

Adiabatic shear banding instability in bulk metallic glasses

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In this letter, a linear instability analysis was performed to highlight the mechanism of formation of adiabatic shear banding instabilities in bulk metallic glasses (BMGs). It is found that this instability is determined by the free volume coalescence-diffusion Deborah number. The most important findings are that both free volume coalescence softening and adiabatic heating softening exert an influence on the formation of adiabatic shear banding instability in BMGs, and higher strain rate promotes the growth of instability. These results are of particular significance in understanding the mechanism of formation of shear bands in BMGs. © 2005 American Institute of Physics.

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Recently, bulk metallic glasses (BMGs) have attracted large interest due to their unique physical, mechanical, and chemical properties.^{1–3} However, plastic deformation of BMGs at high stresses and low temperatures (e.g., room temperature) is prone to be localized into shear bands. Two important hypotheses, namely free volume softening^{4–8} and local adiabatic heating softening,^{9,10} have been proposed to explain the formation mechanism of shear bands in BMGs. However, the precise physical nature of the mechanism of formation of shear bands in BMGs still remains unclear. Furthermore, it is noted that these investigations are mainly focused on quasistatic conditions. However, considerable research work has demonstrated that the formation of shear bands in BMGs is a rate-dependent process.^{11–13} In this connection, particularly, Johnson and co-workers recently reported the striking findings that Zr-based bulk metallic glass matrix composite exhibited a peculiar “self-sharpening” phenomenon in the course of penetration.¹⁴ This self-sharpening behavior results from localized adiabatic shear banding, which is a typical dynamic shear instability phenomenon in materials at high strain rate. Though great progress in understanding adiabatic shear banding instability in crystalline materials has been made during past several decades,¹⁵ the physical nature of adiabatic shear banding instability in BMGs has not previously been identified.

Here, the dynamic thermoplastic instability of BMGs in one-dimensional simple shear is analyzed using linear stability analysis. The onset criterion and the formation mechanism of adiabatic shear banding instability are clearly revealed.

Consider dynamic thermomechanical deformation of a bulk metallic glass in one-dimensional simple shear, i.e., deformation can only occur in the direction of the x -axis direction but there may have a gradient along the y axis. The governing equations for this problem can be written as

$$\tau = f(\gamma, \dot{\gamma}, \theta, \xi), \quad (1a)$$

$$\frac{\partial^2 \tau}{\partial y^2} = \rho \frac{\partial^2 \gamma}{\partial t^2}, \quad (1b)$$

$$\frac{\partial \theta}{\partial t} = \frac{\lambda}{\rho C_v} \frac{\partial^2 \theta}{\partial y^2} + \frac{K \tau}{\rho C_v} \frac{\partial \gamma}{\partial t}, \quad (1c)$$

$$\frac{\partial \xi}{\partial t} = D \frac{\partial^2 \xi}{\partial y^2} + g(\xi, \theta, \tau), \quad (1d)$$

where Eqs. (1a), (1b), (1c), and (1d) are the constitutive equation, the momentum equation, the energy equation, and the diffusion-production equation of the free volume concentration, respectively. In these equations, τ is the shear stress, γ is the shear strain, $\dot{\gamma}$ is the shear strain rate, ρ is the density, θ is the temperature, C_v is the specific heat, λ is the thermal conductivity, K is the Taylor-Quinney coefficient ($K \cong 0.9$), ξ is the free volume concentration, and D is the diffusion coefficient of the free volume concentration. While $g(\xi, \theta, \tau)$ in Eq. (1d) is the net generation rate function of the free volume concentration, the explicit expression of which was given by Spaepen⁴ and Huang *et al.*⁸

