, plastic deformation of MMGs with uniform and isotropic structure relies on the initiation and propagation of shear bands on the yielding plane and shows strong correlations with extrinsic factors, i.e. stress state, sample size, and geometry. Based on



Figure 1. (a) Morphology of the shear band pattern on the lower surface of Pd-based metallic glass punched at a deflection of 0.45 mm as a typical example for ductile MMG (a); (b) for macroscopically brittle Fe-based metallic glass punched at a deflection of 0.15 mm; and (c) morphology of the cross-sectional plane of Zr-based metallic glass punched at a deflection of 0.4 mm. The inset in (a) shows preferential propagation of shear bands.



Figure 2. Schematic illustration of the contrasting patterns of plastic deformation for crystalline material (left, *b* stands for Burgers vector) and metallic glass (right).

experimental observations, the processes of shear bands can be characterized by two parameters, i.e. the shear band density ρ and the critical shear offset λ [14–16].

For crystalline alloys, the correlation between plastic strain and dislocation movement can be expressed by the Orowan equation [21]

$$\gamma = k \cdot \rho \cdot b \cdot l, \tag{1}$$

where γ is the shear plastic strain, k is a correction parameter, ρ is the dislocation density, b is the Burgers vector, and l is the average distance the dislocations traveled. The deformation of crystalline alloys is related to both the density ρ of dislocations and the Burgers vector. Based on the similar geometrical necessity, the plasticity of MMGs may be characterized as

$$\varepsilon^* = \rho \cdot \lambda, \tag{2}$$

in which shear band density ρ and critical shear offset λ stand for the initiation and stable shear capabilities of shear bands, which are the only two ways for plastic deformation of metallic glasses. As illustrated in Figure 3c, the plastic strains of MMGs under uniaxial compression show a linear correlation with equivalent plastic strain ε^* .

The shear band density and the critical shear offsets of Fe-, Zr-, Cu-, and Pdbased MMGs are illustrated in Figure 3a and b. Complementarily, the deformation range of circumferential shear bands is illustrated in Figure 3d. It can be seen that the MMGs with higher plasticity exhibit a larger deformation range, shear band density, and critical shear offset. Especially, the shear band density of the Pd-based MMG and the critical shear offset of the Fe-based MMG differ strongly from what is observed for the other three MMGs. These findings may be related to the differences in global plastic deformation ability and fracture mode of these MMGs, as will be discussed below.



Figure 3. (a) Critical shear offset and (b) shear band density of metallic glasses with different plasticities; (c) correlations between macroscopic plastic strain (under uniaxial compression) and equivalent plastic strain ε^* ; and (d) circumferential shear band range of the four metallic glasses at different deflection.

Notes: For Zr-, Cu-, and Pd-based specimens, the experiments were interrupted at deflections of 0.15, 0.25, 0.35 and 0.45 mm, respectively. For Fe-based specimens, the experiments were interrupted at equivalent deflections of 0.125 and 0.375 mm (equivalent deflection f_e is converted by $f_e/t_e = f_0/t_0$, f_0 and t_0 are experimental deflection and specimen thickness and t_e is the equivalent deflection, 100 µm).

It is widely accepted that shear band spacing (density) is closely related to sample dimension and the ratio of 10:1 (of cross-section to band spacing) is suggested [22]. Considering our results of MMGs with different compositions under SPT, sample dimension seems not to be the only reason. The ratio could be considered as a variable attributed to different composition and plastic deformation capabilities of samples. It could be seen in Figure 3a that, at the same deflection, shear band density of Pd-based MMGs is extremely higher than the other three MMGs. This must be attributed to its higher plastic deformation capability.

In SPT, the Zr-, Cu-, and Pd-based MMG specimens deform in a shear mode, while the Fe-based MMG samples split into pieces under uniaxial compression tests even though all the glasses exhibit much more severe plastic deformation under SPT. Unlike the fracture of other brittle materials originating from fast propagation of cracks, the failure of MMG specimens originates from instability of shear bands resulting in different fracture modes of either shearing or splitting [3,6]. As illustrated in Figure 1a and b, the morphologies of the shear bands in ductile and brittle metallic

glasses differ a lot when approaching fracture. For Zr-, Cu-, and Pd-based MMG specimens, parallel shear bands with certain spacing initiated after yielding along a direction exhibiting an angle with respect to the stress axis. Due to the competition between shear bands during progressing plastic deformation, strain will be carried by fewer and fewer shear bands, as illustrated in the inset of Figure 1a, and finally plastic deformation is localized in a single principal shear band are considered as the global failure of the whole specimen, which is characterized as shear failure mode. For Fe-based MMG specimens, similar shear bands will be initiated after yielding. However, as mentioned before, the stable shear capability of Fe-based MMG is limited and fracture often occurs prior to the plastic strain localization along shear bands. The instability and shearing part of many shear bands is taken as the global failure of the whole specimen which is characterized as splitting failure mode [6].

In summary, through a series of SPTs of four typical MMGs with different plasticities ranging from brittle to ductile behavior, we find that all of them exhibit uniform evolution patterns of shear bands but are characterized by different shear band densities and critical shear offsets. MMGs with better plasticity generally exhibit larger shear band density and critical shear offset. Equivalent plastic strain ε^* defined in SPT makes a considerable parameter for evaluating plasticity of MMGs through the characteristics of shear bands. Moreover, their fracture mode shows a correlation with shear band instability, which is attributed to different stable shear capabilities of the MMGs. Based on these results, it is vital to improve the shear band initiation capability and to make the propagation of shear bands easier for enhancing the plasticity and avoiding unpredictable failure of MMG. This has implications for developing MMGs with both high strength and good ductility.

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