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Strain rate-dependent shear band behavior in bulk metallic glasses

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Abstract. In this article, we review our recent advances in understanding the deformation behavior of a typical tough $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ (Vit 1) bulk metallic glass (BMG), as a model material, under various loading modes and strain rates, focusing particularly on the rate-dependence and formation mechanism of shear-banding. Dynamic and quasi-static mechanical experiments, including plate shear, shear punch and spherical indentation, and continuum as well as atomistic modeling on shear-banding are discussed. The results demonstrate that higher strain rate slows down the annihilation process of free volume, but promotes the free-volume coalescence, which is responsible for the rate-dependent shear banding. The physical origin of shear bands, that is the free volume softening underpinned by irreversible rearrangements of atoms, is unveiled. Finally, some concluding remarks are given.

1. INTRODUCTION

Bulk metallic glasses (BMGs) are a relatively young class of alloy materials envisaged for wide functional and structural applications, exploiting their intriguing physical and mechanical properties [1–7]. However, they often exhibit unusual deformation behavior compared with their crystalline cousins. An example of this is the propensity for localized deformation in the form of shear banding with characteristic thickness of ~ 10 nm [8–13]. The initiation and propagation of shear band incurs the lack of global ambient-temperature ductility or plasticity prior to catastrophic failure [11–14], severely impeding further exploitation of BMGs. Therefore, considerable efforts have been made to investigate the shear bands behavior of BMGs during the past decades [15–18], yet the precise physical nature of the shear band formation in BMGs still remains unclear.

In polycrystalline alloys, the occurrence of shear bands is well known to be attributed to local thermal softening [19]. As for metallic glasses, there have been two potential causes for the onset of shear band instability, that is, free volume creation [15, 16] and local heat generation [20]. The first suggests that, shear-induced dilatation of randomly close-packed atoms causes the coalescence of free volume. This results in a precipitous drop in local viscosity, triggering the shear localization. Alternatively, shear banding events are proposed to be thermal-initiated, similar to adiabatic shear bands (ASBs) in crystalline alloys. This hypothesis stems from the direct observations on vein patterns as well as melted droplets and belts on fracture surfaces of metallic glasses. Actually, the two physical processes mentioned above are naturally coupled during the shear banding formation in BMGs, especially under high strain rates [17, 21–23]. The shear band formation is an instability process that is free-volume softening dominant and thermal assistant [7, 17]. Furthermore, it is recognized that both the dynamics of free volume [15] and the heat generations [19] are rate-dependent processes; hence, the resulting shear bands must be strongly affected by strain rates. The effect of strain rates on shear bands behavior therefore ought to be a primary focus of study in understanding the mechanism of shear banding instability. Our purpose in this article is to present an overview of strain rate-dependent shear band behavior of a typical tough

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$Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ (vit 1), as a model BMG, under various loading modes, paying specific attention to the physical origin of shear-banding instability.

2. RATE-DEPENDENT SHEAR BAND BEHAVIOR

The testing materials is $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ (vit 1) BMGs, whose fabrication can refer to works of Liu et al. [11, 12] and Jiang et al. [14]. In order to investigate whether the strain rate exerts a role in the shear-banding formation in BMGs, we performed different strain rate levels of plate shear, shear-punch, and spherical indentation testing on the Vit 1 specimens [11–13]. The dynamic and quasi-static mechanical tests were carried out with a split-Hopkinson pressure bar (SHPB) apparatus and an MTS-810 machine, respectively. Considering the results obtained in plate shear are almost identical to those in the shear-punch case, here we only present the results of shear-punch, as well as spherical indentation. Figure 1 shows the local shear band patterns around the circular deformation region during shear-punch on the Vit 1 BMGs. It can be found that the number of shear bands is relatively higher at dynamic strain rates (Figure 1a) than that at quasi-static strain rates (Figure 1b). The positive strain rate dependence of shear banding formation is also clearly observed in the spherical indentation case (Figure 2) [13]. It can be seen from this figure that the number density of shear bands around the final indentation at dynamic strain rate is far larger than that at quasi-static case. This rate-dependent shear band behavior is consistent with a series of experimental observations, such as tensile testing by Mukai et al. [24], compressive testing by Liu et al. [9], nano-indentation by Dai et al. [8] and micro-indentation by Jiang et al. [25]. The important question now is the reason why the high strain rates facilitate the shear band formations. According to the free volume theory, the formation of shear bands in metallic glasses is mainly due to the creation of free volume driven by shear stress in some local regions [15]. Actually, the free volume dynamics, including diffusion, annihilation and creation is affected greatly by strain rates [26–28]. In addition, the plastic work-heat conversion induced temperature rise under dynamic loading maybe play an influence on the formation of shear bands [17, 21–23],

