Acta Materialia 111 (2016) 273–282

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

Competition between shear band nucleation and propagation across rate-dependent flow transitions in a model metallic glass

Matthew B. Harris, Lars S. Watts, Eric R. Homer*

Department of Mechanical Engineering, Brigham Young University, Provo, UT, 84602, USA

A R T I C L E I N F O

Article history:
Received 22 January 2016
Received in revised form
12 March 2016
Accepted 24 March 2016

Keywords:
Metallic glass
Shear transformation zone
Modeling
Flow serration
Shear band

A B S T R A C T

Shear transformation zone (STZ) dynamics is used to examine the transition between different regimes of flow serration in the strain rate dependent deformation of metallic glass. To capture the strain rate independent yield strength of Vitreloy 1 at low to moderate strain rates, the model is adapted to include STZ volume and activation energy that decrease with increasing strain rate. The different stages of shear banding are examined in a statistical fashion over six different strain rates ranging from 10^{-5} to 10^{0} s^{-1}, with twelve replicates at each strain rate. Examination of flow serration, shear band nucleation rates, propagation rates, and sliding rates in each simulation find support for the hypothesis that the flow transition is caused by high shear band propagation and sliding rates at low strain rates, and high shear band nucleation rates at high strain rates. The underlying cause for the flow transition is hypothesized to be a strain rate dependent critical shear band nucleus size that increases with increasing strain rate. This critical shear band nucleus size results from the strain rate dependent STZ volume and activation energy, in which very small variations can cause a large change in shear banding behavior.

1. Introduction

Metallic glasses show great promise as lightweight, high-strength, flexible materials due to their impressive mechanical properties [1–3]. However, metallic glasses suffer from poor ductility at room temperature due to their tendency to localize plastic strain into shear bands [2,4,5], which ultimately lead to catastrophic failure. Interestingly, although the yield point of these materials is often independent of strain rate for rates up to 10^2–10^3 s^{-1}, the shear band density and degree of flow serration are highly strain rate dependent [6–8]. A thorough understanding of the mechanisms underlying this phenomena is necessary to enable the development of tougher, more ductile metallic glass composites and alloys.

The different modes of deformation, homogeneous and inhomogeneous, exhibited by metallic glasses are well characterized by examination of Schuh's deformation map, shown in Fig. 1 [6]. The homogeneous regime exists at elevated temperatures and lower strain rates, where the deformation is characterized by viscous flow. The inhomogeneous regime is characterized by localized deformation, typically in the form of shear bands. This regime encompasses temperatures below the glass transition temperature (T_g) at lower strain rates to a much larger temperature range at higher strain rates. Within the inhomogeneous regime, deformation at low strain rates is characterized by strongly serrated flow, meaning that strain accumulates in the material in temporal bursts accompanied by relaxation stress drops resulting in a jagged stress–strain curve [9,10]. Higher strain rates are characterized by moderately serrated flow, and very high strain rates have little or no flow serration. In nanoindentation experiments, Schuh and Jiang independently observed that this reduced flow serration was accompanied by a reduction in the appearance of shear steps in the surface of the material around the indenter [11,12]. At the lower strain rates, the plasticity is localized into only a few shear bands; at higher strain rates the plasticity is dispersed across many shear bands. It has been hypothesized that this change from few to many shear bands at increasing strain rate is due to competition between shear band nucleation and propagation [7]; when individual shear bands nucleate and propagate quickly relative to the strain rate, the stress in the surrounding material is reduced, suppressing additional shear band nucleation. However, when shear bands do not accommodate strain quickly enough to relieve stress in the material, multiple shear bands occur to reduce the stress.

The process by which individual shear bands nucleate,

* Corresponding author.
E-mail address: eric.homer@byu.edu (E.R. Homer).

http://dx.doi.org/10.1016/j.actamat.2016.03.066
1359-6454/

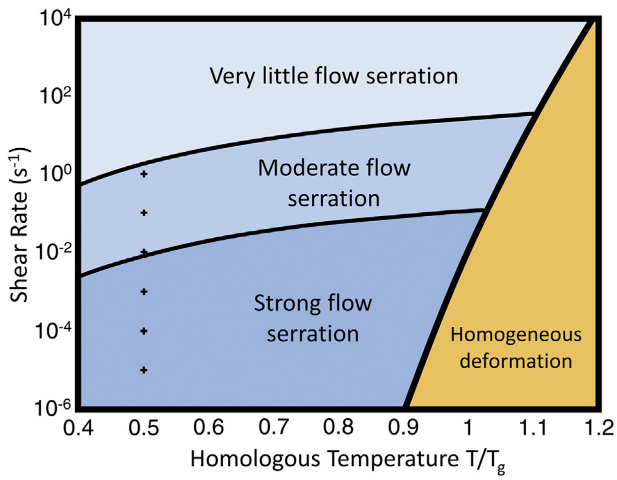

Fig. 1. General deformation map for metallic glasses as a function of homologous temperature and applied strain rate, adapted from Schuh [6]. Points investigated in this paper are marked with a '+' on the deformation map.

