

Mesoscale modeling of amorphous metals by shear transformation zone dynamics

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Abstract

A new mesoscale modeling technique for the thermo-mechanical behavior of metallic glasses is proposed. The modeling framework considers the shear transformation zone (STZ) as the fundamental unit of deformation, and coarse-grains an amorphous collection of atoms into an ensemble of STZs on a mesh. By employing finite element analysis and a kinetic Monte Carlo algorithm, the modeling technique is capable of simulating glass processing and deformation on time and length scales greater than those usually attainable by atomistic modeling. A thorough explanation of the framework is presented, along with a specific two-dimensional implementation for a model metallic glass. The model is shown to capture the basic behaviors of metallic glasses, including high-temperature homogeneous flow following the expected constitutive law, and low-temperature strain localization into shear bands. Details of the effects of processing and thermal history on the glass structure and properties are also discussed.

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1. Introduction

Amorphous metals exhibit a rich diversity of deformation behavior, with significant differences from classic crystalline deformation behavior [1,2]. For example, at high homologous temperatures amorphous metals behave as supercooled liquids and display homogeneous deformation that is Newtonian over a broad range of low stresses. At somewhat higher stresses their rheology becomes non-Newtonian, but follows an exponential stress dependence rather than the power-law common to crystalline metals. On the other hand, at low temperatures and high stresses, amorphous metals deform in a highly inhomogeneous fashion where plastic strain tends to localize into nanoscale shear bands that encourage catastrophic failure.

Central to understanding this diverse behavior in amorphous metals are the deformation mechanisms that act on a microscopic level. The shear transformation zone (STZ)

proposed by Argon [3] has emerged as a useful mechanistic picture in which the unit process of deformation is a collective motion of a few atoms that rearrange to achieve a characteristic shear strain, γ_0 , under an applied shear stress, as shown in Fig. 1. The STZ is viewed as a stress-biased, thermally activated event, permitting simple rate laws for STZ activation to be written in terms of state variables, including stress, temperature and local structural order parameters such as free volume [4]. One advantage of defining a unit STZ process in this way is that by appropriately modeling the dynamics of these events, one may overlook the local details of individual atomic motions, while still capturing the fundamental physics of deformation. For example, by assuming that STZs operate independently of one another, one can readily calculate the average behavior of STZs in the system. This approach yields an analytical solution for the steady-state flow law of a homogeneously deforming amorphous metal, with a hyperbolic-sine stress dependence that is commonly seen in experiments [1,5].

On the other hand, the more complex and interesting behaviors associated with shear localization and fracture,

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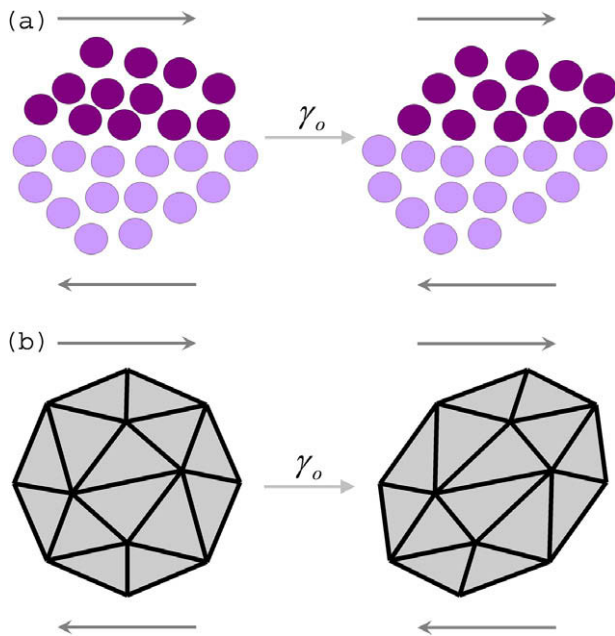


Fig. 1. (a) Shear transformation zone, or STZ, where several dozen atoms shear inelastically under an applied shear stress; (b) an idealization of an STZ on a continuum mesh.

for example, require the collective action of many STZs, which may no longer be assumed to operate independently of one another. In this situation, the rate law for STZ activation must be supplemented with details of how STZs interact, and how their operation redistributes stress and free volume in the system [4]. Without a priori knowledge of STZ interactions, there is as yet no clear connection between local atomic motions and the macroscopic deformation behavior of amorphous metals undergoing shear localization [6].

