Temperature-dependent shear band dynamics in a Zr-based bulk metallic glass

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Flow serrations recorded during inhomogeneous deformation of $Zr_{52.5}Ti_5Cu_{17.9}Ni_{14.6}Al_{10}$ (Vit105) were studied during compression testing at temperatures between -40 and 60 °C. The shear band velocities determined exhibit a pronounced temperature dependence covering nearly two orders of magnitude. The velocities follow an Arrhenius-type behavior with an associated activation energy of 0.3 ± 0.05 eV. The results demonstrate a thermally activated mechanism of shear band propagation, which is similar to the behavior of other, nonmetallic amorphous materials. © *2010 American Institute of Physics*. [doi:10.1063/1.3309686]

While the mechanical properties of bulk metallic glasses have been studied for many years,[1] the underlying deformation mechanisms remain the subject of vivid debate. At low homologous temperatures, i.e., well below their glass transition temperature, metallic glasses deform by flow localization with the entire plastic strain being confined to shear bands with a thickness of a few tens of nanometers.[2] It is commonly understood that this process of flow localization involves a significant softening of the material within the shear band.[3] This local drop in viscosity has been attributed either to significant heating during shear banding[4] or to a local dilatation of the atomic structure, i.e., a volume expansion under the applied stress.[5,6]

Experimental evidence for significant local heating during shear banding has been reported in the work of Greer *et al.*, and a model for the temperature rise within shear bands has been established.[7] The model is based on the dissipation of the stored elastic energy as heat within a confined zone of the material. In order to yield feasible temperature rises, it is suggested that shear band operation occurs within time periods of nano to microseconds, i.e., close to the speed of sound. Attempts have also been made to follow the process of shear banding *in situ* during mechanical testing[8–10] using optical microscopy equipped with high-speed cameras. From these experiments it was concluded that shear bands formed rapidly in time periods of less than a few milliseconds. However, this only corresponds to an upper time limit due to the resolution of the tests.

More recently, Wright *et al.*[11] and Chen *et al.*[12] used high-sensitivity strain gauges in combination with high acquisition rates (kilohertz) to accurately measure the strain bursts during serrated plastic flow of bulk metallic glasses at room temperature. The temporal resolution of these experiments was well below 1 ms. The strain bursts were reported to occur over time periods ranging from 0.4 to 1.5 ms with corresponding shear band velocities of the order of 10^{-3} to 10^{-4} m/s, i.e., much lower than the speed of sound in these materials. In this study, the temperature dependence of the velocity associated with these strain bursts will be presented.

Uniaxial compression tests were conducted using cylindrical samples of glassy $Zr_{52.5}Ti_5Cu_{17.9}Ni_{14.6}Al_{10}$ (Vit105)

with a diameter of 3 mm. The samples were produced by arc-melting the constituent elements (purity >99.9%) in a Ti-gettered argon atmosphere (99.9999% purity) and subsequently suction casting. Mechanical tests were conducted with samples of 5 mm length in the serrated flow regime. Hence for temperatures between 60 and -30 °C a strain rate of 10^{-3} s^{-1} was deployed, while for a single test at -40 °C the strain rate was reduced to 10^{-4} s^{-1}. An extensometer bridging the upper and lower compression plates was used to record the displacement, and a piezoelectric load cell was employed to measure the load during the tests. Data was acquired at rates of 10 kHz using an analog-to-digital converter with a moving average filter over eight consecutive points. As pointed out in Ref. 11 these means are essential to record load and displacement accurately during dynamic stress drops and strain bursts. In fact, a preliminary compression test on a brittle Si-wafer revealed a time resolution of 300 μs for individual load drops for the specific set-up used in these experiments.

