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Dynamic properties of major shear bands in Zr–Cu–Al bulk metallic glasses

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ABSTRACT

We present a systematic investigation of shear-band dynamics as a function of chemical composition in the $Zr_xCu_{90-x}Al_{10}$ ($x = 45–65$) metallic glass system. We investigate aging dynamics in the non-serrated flow regime, shear-band velocities in the serrated flow regime, the transition between these two flow modes, and the transition from ductile to brittle behavior. We find that the activation energy for shear-band propagation is largely determined by the underlying time scales of the shear process, and that temperature-dependent stress drops only play a minor role. The activation energy as a function of composition can be linked to the bonding strength between the fastest diffusor, Cu, and its coordinating atoms, represented by the ratio of strong Cu–Zr to weaker Cu–Cu bonds. This indicates that the resistance to accelerated shear, i.e. the apparent activation barrier, is primarily controlled by a chemical nearest-neighbor effect.

1. Introduction

The amorphous structure of bulk metallic glasses (BMGs) possesses no translational symmetry or long-range order and consequently no lattice defects such as dislocations, which can mediate substantial amounts of plastic flow. Compared to crystalline metals, strain hardening or extended tensile ductility is also absent in BMGs. However, BMGs are by far less brittle than oxide glasses, because other inelastic processes can inhibit or delay crack initiation and propagation. It has been proposed that these processes proceed at the atomic scale and enable structural transitions via creation or annihilation of free volume [1], activation of shear transformations [2,3], or beta relaxations [4,5]. These atomistic processes facilitate the formation of narrow layers of strain-weakened material, known as shear bands [6], which for some BMGs efficiently absorb energy upon deformation and thus toughen the material. Thanks to shear-band formation, BMGs are for instance relatively flaw-insensitive, which is manifested by a large Weibull modulus [7,8]. In addition, considerable plastic deformation can be achieved under loading conditions other than uniaxial tension, e.g. bending [9–12], shearing [13], compression [14,15], or in fracture toughness measurements [16]. Deeper understanding of shear bands is therefore key to creating new design strategies for developing BMGs and BMG structures with improved mechanical properties, and motivates ongoing physical characterization of individual shear bands [17]. To this end, we have studied the dynamics of single shear bands under compression in the Zr–Cu–Al BMG system as a function of temperature and composition. More specifically, in this study we investigate (i) shear-band aging during non-serrated flow; (ii) the size and time scales of serrated flow; and (iii) the transitions from non-serrated to serrated flow and from ductile to brittle behavior. We explore the influence of chemical composition on the physics of shear-band propagation within the ternary Zr–Cu–Al BMG system. We subsequently compare the temperature-dependent shear-band dynamics of these alloys and relate them to several key BMG properties, namely glass transition temperature T_g, topology, bonding characteristics, and elastic constants. All these properties are believed to strongly influence the alloys' thermo-mechanical stability.

2. Inhomogeneous flow of metallic glasses

Before presenting the experimental details and results we will highlight selected aspects of the various inhomogeneous flow responses of BMGs, which will also form the basis of the subsequent analysis. For this purpose, Fig. 1 schematically depicts the dependence of malleability and flow response on temperature.

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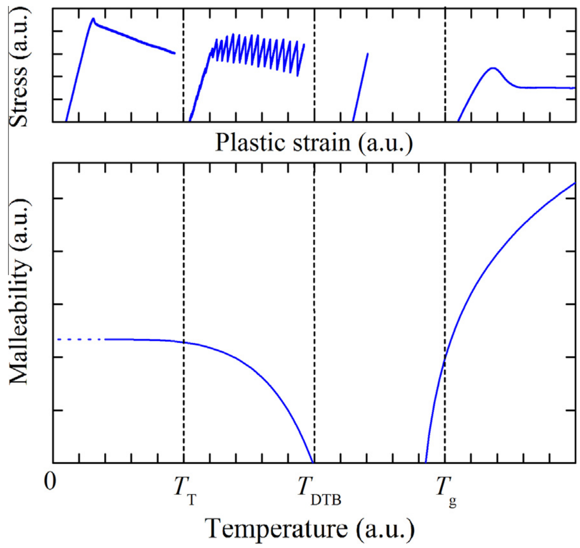

Fig. 1. Schematic plot of metallic glass malleability and flow behavior as a function of temperature. With increasing temperature, flow changes from inhomogeneous, non-serrated to inhomogeneous, serrated flow at the temperature T_T, becomes brittle above ambient conditions (i.e. above the ductile-to-brittle temperature T_{DTB}), and finally gains homogeneous malleability when approaching and crossing T_g.