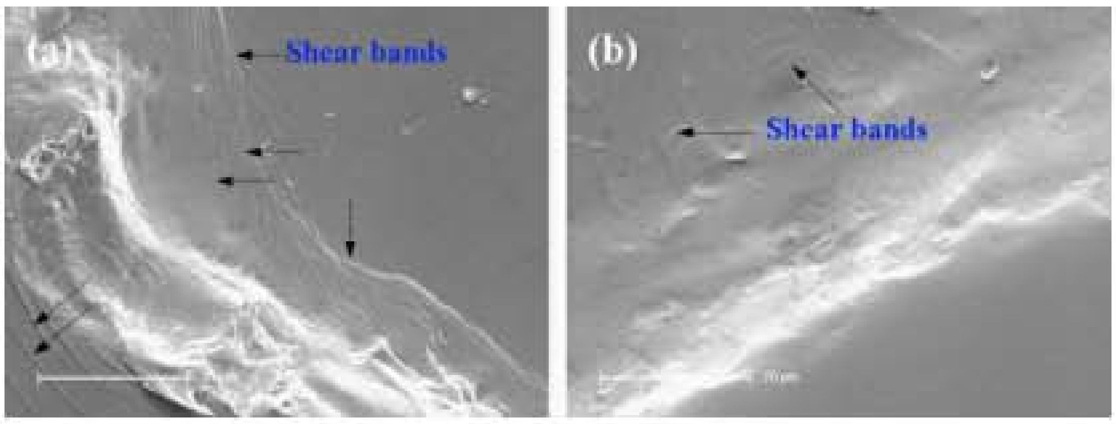

Figure 1. Shear bands patterns during shear-punch under (a) dynamic and (b) quasi-static strain rates [12].

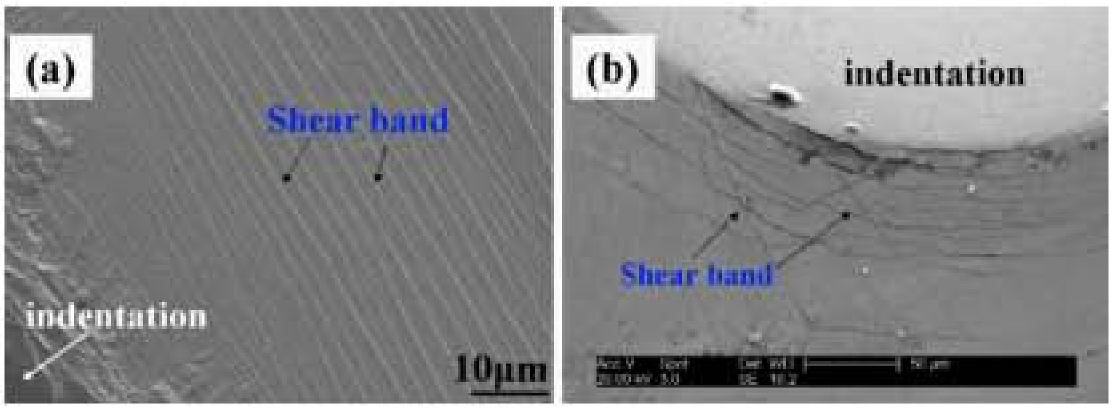

Figure 2. Shear bands patterns during spherical indentation under (a) dynamic and (b) quasi-static strain rates.

even though the evolution of free volume is generally believed to be dominated. It is urgent to develop a coupled thermo-mechanical model that can simulate both stress-driven and thermal-induced shear banding behavior of strain rate dependence.

3. MECHANICS OF SHEAR BANDING

In order to highlight the essential physical argument, we consider a coupled thermo-mechanical deformation of a BMG undergoing one-dimensional simple shearing. The governing equations for this problem can be written as [17]

$$\tau = \psi(\gamma, \dot{\gamma}, \theta, \xi) \tag{1}$$

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

$$\frac{\partial \theta}{\partial t} = \kappa \frac{\partial^2 \theta}{\partial y^2} + A\tau \frac{\partial \gamma}{\partial t} \tag{3}$$

$$\frac{\partial \xi}{\partial t} = \mathrm{D} \frac{\partial^2 \xi}{\partial y^2} + \mathrm{G}(\xi, \theta, \tau) \tag{4}$$

where Equation 1 is the constitutive Equation 2 is the Cauchy momentum equation, Equation 3 the temperature evolution equation, and Equation 4 the free volume evolution equation following Huang et al. [26]; In these equations, τ is the shear stress, γ is the shear strain, $\dot{\gamma}$ is the shear strain rate, θ is the temperature, ξ is the free volume concentration [26–28], κ is the thermal diffusivity ($\kappa = \lambda/\rho C_v$, here λ, ρ and C_v being respectively the thermal conductivity, the mass density and the specific heat), A is a constant related to the Taylor-Quinney coefficient (β_{TQ}), given by $A = \beta_{\mathrm{TQ}}/\rho C_v$, D is the diffusion coefficient of free volume concentration, and $G(\xi, \theta, \tau)$ is the net creation rate of free volume, the explicit expression of which was presented by Spaepen [15].