Figure 1 shows the upper part ($\sigma > 1$ GPa) of selected stress-strain curves for temperatures of 25, 0, and -25 °C.
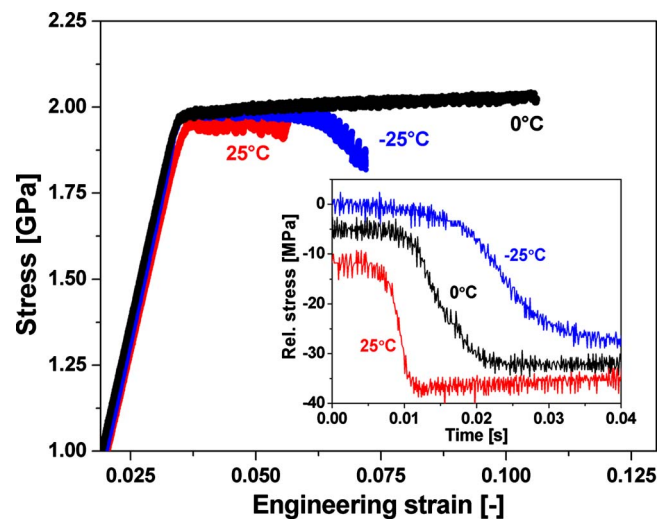

FIG. 1. (Color online) Stress-strain curves of Vit105 samples tested at 25 °C, 0 °C and -25 °C at a strain rate of 10^{-3} s^{-1}. Inset: individual serrations, plotted as relative load vs. time, showing an increase in load drop duration with decreasing temperature.

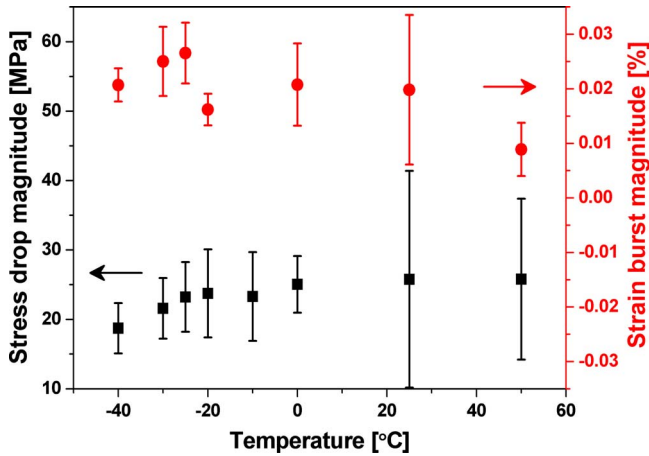[a] Electronic mail: david.klaumuenzer@mat.ethz.ch.

FIG. 2. (Color online) Mean stress drop and mean strain burst magnitude as a function of temperature, revealing a decrease in stress drop size (for $T < -20\ °C$) and a weak increase in strain burst magnitude with decreasing temperature.

FIG. 3. (Color online) SDJ velocity as a function of engineering strain for the samples tested at 0 °C and −25 °C. At −25 °C, the sample shows a distinct increase in SDJ velocity, coinciding with a progressive decrease in flow stress level (see Fig. 1). At 0 °C, where the flow curve in Fig. 1 exhibits a constant stress level, the SDJ velocity also remains constant as a function of strain.

An enlarged view of stress drops selected from these serrated flow curves at similar strains is displayed in the inset. A three-stage mechanism is apparent from each of the stress drops displayed. The three stages may be attributed to acceleration, steady-state and deceleration.[13,14] More importantly, it can be clearly seen that the duration of each individual stress drop increases with decreasing temperature, while the magnitude of the stress drop remains approximately constant. The duration of the steady-state stage increases from approximately 1 ms at 50 °C to just below 100 ms at −40 °C, showing a distinct trend as a function of temperature independent of applied strain rate.[12] A careful comparison between the durations of stress drops and corresponding strain bursts revealed no difference between the two. An analysis of the uniaxial displacement jump magnitude (in units of strain) associated with each individual stress drop reveals little or no increase with decreasing temperature, as displayed in Fig. 2, whereas the stress drop magnitude decreases only for lower temperatures ($T < -20\ °C$) and otherwise remains constant.

