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A new constitutive model for shear banding instability in metallic glass

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ABSTRACT

Inelastic deformation of metallic glass is through shear banding, characterized by significantly localized deformation and emerged expeditiously under certain stress state. This study establishes a new constitutive model addressing the physical origin of the shear banding. In the modeling, the atomic structural change and the free volume generation are embodied by the plastic shear strain and the associated dilatation. The rugged free energy landscape is adopted to naturally reflect the rate-independent flow stress and flow serrations. Based on this, the conditions for the onset of shear banding instability are established, which enables the explicit calculation of the shear band inclination angle and its extension speed. The study concludes that shear band angle is significantly influenced by the diltancy factor and pressure sensitivity, that a shear band does not increase its thickness once emanated from a deformation unit, that the spreading speed of a shear band is intersonic, and that more shear bands, which lead to higher ductility, can be induced by high strain rates or by the introduction of a second material phase. The analysis also demonstrates that the ductility of metallic glass depends on the sample geometry and/or the stress state.

1. Introduction

When metallic glass is loaded, either quasi-statically or dynamically, the formation of shear bands and the localized deformation are the most striking phenomenon which has never been observed in crystalline counterparts. It was therefore believed that the shear bands manifest the major distinction between metallic glass and crystalline metals in terms of atomic structures and their response to external loading. In crystalline metals, lattice defects can easily be nucleated and transmitted, resulting in a low yield stress. In contrast, the plastic deformation of metallic glass has to be the cooperative rearrangements of clusters of atoms, leading to a much higher yield stress. Furthermore, in crystalline metals the lattice defects can be effectively pinned by obstacles like grain boundaries, stacking faults and solute atoms, which brings about strain-hardening and large ductility. In metallic glass, however, once the rearrangement of atoms is activated at a critical stress level, it spreads across the material and traps the deformation, and hence causes the material's brittleness. The plasticity and strain-hardening of crystalline metals have been successfully explained by dislocation dynamics. However, the fundamental understanding of the nucleation, propagation and annihilation of shear bands in metallic glass is still lacking. Questions like how fast a shear band extends or at what conditions a shear band nucleates or annihilates have not yet been convincingly answered.

While the experimental evidence on the physical origin of shear band remains inconclusive, the deformation mechanisms of metallic glass have been investigated theoretically, such as Steif et al. (1982), Huang et al. (2002) and Jiang and Dai (2009). Based on the free volume theory (Spaepen, 1977), they ascribed the inhomogeneous deformation to the shear-induced dilatation which leads to the reduction of viscosity. The adiabatic thermal softening was the secondary effect in the analysis by Jiang and Dai (2009). By assuming a preexisting band with slightly higher initial free volume concentration, Huang et al. (2002), Jiang and Dai (2009) and Gao et al. (2007) studied the instability in the material. They ascribed the instability to the precipitous drop of viscosity within the shear band as the shear stress reached a critical value. Their model has been prevailing in finite-element simulations (Su and Anand, 2006a; Thamburaja and Ekambaram, 2007; Yang et al., 2006), aiming to more precisely simulate the large deformation of metallic glass at high temperature or to investigate the shear band activation and fracture at low temperature (Tandaiya et al., 2009).

In the aforementioned modeling of metallic glass, the material was assumed to be viscoelastic. The free volume concentration, which varies with the stress state, serves as an internal variable to correlate the microstructure defect with the macroscopic deformation rate. This assumption is useful in establishing high-temperature stress–strain relationships, in which the stress

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overshoot and the non-Newtonian behavior can be well described (Thamburaja and Ekambaram, 2007). However, the direct extension of this theory to a low-temperature scenario has faced significant challenges.

The first challenge is that the viscoelasticity within the theory makes the flow stress at low temperature significantly rate-sensitive (Jiang and Dai, 2009), while experimental evidence clearly shows that the yield stress of metallic glass is insensitive to strain rate (Schuh et al., 2007). To resolve this problem, Anand and Su (2005) simply assumed that the yield surface is weakly dependent on or independent of the strain rate. However, this assumption breaks the connection between the microstructure defects and the macroscopic deformation rate.

In addition to the rate-dependency, the previous models cannot describe the serrations (or pops) at experimental stress–strain curves, which was ascribed to the shear band nucleation and annihilation (Song et al., 2008; Wang et al., 2009a). Both the viscoelastic model and the elastoplastic model render smooth stress-strain curves and merely a single load drop after the formation of catastrophic shear bands. Therefore, it is necessary to develop a new model to describe the physical origin of these serrations.

The third challenge is the shear band propagation. To our knowledge, no method for calculating the speed of shear band is available. The estimation of shear-banding speed from experimentally measured data varies from a few meters per second (Wright et al., 2009) to the speed of a shear wave (Lewandowski and Greer, 2006), supported by the dynamic strain measurement (Wright et al., 2009), high-speed photography (Sunny et al., 2009) and molecular dynamic simulations (Cao et al., 2009).

The present study will take up the above challenges by developing a new theoretical model that not only considers viscous deformation rate in BMG but also the associated atomic structural change of the material. The free energy undulating with the peaks and basins will be treated as the evolution of the material's atomic structure.

