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Prediction of shear-band thickness in metallic glasses

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We derive an explicit expression for predicting the thicknesses of shear bands in metallic glasses. The model demonstrates that the shear-band thickness is mainly dominated by the activation size of the shear transformation zone (STZ) and its activation free volume concentration. The predicted thicknesses agree well with the results of measurements and simulations. The underlying physics is attributed to the local topological instability of the activated STZ. The result is of significance in understanding the origin of inhomogeneous flow in metallic glasses.

Keywords: Metallic glasses; Shear band; Shear transformation zone; Free volume

The shear-banding-mode plastic flow of metallic glasses (MGs) at ambient temperature continues to fascinate and challenge scientists [1–5] because of its physical origin and practical implications. The free volume creation [6] and local heating generation [7], in which shear-band thickness is an important factor [2,8], are two potential causes of shear-banding instability in MGs. Here, the shear-band thickness is the characteristic width of the strain localization normal to the shear plane, and is not involved in the ultimate failure. In general, the thickness of shear bands in MGs is restricted to a rather narrow range from several to 10 or more nanometers, regardless of chemical components and loading methods (including tension, compression, bending, indentation, rolling, etc.); this has been widely found by direct experimental observations [9–15], or by numerical simulations [16–18]. Such localization of plastic flow, far smaller than the thickness (10–500 μm) of adiabatic shear bands (ASBs) in conventional alloys [19], suggests that the shear bands in MGs have a structural, rather than a thermal, origin [1,2,8]. Furthermore, the coupled thermomechanical analysis of shear-banding instability in MGs reveals that the onset of this instability is mainly controlled by local free volume softening [20] via discrete atomic jumps [6] or cooperative arrangement of local atomic clusters, termed the "shear transformation zone" (STZ) [21] or "flow defect" [22]. The STZ is the fundamental unit process underlying plastic deformation associated with the free-volume evolution. Although the study of thickness provides insight into the origin of shear-banding instability, the theoretical prediction of the shear-band thickness itself in MGs lags well behind that of ASBs in crystalline alloys.

Very recently, Joshi and Ramesh [23] have predicted a shear-band thickness of about 10–50 nm, based on a rotational plastic deformation mechanism in nanocrystalline materials at grain sizes approaching the amorphous limit (~2 nm). The lower bound of their predicted thickness agrees well with the shear-band thicknesses for many MGs [2]. This means that the flipping of STZ may be valid for the shear localization process in MGs. In addition, finite STZ sizes of about 1–2 nm (not reaching 2 nm) have been identified by many recent works [24–28]. Interestingly, the "10-time-rule" in granular materials [29] seems to be roughly satisfied in MGs, i.e. the shear-band thickness is approximately 10 times the STZ size, implying a similar shear instability mechanism between the two materials. However, the quantitative relationship between the thickness of the shear band and the size of the STZ is still under investigation, and the underlying precise physics that dominates the shear-band thickness is not clear. In this paper, we present an explicit expression of the thickness of shear banding based on shear instability due to STZs in metallic glasses. Its underpinning nature is discussed.

Plastic deformation of MGs occurs by the cascade of STZs or flow defects [3,21,22,30]. Subjected to an

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external shear stress τ, an STZ with activation volume Ω_a undergoes a characteristic shear strain $\gamma_a(\approx 1)$at a rate that depends on τ. The concentration of STZs C_ξ, namely the fraction of material that is available to STZ operations in a unit volume element, is statistically related to the free volume concentration ξ by $C_\xi = \exp(-1/\xi)$ [3,22]. Thus, the STZ operations in unit volume element can be characterized by the evolution of ξ as [20,31]:

$$\frac{\partial \xi}{\partial t} = D_\xi \frac{\partial^2 \xi}{\partial y^2} + G(\tau, \xi), \tag{1}$$

where D_ξ is the diffusion coefficient of free volume concentration [31], and the net creation rate function G is the combined rate of annihilation and generation of free volume, and is taken to be dependent on the local concentration of free volume ξ, and the shear stress τ [6]. The explicit expression of G was given first by Spaepen [6], as follows:

$$G(\tau, \xi) = \frac{1}{\chi} v_0 \exp\left[-\frac{1}{\xi}\right] \exp\left[-\frac{\Delta G^m}{k_B T}\right] \times \left\{ \frac{2k_B T}{\xi v^* S}\left[\cosh\left(\frac{\tau\Omega}{2k_B T}\right) - 1\right] - \frac{1}{n_D} \right\}, \tag{2}$$