A further difficulty for modeling strain localization in amorphous metals is that the process involves time and length scales that span many orders of magnitude. For example, local atomic motions, including STZ activation, occur on a timescale of about 10^{-12} – 10^{-11} s, while shear band formation occurs over periods of 10^{-5} – 10^{-3} s in experiments [7,8]. Similarly, shear band thickness is usually found to be of order 10^{-8} – 10^{-7} m [9,10], with typical shear offsets that can be much larger, 10^{-6} m or greater [11,12]; both of these values are much larger than the size of an STZ at $\sim 10^{-10}$ – 10^{-9} m [13,14]. These facts suggest that shear band formation involves a slow cooperative process involving a great many STZs.

This disparity in time and length scales creates difficulties for clean experimentation, and even more for modeling the full range of glass behaviors under experimentally relevant conditions. For example, molecular dynamics simulations exquisitely track atomic motion [15–25], but are intrinsically limited to small length scales and, more importantly, to very short time scales. This restricts their ability to capture large-scale events that occur on long time scales, including glass formation by cooling from the melt at

experimental rates. Although shear localization is seen in many atomistic simulations of amorphous systems [24,26–31], it generally requires very driven systems that cannot be easily compared to experiments. On the other hand, continuum simulations have the ability to access much larger system sizes and longer time scales through the development of constitutive relations and the use of finite element analysis (FEA) [32,33]. These models are especially powerful for modeling complex geometries with realistic boundary conditions, but they are limited by the constitutive relationships on which they are constructed, which can only capture the specific physics that they have been designed to model.

In order to access deformation behavior intermediate to these two modeling techniques, there is a need for meso-scale models based upon an ensemble of characteristic events such as the STZ. A coarse-graining approach of this type was proposed by Bulatov and Argon [34], who developed a lattice STZ model in which each lattice element represented a single potential STZ. The activation or shearing of any single STZ led to the redistribution of stress and strain in the system, which in turn affected the rate of activation for subsequent STZ operations. The selection of STZs for activation and the time evolution of the system were controlled through a kinetic Monte Carlo algorithm [34–36]. This model reproduced both homogeneous and inhomogeneous modes of deformation and accessed significant time scales. One clear limitation of this model, however, involved the use of a fixed lattice geometry, which cannot capture the spatial evolution, or shape change, of the system. In addition, Bulatov and Argon's use of Green's functions to determine the stress and strain distributions in the system improved computational efficiency but limited their ability to model complex geometries and stress states.

The purpose of this paper is to develop a new mesoscale modeling technique that we term “STZ dynamics” modeling. This approach considers STZ activation as a stochastic, stress-biased, thermally activated event which obeys a specific rate law and uses the kinetic Monte Carlo method to control the evolution of the system. We employ FEA to solve the elastic strain distribution in the system, by which the STZs communicate with one another. In this manner, we are able to access longer time and length scales than those associated with atomic motions. Our model takes its inspiration from the lattice model of Bulatov and Argon [34], but expands upon it in the sense that our use of FEA permits arbitrary shape changes, complex geometries and boundary conditions, greater freedom in the definition and activation of STZs, and a close connection to experimental conditions. In this paper, we present our basic methodology, then proceed to develop a specific two-dimensional implementation as a demonstration of the method. We explore the thermal response and effects of processing, the rheological nature of deformation at high temperatures and shear localization at low temperatures. Lastly, a compilation of data from many simulations is

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