2. Constitutive modeling

2.1. Thermodynamics requirement

Consider the variation of free energy Φ of the atomic subsystems in metallic glass over the atomic coordinates as a hypersurface in a high-dimensional space. If the change of atomic coordinates due to the far-field shear stress τ is in a corporative manner and can be described by one or several proportional parameters, say the shear strain γ, a path of deformation can be identified on the hypersurface. This path has peaks and valleys, corresponding to many activated states and basin states. The second law of thermodynamics requires non-negative dissipation rate (Maugin, 1992), which reads

$$(\tau - \partial\Phi/\partial\gamma)\dot{\gamma} \geqslant 0. \tag{2.1}$$

Integrating Eq. (2.1) yields

$$Q \equiv \text{dissipation} = \int_{\gamma_1}^{\gamma_2} \tau d\gamma - (\Phi|_{\gamma=\gamma_1} - \Phi|_{\gamma=\gamma_2}), \tag{2.2}$$

where $\gamma = \gamma_1$ and $\gamma = \gamma_2$ represent two different atomic structures in the adjacent basins along the deformation path. Particularly, if $\Phi|_{\gamma=\gamma_1} = \Phi|_{\gamma=\gamma_2}$, the external work $\int_{\gamma_1}^{\gamma_2} \tau d\gamma$ associated with this transition is totally dissipated. $\gamma_0 = \gamma_2 - \gamma_1$ is regarded as the plastic strain since it refers to the irreversible change of atomic structures. It is worth highlighting that the jump from one energy basin to another is a dynamic process once the energy barrier is overcome. In experimental observations, γ_0 is embodied by the strain burst in a stress-mediated process. This intermittence, which has also been revealed in crystalline materials (Dimiduk et al., 2006), may be considered as the fundamental feature of plastic deformation.

In order to satisfy Eq. (2.1), we follow Eyring's concept (Eyring, 1936) to express the strain rate as:

$$\dot{\gamma} = \dot{\gamma}_0 \sinh((\tau - \partial\Phi/\partial\gamma)/\tau_0), \tag{2.3}$$

where $\dot{\gamma}_0$ is a reference strain rate and τ_0 is a reference stress. τ_0 may be further expressed as $\tau_0 = K_B T/\Omega_0$, where K_B and T are Boltzmann constant and temperature, respectively, and Ω_0 is the activation volume. Eq. (2.3) renders the strain rate effect of the system. It is noted that if τ_0 is sufficiently small (say less than 5% of the quasi-static yield stress of the material), the yield stress is then dictated by the local maximum of $\partial\Phi/\partial\gamma$. Any significant deviation from the equilibrium (*i.e.*, $\tau = \partial\Phi/\partial\gamma$) should invoke fast atomic motion to re-establish the equilibrium. Noting that the free energy landscape is rate-independent, the local maximum of $\partial\Phi/\partial\gamma$ is also rate-independent. We conjecture that this is the main cause of rate-independency of the yield stress when deforming metallic glass at low rate and low temperature. This conjecture is consistent with the accounts proposed by Johnson and Samwer (2005) and by Schuh et al. (2007). According to Pan et al. (2008), the activation volume Ω_0 of zirconium-based metallic glass is approximately $0.1 \sim 0.3\text{nm}^3$ corresponding to the volume of the shear transformation zone $2.5 \sim 6.6\ \text{nm}^3$. Therefore, at room temperature τ_0 is 10–40 MPa, which is indeed much smaller than the shear strength of metallic glass.

Eq. (2.3) leads to negligible but still positive rate sensitivity. Although from some dynamic experiments, negative strain-rate sensitivity was concluded (Li et al., 2003; Trexler and Thadhani, 2010), we think that it may be induced by artifacts (*e.g.*, stress concentrations) in dynamic experiments as pointed out by Sunny et al. (2007). Li et al. (2003) ascribed the negative rate sensitivity to the early development of a shear band from a local weak region with the yield stress lower than the macroscopic yield stress. In quasi-static case, one is still able to obtain the increase of macroscopic stress due to the relaxation and response of overall material. But for dynamic case, such an early shear band immediately leads to fracture due to the large kinetic energy. In this sense, the negative rate sensitivity refers to the local failure strength rather than the relationship between stress and strain rate. Gu et al. (2003) ascribed the negative rate sensitivity to the adiabatic heating, which in constitutive level is thermal softening rather than negative rate sensitivity at a constant temperature.

If the difference between the driven stress τ and the internal resistance $\partial\Phi/\partial\gamma$ is smaller than τ_0, the system behaves like a Newtonian flow; *i.e.*, $\tau - \partial\Phi/\partial\gamma \approx \tau_0\dot{\gamma}/\dot{\gamma}_0$. For a quasi-static stable process, $\dot{\gamma}$ approaches zero. The measured stress then reflects the internal resistance to the structural change, *i.e.*,

$$\tau = \partial\Phi/\partial\gamma. \tag{2.4}$$

It should be noted that Eq. (2.4) is only applicable before the onset of the shear band, since the deformation within the shear band must be dynamic.

2.2. The kinetics within a shear band

The inelastic deformation of metallic glass is generally embodied by the corporative rearrangement of the atomic subsystems. A two-dimensional schematic of such rearrangement is shown in Fig. 1(a). The figure illustrates an atomic process that accommodates a plastic shear strain γ_0. We try to unify the two distinct views of inelastic deformation of metallic glass, namely, the "shear transformation" after Argon (1979) and the "atomic jump" after Spaepen (1977). According to Argon (1979), the fundamental unit process underlining inelastic deformation is achieved by the shear distortion of a cluster of atoms (in dark grey color) from one relatively low energy configuration (above the arrow) to a second