Uniaxial tensile test on an amorphous solid with embedded quasi-crystallites: a molecular dynamics study

Y.F. Shi, M.L. Falk*

Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI 48109–2136, USA

Abstract

Molecular dynamics simulations of uniaxial tension in a two-dimensional model of a metallic glass exhibit shear localization. The structure of this model system is characterized based on the short range ordering, arising from the underlining quasi-crystalline packing order. Atoms with quasi-crystalline order cluster together to form quasi-crystallites, which embed inside the amorphous matrix. Regions of the sample with quasi-crystalline order tend to have more resistance to deformation, while regions with pure amorphous structure tend to deform more easily. The existence of quasi-crystallites inside the glass, and their evolution during deformation, appears to induce the instability of shear banding in this system.

Keywords: Molecular dynamics; Amorphous; Quasi-crystal; Shear localization; Shear bands; Metallic glasses; Uniaxial tension

1. Introduction

Metallic glasses can be produced by a variety of processing routes, ranging from casting at relatively low cooling rates of a few K per second in the case of bulk glass formers [1,2] to splat quenching at elevated cooling rates [3] to ion beam assisted deposition, an extremely energetic non-equilibrium process [4]. Since glasses, unlike crystals, do not naturally conform to a small number of identifiable and well-defined ground state structures, it is generally expected that they can exhibit a range of mechanical properties depending on processing.

Localization plays an important role in the mechanical response of metallic glasses. Particularly under uniaxial tension the tendency to localize can result in dramatic failure via fracture along a single shear band [5]. This failure mode can prevent any apparent hardening in tension, limiting the structures in which metallic glasses can be employed as structural materials.

Recently a number of investigations have shown nano-scale crystallites and quasi-crystalline order in BMG formers. The quasi-crystallites in Zr-based metallic glasses appear not only to stabilize the glassy state [6,7], but also to enhance the ductility and strength of the glass [8]. Furthermore, icosahedral clusters could be a fundamental building block for liquids and glasses [9]. In this work, we seek to relate the atomic structure, particularly the short range ordering (SRO), to the mechanical properties of a model metallic glass former.

2. Sample preparation and testing

We have performed two-dimensional molecular dynamics simulation on a binary alloy that consists of two species, which we will refer to as S and L for small and large, interacting via a Lennard-Jones potential of the form. The system contains 20 000 atoms. We chose our composition, $N_L{:}N_S = (1+\sqrt{5}){:}4$ to be consistent with other studies of this system. The glass transition temperature (T_g) of this system is known to reside approximately $0.325\ \epsilon_{SL}/k$, where ϵ_{SL} is the energy well depth for interaction between S and L atoms, and k is the Boltzmann factor. For the sake of comparison, temperatures will be measured in units of T_g. A detailed description of the simulation methodology is given in [10].

The sample was created by starting from supercooled liquids equilibrated at about $1.08T_g$. Subsequent to equilibration the temperature of the liquid was reduced to 9.2% of T_g. The quenching rate in this report is

* Corresponding author. Tel.: +1 734 615 8086; Fax: +1 734 763 4788; E-mail: mfalk@engin.umich.edu

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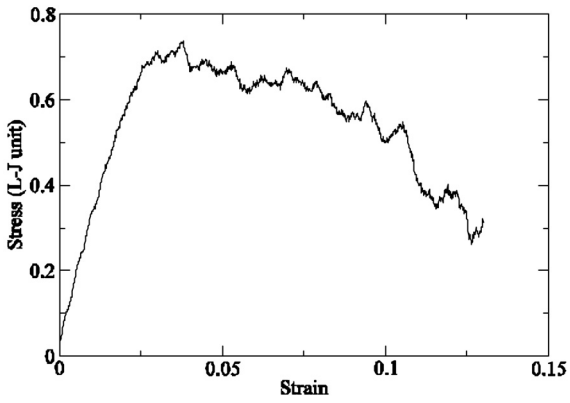

Fig. 1. Stress–strain curve for a model glassy sample in a uniaxial tensile test.

1.97×10^{-4} T_g/t_0, where t_0 is the internal Lenard-Jones time unit which is approximately an atomic vibration period [10]. During the uniaxial tensile test the top and bottom boundaries were maintained as periodic boundaries. The left and right boundaries were free surfaces. The strain was imposed by rescaling the boundaries and the positions by a small amount in the yy direction at each time step at a constant strain rates of 10^{-4} $(1/t_0)$.

