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Examining the initial stages of shear localization in amorphous metals

Eric R. Homer

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

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Abstract

A mesoscale simulation by shear transformation zone (STZ) dynamics is used to analyze the initial stages of shear localization in amorphous metals, of which many details remain unresolved due to the difficulty in accessing the appropriate time- and length-scales. Examination of a constant strain-rate tensile test of a model amorphous metal reveals four different stages in the microscopic processes that lead to formation of a shear band. These stages are identified as: (i) STZ clustering, where potential nucleation sites form as STZ activations cluster in space; (ii) growth following nucleation, where a nascent shear band exhibits a propagating front that defines the shear band path; (iii) relaxation thickening, where the shear band thickens and relaxes the system down to the flow stress; and (iv) flow thickening, where the shear band exhibits prolonged thickening at the flow stress. The results are consistent with the literature but suggest that a shear band is defined by a front that propagates very quickly with negligible accumulated strain. This propagating front likely occurs below the resolution of current methods that only observe simultaneous slip in a shear band where significant strain can be accumulated at much slower rates. Analysis of a thermodynamic model also suggests a specific critical stress that is required to nucleate a shear band, after which the shear band is allowed to grow unconstrained.

Keywords: Metallic glass; Shear bands; Micromechanical modeling; Nucleation; Shear transformation zone

1. Introduction

Despite several decades of research, the poor ductility in amorphous metals continues to be one of the primary factors impeding their adoption in structural applications. These metals are particularly attractive because their inherent lack of structure can lead to impressive values of the yield strength, among other notable properties [1]. However, these metals usually fail catastrophically upon yield when pulled in tension, or exhibit little to no strain hardening when compressed. Recent advancements in glass composition [2–6], amorphous matrix–crystalline composites [3,7–13] and even cold work [14–16] have lead to considerable improvements in ductility, but have not addressed the underlying cause behind the nucleation, formation and propagation of shear bands. Once a shear band nucleates, there is very little that can stop its propagation. Thus, if ductility is to be improved, the very earliest stages of nucleation and shear band formation must be better understood.

The underlying unit of deformation in amorphous metals is believed to be the shear transformation zone (STZ), which involves the collective and inelastic shearing of a group of atoms [17]. In his original proposal of the STZ, Argon suggested that the repeated activation of shear events (STZs) at neighboring sites leads to bifurcation of the accumulated strain and, ultimately, formation of a shear band [17]. In more recent work, Schuh et al. suggested that multiple processes are involved in shear band formation, namely: individual STZ activations, formation of STZ clusters into a nucleus, and the transition of the nucleus into a full shear band [18]. These theories are supported by other similar works that suggest that shear bands are formed through stress-assisted nucleation events [19,20].

The challenge in proving these theories and actually measuring the nucleation and propagation of shear bands

E-mail address: eric.homer@byu.edu

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is one of time- and length-scales. Shear bands tend to propagate over 10^{-6} m distances [18,21,22] on 10^{-3} s time-scales [23–27], while maintaining a thickness of $\sim 10^{-8}$ m [28,29]. The process of shearing the fundamental unit of deformation (STZ) typically involves volumes of $\sim 10^{-27}$ m^3 on timescales of 10^{-12} s [17,30–34]. Thus, full investigation of nucleation and propagation requires the ability to access a very wide range of time- and length-scales, whether by one or more methods.

Due to the challenge of resolving the earliest stages of shear banding, some experimental works focus on statistical analysis of numerous shear band events to infer information about nucleation and the early formation stages [18,27], while others directly observe shear band events during propagation [25,35–41]. For example, instrumented nanoindentation and compression experiments are able to access load–displacement data on time-scales down to 10^{-4}–10^{-5} s [42,43] and 10^{-6} s [24], respectively. The result is inference about certain statistics such as critical nuclei dimensions in the range 10^{-8}–10^{-6} m [18,44,45]. Recent high-speed cameras have even improved direct observation of shear bands to frame rates as high as 5000 s^{-1} [25] and 12,500 s^{-1} [41]. Thus, experiments provide important details about specific parts of the shear band process, but the associated time- and length-scales still limit resolution of the earliest stages of nucleation.