2.1. Non-serrated flow

At liquid nitrogen temperature the quasi-static flow curves of BMGs are smooth (Fig. 1), and malleability is generally larger than under ambient conditions. Such non-serrated flow curves often show pronounced stress-overshoots upon yielding, meaning that the stress at which shear banding is initiated is considerably larger than the stress necessary to maintain the applied strain rate on the shear band. This feature also appears when plastic flow is interrupted, e.g. if the sample is unloaded and subsequently reloaded, or if the applied strain rate is set to zero for a given waiting time t_w. Such controlled interruptions are the basis of so-called slide-hold-slide experiments [18]. Stress overshoots $\Delta\sigma_A$ were found to scale with the logarithm of the waiting time [19]. This behavior is also known in the context of aging in the field of rate- and state-dependent friction [18], and analytically expressed by $\Delta\sigma_A = \beta\ln(1 + t_w/\tau)$, where β is a constant and τ is a characteristic time scale, promoting an increase in $\Delta\sigma_A$ when it decreases.

2.2. Serrated flow

Increasing the temperature (or lowering the applied strain rate) promotes a transition from smooth to serrated flow (Fig. 1). Shear bands are no longer constantly driven at the applied strain rate but show stick–slip behavior [20] with phases of fast propagation (slip) alternating with slow reloading phases (stick). One such cycle is referred to as a serration. It has been shown that the flow transition in various BMGs is thermally activated [21,22]. This means that for a given applied strain rate there is a certain temperature, here denoted as T_T, above which flow is serrated. The transition has been shown to originate from a time-scale match of test and aging dynamics [19,23].

The slip phases are characterized by stress drops and simultaneous strain bursts. Serrations may appear in sequences of irregularly sized stress drops which arise from geometrically constrained hardening, or very regularly during geometrically unconstrained, re-activated propagation of major shear bands [9,24]. Scaling behavior, i.e. a cumulative size distribution which follows a power law, has been reported for BMG serrations. The respective studies, however, did not consider in depth the impact of the degree of geometric constraints on these distributions [25–28].

Unconstrained propagation is associated with a single operating major shear band [23]. This makes it possible to calculate a shear-band velocity from the stress-drop size $\Delta\sigma_S$ (or the displacement jump Δu_0) and the event duration Δt, and to describe how fast shear offsets are generated by simultaneous shearing [29]. The derived shear-band velocities are also thermally activated [23,30,31] and exhibit activation energies which accord with those deduced from an assessment of the flow mode [22,32], as summarized in Fig. 2. The shear-band velocity is directly correlated with the critical strain rate necessary for the transition from serrated to non-serrated flow. The interpolated transition line is given in black. Blue diamonds represent the temperature-dependent shear-band velocities projected to the load axis. The good agreement of the data supports the view that the transition between serrated and non-serrated flow can be ascribed to competing time scales – one determined by the applied strain rate, and the other by the aging dynamics within the shear bands [19,23]. In other words, the shear-band velocity is a measure of how fast the applied strain rate must be in order to attain smooth flow conditions.

2.3. Embrittlement and homogeneous flow

With further increases in temperature the malleability of BMGs decreases drastically (Fig. 1), and the material becomes prone to immediate brittle failure above a certain temperature. This was shown, for example, for Au-based [33] and Zr-based [34] BMGs. This brittle behavior vanishes upon approaching T_g, at and beyond which point homogeneous non-Newtonian or Newtonian flow with the absence of shear bands occurs [34–36].

3. Experimental procedure

The experiments were conducted with $Zr_xCu_{90-x}Al_{10}$ BMGs, where x = 45, 50, 55, 60, and 65. Pre-alloys of the compositions were produced by arc-melting the constituent elements on a water-cooled copper hearth in a 6 N Ar atmosphere. Ten cycles of re-melting and flipping were performed in order to ensure the greatest possible chemical homogeneity. Rods of 2 mm diameter were then prepared via suction-casting in an arc melter in a 6 N argon atmosphere. X-ray diffraction (Struers Powder diffractometer) showed all compositions to be amorphous, and the samples

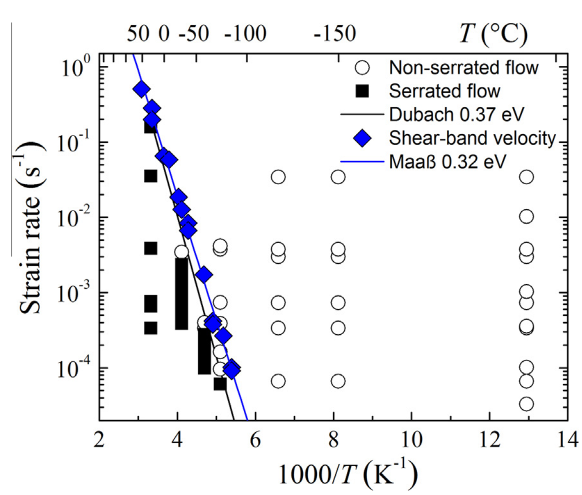

Fig. 2. Critical strain-rate map from Dubach et al. [22], extended by shear-band velocity data from Maaß et al. [23], illustrating the close correlation of the two phenomena of flow transition and shear-band velocity.