where χ is a geometrical factor, v^* is the critical volume or the effective hard-sphere size of an atom, the attempt frequency v_0 is essentially the frequency (approximately the Debye frequency) of the fundamental mode vibration along the reaction pathway [22], ΔG^m is the activation energy, $k_B T$ is the thermal energy, S is the Eshelby modulus ($S = 2(1+v)\mu/3(1-v)$ where μ is the shear modulus v is the Poisson's raio), Ω is the atomic volume, and n_D is the number of diffusive jumps necessary to annihilate a free volume equal to v^*. Meanwhile, the macroscopic plastic strain rate can be written as [3,21,22]:

$$\dot{\gamma}^p = C_\xi \gamma_a H_a, \tag{3}$$

where the net activation frequency H_a of an STZ obeys a rate law of the form [3]: $H_a = v_0\left[\exp\left(-\frac{Q-\tau\Omega_a}{k_B T}\right) - \exp\left(-\frac{Q+\tau\Omega_a}{k_B T}\right)\right]$, here Q is the activation energy barrier for an STZ under an unstressed field [30]. In addition, the momentum balance, in the absence of body forces, requires that [20,31]:

$$\rho \frac{\partial^2 \gamma}{\partial t^2} = \frac{\partial^2 \tau}{\partial y^2}. \tag{4}$$

where ρ is the mass density, and the total shear strain γ can be decomposed into elastic and plastic parts, i.e. $\gamma = \gamma^e + \gamma^p$, here the elastic strain γ^e obeys Hooke's law: $\gamma^e = \tau/\mu$. Eqs. (1)–(4) govern the inhomogeneous deformation of MGs.

Shear banding, as a physically unstable event, is investigated through a linear perturbation analysis, i.e. seeking an inhomogeneous solution with respect to small perturbations to the homogeneous solution. The homogeneous solution $(\tau_h, \gamma_h, \xi_h)$ satisfies $\partial\tau_h/\partial y = \partial\gamma_h/\partial y = \partial\xi_h/\partial y = 0$. For a typical $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ (Vit 1) BMG, Figure 1 shows the stress–strain curve (black) of homogeneous deformation, along with the concentration of free volume vs. shear strain for a strain rate of $10^{-2}\ \mathrm{s}^{-1}$. For small perturbations it is assumed that $(\delta\tau, \delta\gamma, \delta\xi) = (\tau^*, \gamma^*, \xi^*) \exp(\alpha t + iky)$, where $(\tau^*, \gamma^*, \xi^*)$ are small constants that characterize the initial magnitude of the perturbation, k is the wavenumber, and α is related to the initial rate of growth. The stability of the deformation is now determined by the sign of the real part of α: if $\mathrm{Re}(\alpha) < 0$, the shear deformation is stable; if $\mathrm{Re}(\alpha) > 0$, it is unstable. The stability analysis tells immediately that the critical wavelength that may lead to runaway instability is:

$$\lambda_{crit} = 2\pi \left(\frac{D_\xi}{G_\xi^*}\right)^{1/2}. \tag{5}$$

where G_ξ^* is the free volume coalescence rate $\partial G/\partial\xi$ at the critical point of instability. Perturbations with a wavelength smaller than λ_{crit} will die out, whereas the ones with a wavelength larger than λ_{crit} will grow. Based on the homogeneous solution (Fig. 1), we can obtain the

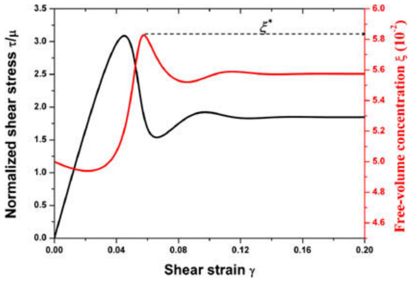

Figure 1. Dimensionless shear stress (black curve) and free volume concentration (red curve) vs. shear strain for the homogeneous deformation at a strain rate of $10^{-2}\ \mathrm{s}^{-1}$; the peak value of free volume concentration is denoted by ξ^*. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

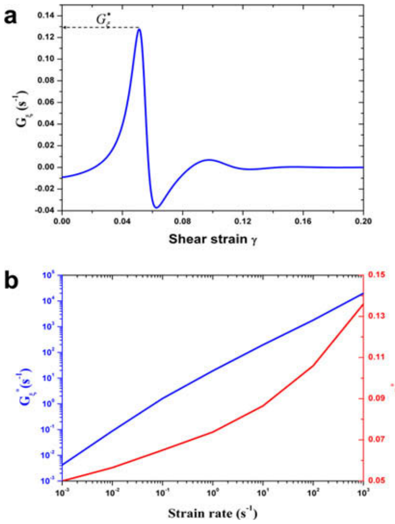

Figure 2. (a) Evolution of coalescence rate G_ξ of free volume concentration with shear strain at a strain rate of $10^{-2}\ \mathrm{s}^{-1}$; its peak value is denoted by G_ξ^*. (b) The effect of applied shear strain rate on G_ξ^* and ξ^*.