To resolve these very limited time- and length-scales, modeling techniques, such as atomistic methods, provide detailed information about the nanoscale motions associated with deformation in amorphous metals. These methods have been integral to resolving the atomic motions, energetics and operating conditions surrounding individual STZs [30–32,46–48] as well as the structural evolution and other effects that influence shear band formation [33,34,47,49–60]. However, due to time- and length-scale limitations (typical dimensions in the range 10^{-8}–10^{-7} m and durations in the range 10^{-9}–10^{-8} s) [34], atomistic simulations have difficulty accessing experimentally relevant deformation rates and times.

Thus, one can turn to mesoscale approaches, which provide methods for bridging the time- and length-scales surrounding the initial stages of shear localization [34,61–65] while preserving the ability to examine the microscopic states that lead to the deformation and shear localization.

In general, the mesoscale approach coarse-grains a system into an ensemble of potential plastic events such as the STZ. The activation of these events is then controlled by an algorithm, such as the kinetic Monte Carlo (kMC) algorithm, and the stochastic activation of numerous individual events leads to macroscopic deformation of the sample. Recent work by the author extended the lattice-based, Green's function solution STZ model of Bulatov and Argon [61] to a finite-element-based STZ model to enable the observation of macroscopic deformation. The flexibility of the framework, referred to as STZ dynamics, has enabled investigation of deformation in two and three dimensions [64,66], correlations between STZs [67], the effects of cyclic strengthening [68] and nanoscale strength distributions [69].

In this work, STZ dynamics is used to examine shear localization in a model nanowire with a specific focus on the earliest stages of the localization. The work details the progression of the deformation starting from potential nucleation sites or clusters of STZs, then nucleation of the shear band and the various stages of propagation that follow. The conditions surrounding nucleation are then analyzed in the context of a thermodynamic model. Together, the simulation results and analytical model provide a detailed examination of the early stages of shear band nucleation and formation, which is discussed in the context of the available literature.

2. Modeling approach

As mentioned previously, the STZ dynamics modeling framework is based on the stochastic operation of coarse-grained STZs. In this framework the STZ mechanism, which represents the collective and inelastic shearing of atoms in response to an applied shear stress, is modeled by applying strains to groups of elements in a finite-element mesh that represent the collections of atoms or STZs. The stress and strain distributions that result from the shearing of STZs are then solved using finite-element analysis (FEA). The entire system is controlled by a modified-kMC algorithm, where individual STZs are selected for shearing based on their local propensity (activation rate), which can be biased by the local stress state. Loading conditions are applied according to standard FEA methods.

The propensity for a given STZ to be activated is based on its activation rate, $\dot{s}$. The activation rate for an STZ to shear in one direction is given by:

$$\dot{s} = v_o \cdot exp\left(-\frac{\Delta F - \frac{1}{2}\tau \cdot \gamma_o \cdot \Omega_o}{kT}\right), \tag{1}$$

where v_o represents the attempt frequency along the reaction pathway (determined from the Debye temperature), ΔF gives the intrinsic barrier height of the STZ transition, which can be biased by the local shear stress, τ, acting on an STZ of volume Ω_o, as it attempts to shear by the magnitude γ_o. The thermal energy in the system is given by kT where k is Boltzmann's constant and T is the temperature. Additional detail regarding the energetics of this equation is available in Ref. [67] and the generalization of Eq. (1) to three dimensions involves the consideration of all unique combinations of shear planes and directions as detailed in Ref. [66].

The modified-kMC algorithm used here differs from the standard kMC approach in that events, or STZ activations, that would occur on time-scales greater than a maximum allowed time step are suppressed and the system simply increments time by the maximum allowed time step without shearing any STZ in that step [68]. Whether an STZ is sheared or not, the system is incremented by the