First, we perform an analysis of homogeneous flow prior to the shear instability, which is important to understand the resultant shear-banding instability process. The homogeneous solution (τ_h, γ_h, ξ_h, θ_h) satisfies that $\partial/\partial y = 0$. Since the rate-dependent shear band formation closely connects with the microscopic free volume dynamics, we can define a dimensionless Deborah number to characterize this trans-scale problem. In the present case, the Deborah number is defined as the ratio between the internal structural relaxation time t_r and the macroscopic imposed time t_e of external loading, that is

$$D_e = t_r/t_e \tag{5}$$

where $t_r = \eta_h/G$ with the viscosity $\eta_h = \tau_y/\dot{\gamma}_h^p$ and shear modulus G, $t_e = (\gamma/\dot{\gamma}_h^p)$. The magnitude of the Deborah number provides an interesting indication. If t_r is very larger compared with t_e, i.e. $D_e >> 1$, we see metallic glasses behaving as a glassy solid. In such case, the structural relaxation annihilation process of free volume is very slow and free volume concentration will grow within the BMG, resulting in shear band formation. However, in the opposite case, i.e. $D_e << 1$, they behave as an ordinary viscous fluid instead of inhomogeneous flow (or shear banding). For the present Vit 1 BMGs, the variation of Deborah number with shear strain at different strain rates is shown in Figure 3a. From the figure, one can find that the values (far more than unit) of Deborah number at high-strain rates are larger than those at low-strain rates in the early deformation stage. The high-strain rate decreases the macroscopic flow-ability. This is the main reason that the shear bands form easier at higher strain rates, which is consistent with our experimental observations.

Shear banding, as a physically unstable event, is investigated through a linear perturbation analysis [19], i.e., seeking an inhomogeneous solution with respect to small perturbations on the above homogeneous solution. The stability analysis [17] tells immediately that the shear-banding instability is mainly controlled by the microscopic free-volume coalescence rate $G_\xi = (\partial G/\partial \xi)_k$, since its diffusion is a very slow process. The temperature rising is a secondary effect in this coupled deformation process, but it in turn promotes the shear instability at the dynamic strain rate [28]. Figure 3b shows the free-volume coalescence rate versus applied shear strain rate for the present Vit 1. It is noted that G_ξ increases with increasing strain rate. Therefore, at higher strain rates, the free-volume grows faster and annihilates slower, which facilitates the formation of shear bands in BMGs. This numerical result agrees well with our above experimental observations for BMGs.