To perform a linear stability analysis, we impose a small perturbation ($\gamma', \tau', \theta', \xi'$) on the smoothly developing homogeneous state ($\gamma_0, \tau_0, \theta_0$), which is a solution of Eq. (1), such that

$$\{\gamma, \tau, \theta, \xi\} = \{\gamma_0 + \gamma', \tau_0 + \tau', \theta_0 + \theta', \xi_0 + \xi'\}, \quad (2a)$$

$$\{\gamma', \tau', \theta', \xi'\} = \{\gamma_*, \tau_*, \theta_*, \xi_*\} e^{at+iky}, \quad (2b)$$

where ($\gamma_*, \tau_*, \theta_*, \xi_*$) are the magnitudes of the perturbation, a is the rate of growth, and k is the wave number. The stability of the deformation is determined by the sign of the real part of a .

Combining Eq. (1) with Eq. (2) yields the following characteristic equation:

$$\alpha^4 + a\alpha^3 + b\alpha^2 + c\alpha + d = 0, \quad (3)$$

where

$$a = [\beta + \rho C_v (Dk^2 - G_\xi) + \rho C_v G_\tau F_0] / \rho C_v, \quad (4a)$$

$$b = [k^2 \omega + \rho \beta (Dk^2 - G_\xi) + k^2 \rho \lambda G_\tau F_0 + K \dot{\gamma} \rho G_\theta F_0] / \rho^2 C_v, \quad (4b)$$

$$c = k^2 [\omega (Dk^2 - G_\xi) + \lambda Q_0 k^2 - K \tau_0 G_\theta F_0] / \rho^2 C_v, \quad (4c)$$

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$$d = k^4 \lambda Q_0 (Dk^2 - G_\xi) / \rho^2 C_v, \quad (4d)$$

and $\beta = K \dot{\gamma} P_0 + \lambda k^2 + R_0 C_v k^2$, $\omega = \lambda R_0 k^2 + \rho C_v Q_0 - K \tau_0 P_0$. Whereas $Q_0 = (\partial \tau / \partial \dot{\gamma})_0$, $R_0 = (\partial \tau / \partial \dot{\gamma})_0$, $P_0 = -(\partial \tau / \partial \theta)_0$, $F_0 = -(\partial \tau / \partial \xi)_0$, $G_\xi = \partial g(\xi, \theta, \tau) / \partial \xi$, $G_\theta = \partial g(\xi, \theta, \tau) / \partial \theta$, and $G_\tau = \partial g(\xi, \theta, \tau) / \partial \tau$. According to the Routh-Hurwitz theorem,¹⁶ if $d < 0$ then at least one of the roots of Eq. (3) has a positive real part, which indicates that unstable deformation occurs. Hence, the onset criterion for this adiabatic shear instability can be obtained

$$\text{De} = \frac{t_D}{t_G} > 1, \quad (5)$$

where $t_D = 1/Dk^2$ is the characteristic time for the free volume diffusion, and $t_G = 1/G_\xi$ is the characteristic time for the free volume coalescence. Whereas De is called the free volume coalescence-diffusion Deborah number, which measures the competition between the free volume coalescence and the free volume diffusion. Obviously, the competition between these two microscopic rate-dependent processes controls stability. If $\text{De} > 1$, i.e., the free volume coalescence is faster than the free volume diffusion, perturbation will grow exponentially and deformation becomes unstable, whereas for the opposite case, perturbation will die out and deformation remains stable.

It is interesting to find that the quasistatic instability criterion derived by Huang *et al.*⁸ can also be expressed as Eq. (5). However, the momentum and energy equations were not considered in their quasistatic analysis. It is noted, although the momentum and energy equations were incorporated into the governing equations for the present dynamic shear instability problem, whether instability occurs or not is not related

$$t_c = \frac{2\rho C_v R_0}{K\tau_0 P_0 - \rho C_v Q_0 + \rho C_v R_0 G_\xi + \sqrt{(K\tau_0 P_0 - \rho C_v Q_0 - \rho C_v R_0)^2}}. \quad (6)$$