propagate, and arrest has been the subject of continued investigation. The explanation of this process begins with the fundamental unit of deformation in metallic glasses, which is accepted to conform to the shear transformation zone (STZ) theory introduced by Argon [13]. The STZ involves the collective and inelastic rearrangement of several dozen atoms in response to an applied shear stress. The action of one STZ causes an increase in the local stress field along the direction of shear, creating preferential sites for the activation of additional STZs [14,15]. Models applying Argon's STZ theory have differed on how shear bands form and propagate from an initial group of STZs, with three main viewpoints being most prominent. First, some model the shear band as a percolating boundary that reaches a critical concentration of STZs before initiating simultaneous slip along the plane of highest resolved shear stress [16]. Second, shear bands are modeled as a propagating zone of rejuvenated glass, followed by a zone of glue-like material, and finally followed by liquid material, as adiabatic heating decreases the local strength [17]. Third, others model a two-step process, with a shear band nucleating from a small cluster of STZs, and propagating quickly through the sample before initiating simultaneous slip [18,19]. Recent work by Qu et al. has shown that metallic glass samples pulled to very low levels of plastic strain show signs of partially propagated shear bands [20], lending further credibility to the second and third theories. The two-step theory, as explained by Homer, Schuh, Greer and others [6,15,18,19,21], can be subdivided into three stages for the progression of deformation in metallic glasses:

1. Nucleation: STZs activate, cluster, and make up the growing nuclei of competing shear bands
2. Propagation: When a shear band nucleus reaches a critical size, it begins to rapidly grow, dominating plasticity in the region
3. Sliding: Stress relaxation occurs as the fully developed shear band thickens and accumulates additional plasticity in the form of shear band slip, until the applied load decreases enough for slip to arrest

Once a shear band has arrested the free volume generated by the action of STZs remains and allows it to be preferentially reactivated [22–24]. In other works, stages 1 and 2 are generally referred to as shear band initiation, while stage 3 is referred to as shear band propagation. In this paper, shear bands are analyzed for their progression through all three stages. Stage 1, nucleation, ends when a shear band becomes dominant, stage 2 continues until the shear band reaches the full width of the simulation, and stage 3, sliding, encompasses all plasticity that takes place on the band after it is fully propagated.

Investigating the transition between different flow serration regimes requires a collection of shear band events to be studied in a statistical manner so an understanding can be gained of how the mechanics of shear band formation influence flow serration. Researchers have used several different approaches to resolve shear band events in experimental setups. For example, high-speed cameras have been able to capture shear band sliding, and measure shear band velocities [25]. They also show that flow serration is often the result of the same shear band being activated multiple times, rather than unique shear bands for each event [22]. Analysis of pop-in stresses during nanoindentation enabled estimation of STZ volumes and rate effects [26,27]. Although this information is very useful, such experimental methods are unable to reveal the details of what is happening at the STZ level in shear band nucleation and propagation; the time and length scales of individual STZs are too small and fast for current measurement resolutions to capture directly, and indirect measurements do not give a complete picture.

Modeling techniques provide unique insight into the possible processes of shear band formation. Atomistic simulations do well at simulating the action of individual STZs, capturing the onset of shear localization in metallic glass [28]. They can measure the STZ volume for various glass compositions, and have shown that the instability of shear bands arises from structural disordering in an STZ, rather than thermal softening [19,29]. Constitutive models do well at recreating the macroscopic behavior of metallic glass. By treating the glass as a continuum material, rather than trying to simulate each individual atom or STZ, they enable more complicated structures and loads to be modeled, within the limits of the constitutive model's scope [30,31]. Mesoscale models are needed to investigate the range of time and length scales intermediate to molecular dynamics and constitutive models [28]. One such mesoscale model is the STZ dynamics model developed by Homer and Schuh [32]. The STZ dynamics model is able to capture a broad range of time scales associated with shear band events in an efficient manner by using a kinetic Monte Carlo algorithm [14]. It has been used to simulate both 2D and 3D metallic glass structures; it predicts a propagating shear band, and captures the transition from inhomogeneous to homogeneous flow at the glass transition temperature [21,33]. It has even been adapted by Li to account for free volume generation due to STZ activity [34]. Since this model is capable of simulating the nucleation and growth of multiple shear bands, and these are the parameters of interest, we use the STZ dynamics model for our investigation of flow serration regimes in metallic glasses.

In this work, the STZ dynamics model is adjusted to maintain a constant yield point over strain rates of 10^{-5}–10^{0} s^{-1}, consistent with the behavior of Vitreloy 1, and other metallic glasses [6,8,35]. With the adjusted model parameters, we examine flow serration and the early stages of shear band nucleation and propagation across a range of strain rates, with multiple simulations at each strain rate to determine statistical variance. Discussion of the results shows support for the hypothesis of competing shear band nucleation and propagation rates, and is focused on determining the underlying causes of this interaction. A hypothesis is developed to explain the simulated behaviors, and its implications are explored in the conclusion.