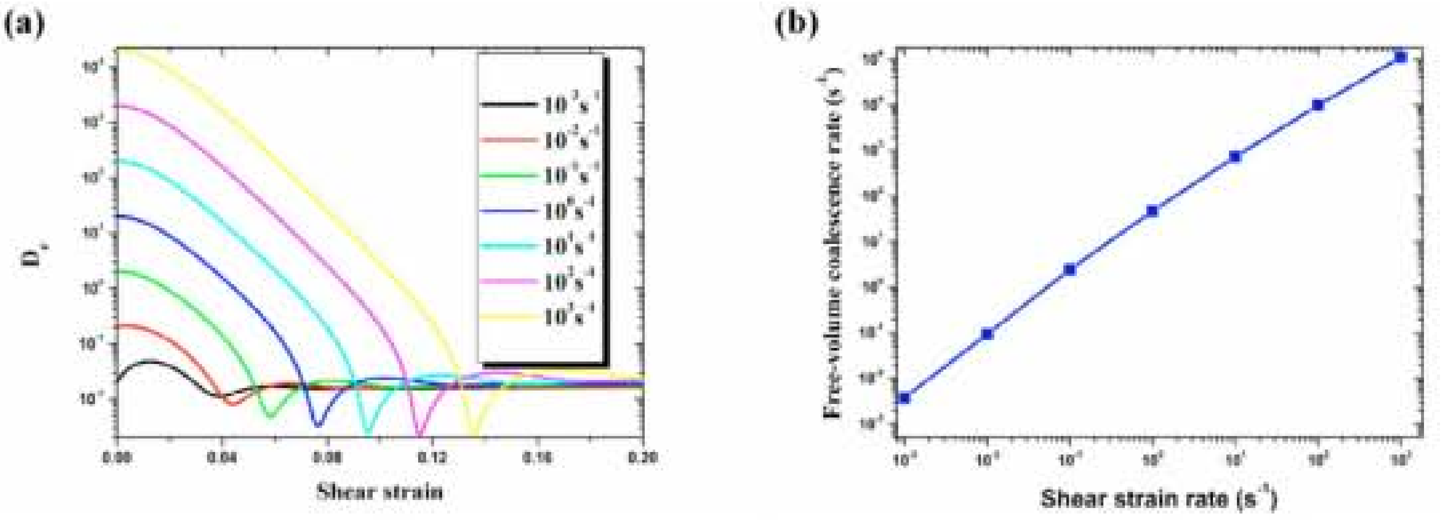

Figure 3. (a) The Deborah number varies with the shear strain under different strain rates. (b) The free volume coalescence rate versus applied shear strain rates.

4. ATOMISTIC MODELING

Based on the experimental observations on rate-dependent shear band formation, the coupled thermomechanical analysis of shear-banding instability in BMGs reveals that the onset of this instability is mainly controlled by local free volume softening. Meanwhile, there is general consensus that the local free volume motions via discrete atomic jumps [15] or cooperative arrangement of local atomic cluster, termed "shear transformation zone" (STZ) [16] or "flow defect" [29]. Therefore, it is interesting to directly model whether this irreversible structural rearrangement at atomic scale can result in the shear banding in BMGs. Here, we rely on the molecular dynamics (MD) method to simulate the rate-dependent shear banding behavior in BMGs undergoing spherical indentation. In our MD simulations, two-dimensional binary $Cu_{46}Zr_{54}$ MGs which contains 250,000 atoms were used. In this system, atoms interact via a modified Lenard-Jones (L-J) 4–8 potential; the motion of each atom was evaluated by integrating the Newtonian equations of motion using velocity-Verlet method with a time step of 1 fs. To obtain glassy structures, the melt-quench procedure was used, finally forming a sample with the size of 195×105 nm^2. Periodic boundary conditions were used in all two directions. The details of the subsequent indentation simulations are available in the work of Jiang et al.[18].

We use the parameter $D_{\min}$, introduced by Falk and Langer [29], to identify such rearrangement. $D_{\min}$ values of all atoms during each loading displacement interval (0.1 Å) were calculated. We selected 1.5 Å, about half of the average distance between a Cu atom and a Zr atom in samples [30, 31], as a cutoff of $D_{\min}$ to characterize the rearrangements that make up a plastic event at all strain rates. During indentation, the average $D_{\min}$ larger than 1.5 Å under three strain rate levels is displayed in Figure 4a. Obviously, we find that the evolution of $D_{\min}$ is strongly dependent on strain rates. With the strain rates decreasing from 10^{10}s^{-1}, 10^{9}s^{-1} to 10^{8}s^{-1}, the $D_{\min}$ becomes larger, whereas their temporal distribution becomes much more inhomogeneous.

According to the result, we can conclude that, during a displacement interval, at high strain rate, few atoms simultaneously participates in the irreversible rearrangement, forming many small shear events, and at low strain rate, many rearranged atoms construct few larger-scale shear events. During whole loading process, the large-scale shear events take place discretely, while the small-scale shear events are prone to occur continuously. This kind of shear events finally leads to definite shear-banding at the maximum indenting depth, which is displayed in Figures 1b–1d, corresponding to strain rates of $10^{10}\mathrm{s}^{-1}$, $10^{9}\mathrm{s}^{-1}$ and $10^{8}\mathrm{s}^{-1}$, respectively. The patterns are drawn by coloring the atoms according to their $D_{\min}$ values; here, the darker the color, the larger $D_{\min}$ value. The MD simulation clearly shows that more and thinner shear bands formed at high strain rate, while fewer and coarser shear bands nucleated at low strain rate. This result agrees well with our present and a series of otherwise experimental observations for real metallic glasses under indentation [8, 25, 32, 33].