The velocity associated with these discrete shear banding events may be calculated in two different ways depending on the mechanism of shear band propagation. If the entire displacement is assumed to form by instantaneous shearing along a principal shear plane inclined at 45° to the compression axis, a shear displacement jump (SDJ) velocity (v_{SDJ}) may be calculated directly from the displacement signal by dividing the shear offset $\sqrt{2}\Delta l$ by the shear event duration Δt, where Δl is the measured uniaxial displacement. Alternatively, shear banding might be envisaged to occur by the successive propagation of a shear front on a shear plane across the width of the sample. The associated velocity of shear front propagation (SFP) is given by $v_{SFP} = \sqrt{2}d/\Delta t$, where d is the diameter of the sample. Based on various experiments, both types of mechanisms have been suggested.[8,10]

Figure 3 shows a plot of the SDJ velocity as a function of strain for compression tests conducted at 0 °C and −25 °C. The sample tested at 0 °C was not tested to failure and exhibited a stress plateau in the flow curve for which a constant SDJ velocity is observed. In contrast, at −25 °C the sample was tested to failure and showed a typical drop in the level of flow stress just prior to failure. Coinciding with this
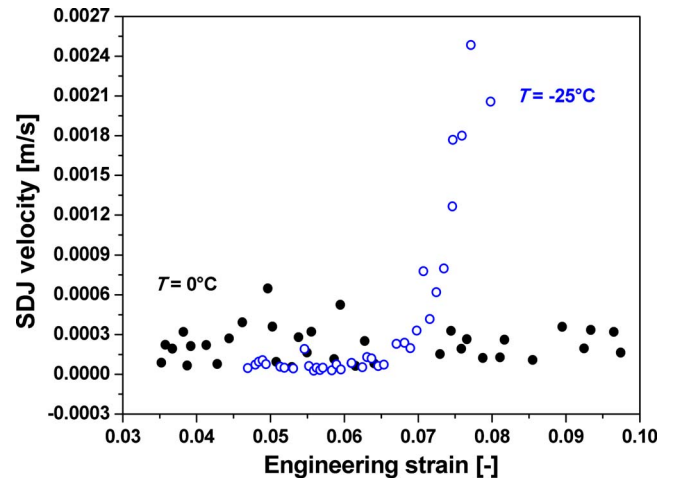
decreasing flow stress, a sharp increase in SDJ velocity is observed (see Fig. 3). An increasing shear band propagation velocity as a function of strain has also been reported for room-temperature measurements[12] and may be associated with an accumulation of free volume within shear bands following their repeated reactivation.[15]

Figure 4 shows a logarithmic plot of SDJ and SFP velocities as a function of inverse temperature. A clear Arrhenius-type behavior is observed and the SFP velocity exceeds the SDJ velocity by approximately three orders of magnitude. The latter is in agreement with the results in Ref. 11. However, all velocity values determined are well below the speed of sound (of the order of 10^3 m/s), which would reflect the time-scales used in modeling the high-temperature rises in shear bands. More importantly, the velocities decrease over two orders of magnitude as the temperature is decreased from 60 °C to −40 °C, emphasizing the strong influence of temperature on the shear band dynamics, as also proposed by Li *et al.*[16] from qualitative experimental results. For the lower temperatures, the observed SDJ velocities tend
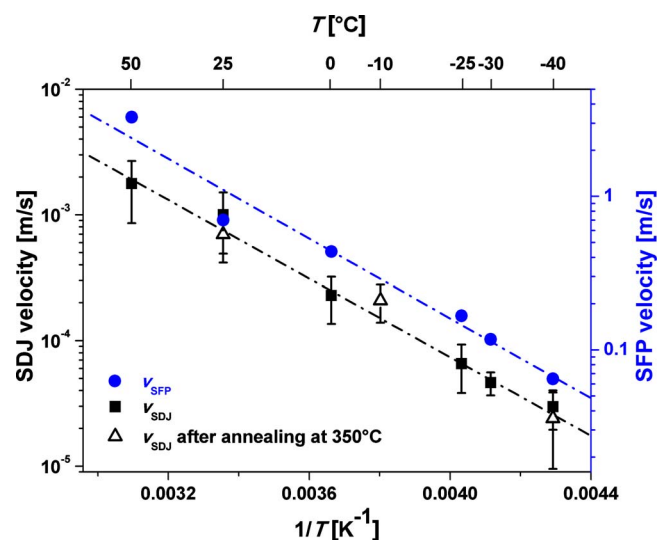

FIG. 4. (Color online) SDJ and SFP velocities as a function of inverse temperature, showing Arrhenius-type behavior.

toward 10^{-5} m/s, which is much lower than any value reported previously.[11,12] Above a critical temperature of 65 °C, the samples become brittle, while a strain rate dependent lower limit in temperature is encountered at the transition from serrated to non-serrated flow, which is due to the SDJ velocity being overwhelmed by the crosshead velocity applied in the test.