It can readily be seen from Eq. (6) that besides the free volume softening (G_ξ), strain hardening (Q_0), and strain rate hardening (R_0), thermal softening (P_0) also exerts a significant influence on the characteristic time. This is quite different from the quasistatic case where the sole softening effect is free volume coalescence.⁸ Furthermore, we find from Eq. (6) that strain hardening and strain rate hardening retard the perturbation growth, whereas thermal softening and free volume softening accelerate the growth. According to the relative importance of the free volume softening and the thermal softening, the critical characteristic time given by Eq. (6) can be converted into the following two simple expressions. If the free volume softening is dominant, i.e., $K\tau_0 P_0 - \rho C_v Q_0 < \rho C_v R_0 G_\xi$, then the critical characteristic time simplifies to

$$t_c = \frac{1}{G_\xi}. \quad (7)$$

If thermal softening is dominant, i.e., $K\tau_0 P_0 - \rho C_v Q_0 > \rho C_v R_0 G_\xi$, then the critical characteristic time is expressed as

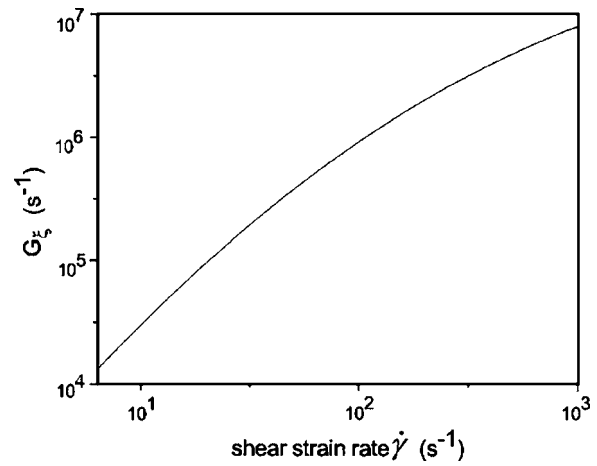


FIG. 1. Variation of free volume coalescence rate G_ξ with shear strain rate.

explicitly to the thermal softening and the strain rate according to Eq. (5). So, a question naturally arises: do these factors exert any influence on the initiation of adiabatic shear banding instability? Actually, these factors influence instability markedly in some other ways which will be demonstrated later.

Of all instability modes meeting the critical condition of Eq. (5), one with the maximum perturbation growth rate α_m is the dominant instability mode. The critical characteristic time for this dominant instability mode can be characterized by $t_c \cong 1/\alpha_m$.¹⁷ The maximum growth rate α_m can be obtained by solving the characteristic Eq. (3). After estimating the quantity order and ignoring the secondary small terms, the critical characteristic time of instability, t_c , can finally be written as

$$t_c = \frac{R_0^*}{\dot{\gamma}_0} \frac{\rho C_v}{K\tau_0 P_0 - \rho C_v Q_0}, \quad (8)$$

where $R_0^* = \partial \tau / \partial \ln(\dot{\gamma} / \dot{\gamma}_0)$ is the strain rate sensitivity coefficient of materials, and $\dot{\gamma}_0$ is the current strain rate. It is very interesting that the expression of the characteristic time for the dominant thermal softening case, i.e., Eq. (8), is totally identical with that of the classical adiabatic shear instability for crystalline materials where thermal softening is the sole factor leading to instability.¹⁷

Now let us turn to the discussion of the strain rate effect on instability. Figure 1 shows the variation of free volume coalescence rate G_ξ with strain rate for a model material of $\text{Zr}_{41.2}\text{Ti}_{13.8}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5}$ bulk metallic glass. From this figure, it can be found that G_ξ increases with increasing strain rate. Hence, it can readily be found that from Eqs. (7) and (8) that the critical characteristic time of instability for both cases decreases with increasing strain rate. This might be the main reason that shear band instability is more probable at high strain rates. This result is consistent with the available experimental observations.¹¹⁻¹³

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