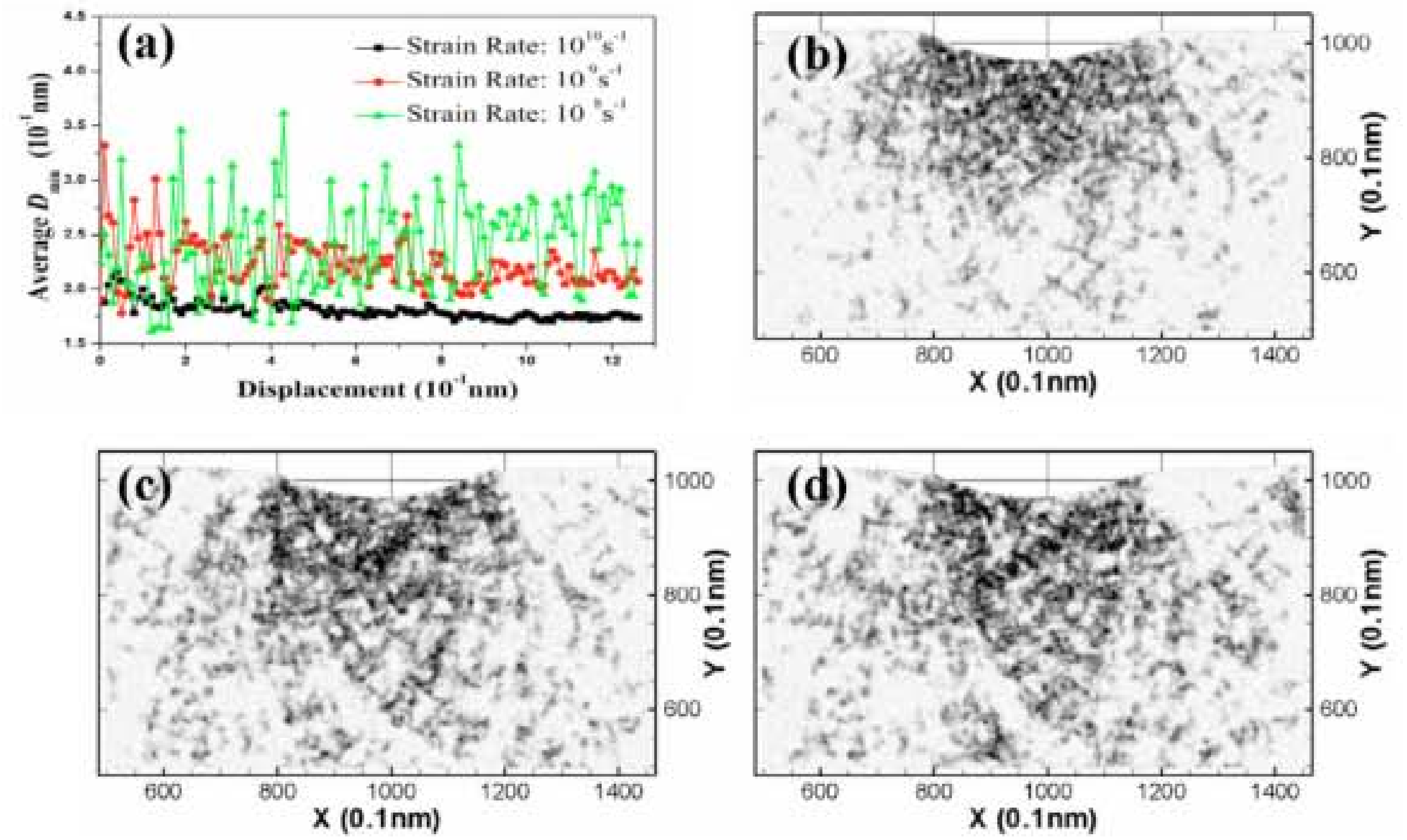

Figure 4. The rate-dependent $D_{\min}$ evolutions (a) during indentation and shear band patterns (b-d) of the maximum indenting depth. The strain rate decreases from (b-d); (b) $10^{10}\mathrm{s}^{-1}$, (b) $10^{9}\mathrm{s}^{-1}$ and (d) $10^{8}\mathrm{s}^{-1}$.

5. CONCLUSIONS

In this paper, experimental observations on the effect of strain rate on the formation of shear banding are first presented. From these experimental phenomena, a coupled thermal-mechanical shear banding formation is modelled within the context of continuum mechanics, during which the evolutions of both free volume and temperature are simultaneously taken into account. Our theoretical analysis demonstrates that, the macroscopic rate-dependent shear band behaviour is mainly dominated by the microscopic free volume dynamics. Higher strain rates promote the free-volume coalescence or slow down its annihilation. This is responsible for the simultaneous formation of shear bands in dynamic cases. Furthermore, we perform direct MD simulation on shear banding formation during spherical indentation of a binary $Cu_{46}Zr_{54}$ MG system by