In addition to the as-cast samples, selected specimens were annealed at 350 °C under an Ar-atmosphere for 12 h to investigate the possible influence of initial free volume content on the shear band dynamics. From Fig. 4 it is evident that the annealed samples, tested at 25 °C, −10 °C and −40 °C, exhibit the same trend as the as-cast samples, and that the initial free volume content has little or no influence on the thermally-activated process governing the velocity of shear-band propagation. This may be explained by the fact that after the first operation of a shear band in both the as-cast and annealed samples the same high level of free volume is reached locally. There is hence no effect on the subsequent reactivation of the same shear band.

By assuming that in both boundary cases for calculating the shear band velocities considered here, the velocity is proportional to the characteristic shear strain rate $\dot{\gamma}$ associated with shear transformation zones, a classical rate equation can be directly applied to the results obtained,[5] i.e.,

$$v \propto \dot{\gamma} = \dot{\gamma}_0 \exp(-\Delta G / k_B T), \tag{1}$$

where $\dot{\gamma}$ is the shear rate, $\dot{\gamma}_0$ is the characteristic strain rate depending on the attempt frequency of the process, ΔG is the free energy barrier, k_B is the Boltzmann constant, and T is the temperature. Fitting the data obtained in Fig. 4 yields an activation energy of 0.3 ± 0.05 eV. Similar values were determined from simulation studies by Mayr[17] as well as Rodney and Schuh.[18] For a relatively low temperature of 10 K, Mayr found that for shear transformation zones (STZs) in a BMG, significant plastic relaxation was observed to occur at excitation energies of ∼0.32 eV. Similarly, Rodney and Schuh determined the activation energy distribution in a metallic glass showing peak frequencies near 0.4 eV. Despite the fact that the data presented in this work is obtained from the analysis of shear band dynamics and not from the behavior of spatially confined STZs at low temperatures, it is reasonable to assume that the underlying rate-limiting mechanism of a discrete shear event is based on STZ operation, which validates this comparison.

The activation energy determined in this work is also similar to the one associated with the transition from serrated to non-serrated flow.[19,20] While in the original works these activation energies could not be attributed to any underlying deformation mechanisms, it is now clear that the transition from serrated to non-serrated flow is governed by the thermal activation of shear banding in metallic glasses, whereby the critical combinations of temperature and test velocity identified in Refs. 19 and 20 directly reflect the temperature dependence of the SDJ velocity.

It is also important to note that the velocity values presented in this work represent the true steady-state, thermally equilibrated materials response, despite the highly dynamic behavior of the metallic glass. This is due to the fact that for a discrete shear event during serrated flow, deformation of the sample occurs under unconstrained conditions with respect to strain rate. This condition results from the fact that

the discrete macroscopic plastic strain is a consequence of the elastic recovery of the machine displacement, which occurs at velocities of the order of 10^3 m/s (i.e., the speed of sound), and is thus much higher than the SDJ velocities reported here. Additionally, from a comparison of the SDJ velocities to those modeled by Cheng *et al.*,[21] it becomes apparent that the influence of temperature rise leading to an autocatalytic acceleration of the shear band is insignificant, since the tests conducted here lie within the regime of "cold shear banding."

It is also noteworthy that similar behavior to that demonstrated in Fig. 4 has been observed for the shear band growth velocities in amorphous polystyrene[22] in which the mechanism of shear band operation occurs by a successively propagating shear front. For polystyrene the activation energy determined is approximately one order of magnitude higher and the shear band growth velocities are six orders of magnitude smaller than the corresponding quantities for the metallic glass investigated here over a comparable temperature range. Thermally-activated shear band dynamics therefore seems to be a common feature of amorphous materials even for different chemical bonding.

In summary, this study shows that the shear band velocity in a Zr-based metallic glass is strongly temperature dependent and exhibits an Arrhenius-type behavior within the temperature regime investigated. An associated activation energy of 0.3 ± 0.05 eV was determined, in good agreement with recent simulation studies. Further comparison of the shear band dynamics of metallic glasses with those of non-metallic amorphous materials is suggested.

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