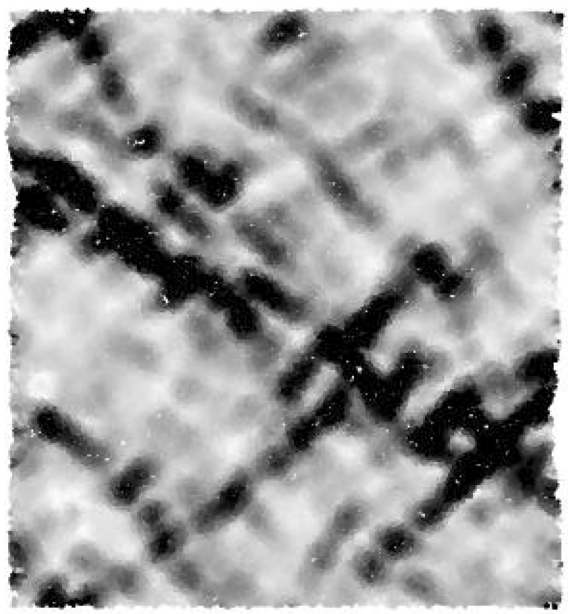

Fig. 2. Deformation mapping for a glassy sample at 5% strain in a uniaxial tensile test. Black corresponds to 10% deviatoric strain, white corresponds to 0% deviatoric strain. Load is applied in y-direction and x-surfaces are stress free.

3. Results

Figure 1 shows the stress–strain curve for a uniaxial tension test of a model glassy sample. Stress appears to be increasing linearly with strain at strains up to 2%, after which the sample undergoes plastic yielding. Serrated flow is evident which corresponds to individual nucleation or propagation of shear bands. Figure 2 shows the distribution of local deviatoric strain, which we call deformation mapping, at 5% strain. The deviatoric strain is extracted through a procedure described in [10]. Shear bands are forming at about 45° with respect to the loading direction, which corresponds to the maximum shear stress direction.

Now we examined the dependence of the localization on the atomic scale structure of the samples. To accomplish this we have adapted an analysis from [11] that utilizes the fact that this system has an underlying quasi-crystalline state that can be entropically stabilized. Although the quasi-crystalline states are not the true ground state [12], their energies are only slightly higher than the crystalline states and are certainly energetically more favorable over the amorphous state. In [11] it was noticed that the quasi-crystal is composed of nine local atomic motifs. We refer to atoms which reside in one of those motifs as stable atoms and to other atoms as unstable atoms. However, during a mechanical test, atoms could frequently transit from a stable state to an unstable state or vice versa. In order to minimize the fluctuations in determining the structural identity, we further divide all atoms, using their first shell neighbors, into four stability classes: S-atoms (stable atoms with all stable neighbors), s-atoms (other stable atoms), U-atoms (unstable atoms with all unstable neighbors), u-atoms (other unstable atoms). Therefore quasi-crystallites are composed of S-atoms, while purely amorphous material consists of U-atoms. By this analysis it is apparent that the uniform glassy sample is in fact structurally heterogeneous and contains regions of short range ordering.

Next, the probabilities of deformation for each atom with respect to its stability class are shown by cumulative shear histogram in Fig. 3. The value on the graph shows the fraction of atoms of a particular class that have undergone deformation equal to or less than the strain denoted on the x-axis. Therefore, the cumulative histograms show that 80% of S-atoms have a deviatoric shear strain smaller than the nominal strain as opposed to 73% of s-atoms, 70% of u-atoms and 62% of U-atoms. Not surprisingly, the most stable atoms, S atoms, have the lowest probability to deform; the most unstable atoms, U-atoms, have the highest probability to deform. However, due to the fluctuation of the local stress state and the stochastic nature of plastic deformation, quasi-crystallites may deform and pure amorphous regions do not all deform.

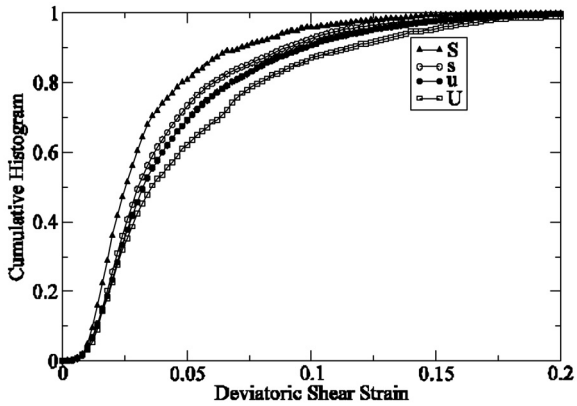

Fig. 3. Cumulative shear histogram for all atoms of a glassy sample at 5% strain. The atoms are classified to four groups based on their stable structure type at 0% strain.

4. Conclusions

A number of the stable metallic glass formers, such as Zr-based metallic glasses, precipitate quasi-crystals upon annealing. It has been proposed that small regions with quasi-crystalline order may be important for the stability of the amorphous state in these glasses [6,7]. In addition it has been asserted that deformation takes place primarily in the amorphous region of the material [13]. In our model system we have observed that the dispersed quasi-crystalline arrangements play a critical role in controlling the qualitative nature of deformation in the material. The structurally stable atoms tend to have greater resistance to deformation. During plastic deformation, the conversion of material from stable state to unstable state may play a crucial role in the softening process that leads to the shear banding instability. However, it remains unclear whether this is true for all metallic glasses, or only those in which the stability of the amorphous phase arises from an underlying quasi-crystalline phase.

Acknowledgments

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