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Slow relaxation dynamics in binary glasses during stress-controlled, tension-compression cyclic loading

Nikolai V. Priezjev*

Department of Mechanical and Materials Engineering, Wright State University, Dayton, OH 45435, United States
National Research University Higher School of Economics, Moscow 101000, Russia

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ABSTRACT

The effect of cyclic loading on relaxation dynamics and mechanical properties of metallic glasses is studied using molecular dynamics simulations. We consider the Kob-Andersen three-dimensional binary mixture rapidly cooled across the glass transition and subjected to thousands of tension-compression cycles in the elastic range. It was found that during cyclic loading at constant pressure, the system is relocated to progressively lower levels of the potential energy, thus promoting greater densification and higher strength. Furthermore, with increasing stress amplitude, the average glass density increases and the minimum of the potential energy becomes deeper, while the elastic modulus is reduced. The typical size of clusters of atoms with large nonaffine displacements becomes smaller over consecutive cycles, which correlates with the gradual decrease in the potential energy. These results are important for thermomechanical processing of metallic glasses with improved mechanical properties.

1. Introduction

Understanding the quantitative correlation between atomic structure and mechanical and physical properties of amorphous materials such as metallic glasses is important for various structural and biomedical applications [1]. It is commonly accepted that deformation of amorphous materials occurs via a series of sudden rearrangements of small groups of particles often called shear transformation zones [2–4]. Interestingly, it was recently demonstrated that the shear modulus as well as local shear transformations can be accurately predicted using the 'flexibility volume', a parameter that combines the information of both static atomic volume and thermal vibrations [5]. The results of atomistic simulations of cyclic nanoindentation of metallic glasses have revealed hardening effects that arise due to local stiffening and densification of the region containing the original yielding path [6–9]. It was also shown that upon cyclic compression, an amorphous frictional granular matter approaches an asymptotic configuration with maximal volume fraction, and the universal reduction in dissipation is determined by frictional losses and changes in the neighbor list [10,11]. However, the influence of complex deformation protocol and sample preparation history on fatigue lifetime, structural changes, and yielding requires further investigation.

Recent molecular dynamics simulation studies of the fatigue mechanism in metallic glasses under tension-compression, strain-controlled cyclic loading revealed that a shear band is initiated at the sample surface due to a slow accumulation of shear transformation zones, followed by a relatively quick propagation of a shear band across the sample [12,13]. In contrast, the results of atomistic simulations of metallic glasses under the uniaxial stress-control mode have shown that the plastic deformation in small-size samples proceeds via network-like shear-transition zones [14]. Furthermore, it was demonstrated that low-cycle fatigue tests on metallic glass nanowires result in work hardening or softening, depending on the applied load, and, after strain-dependent microscopic damage accumulation, a shear band forms rapidly [15,16]. More recently, it was also found that well-annealed metallic glasses, subjected to periodic compressive stress below yield, exhibit softening with either decreasing cycling frequency or increasing stress amplitude [17]. Despite extensive efforts, however, how exactly the yielding transition and shear band formation depend on the cyclic loading conditions (stress versus strain controlled), frequency, and system size remains not fully understood.

In recent years, the mechanical response of amorphous materials subjected to periodic shear was extensively studied using either athermal, quasistatic [18–24] or finite temperature [25–33] molecular dynamics simulations. Under cyclic loading, athermal systems were shown to settle into the so-called limit cycles, where all particles return to their positions after one or several shear cycles [19,20]. Moreover, the number of shear cycles required to reach a steady state increases upon approaching the yield strain from below [18–20]. Above the yield point, periodic deformation of well-annealed glasses results in sudden

* Address: Department of Mechanical and Materials Engineering, Wright State University, Dayton, OH 45435, United States.
E-mail address: nikolai.priezjev@wright.edu.

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formation of a system-spanning shear band after a number of transient cycles and in an increase of the potential energy [12,22,29]. Remarkably, it was recently demonstrated that in contrast to dense amorphous systems, where the yielding transition is associated with a drop of the elastic modulus and enhanced particle diffusion, weakly jammed solids exhibit two-step yielding process; namely, softening at intermediate strain amplitudes and the onset of diffusion at distinctly larger yield strain [30].

In this paper, we investigate mechanical properties and structural relaxation dynamics of poorly annealed binary glasses under periodic tension-compression, stress-controlled loading using molecular dynamics simulations. It will be shown that during several thousand cycles in the elastic range, the amorphous systems continue to explore progressively lower potential energy states and become more dense. The slow relaxation process is associated with small-scale irreversible particle rearrangements that are facilitated by the applied loading. As the stress amplitude increases, the average glass density becomes larger and both the potential energy and elastic modulus are reduced.

The rest of the paper is structured as follows. The details of the molecular dynamics simulation model and the stress-controlled cyclic loading protocol are described in the next section. The numerical results for the time dependence of the potential energy, glass density, and elastic modulus as well as the analysis of nonaffine displacements are presented in Section 3. The main results are briefly summarized in the last section.

2. Details of MD simulations

Molecular dynamics simulations are carried out on a glass former that consists of the non-additive binary mixture (80:20) first introduced by Kob and Andersen (KA) [34] to study properties of the amorphous metal alloy $Ni_{80}P_{20}$ [35]. In this model, the interaction between atoms of types $\alpha, \beta = A, B$ is given by the pairwise Lennard-Jones (LJ) potential:

$$V_{\alpha\beta}(r) = 4\varepsilon_{\alpha\beta}\left[\left(\frac{\sigma_{\alpha\beta}}{r}\right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r}\right)^{6}\right], \tag{1}$$

where $\varepsilon_{\alpha\beta}$ and $\sigma_{\alpha\beta}$ are the energy and length scales of the LJ potential [36]. The interaction parameters for both types of atoms are chosen as follows: $\varepsilon_{AA} = 1.0$, $\varepsilon_{AB} = 1.5$, $\varepsilon_{BB} = 0.5$, $\sigma_{AB} = 0.8$, $\sigma_{BB} = 0.88$, and $m_A = m_B$ [34]. In addition, the cutoff radius is set to $r_{c,\alpha\beta} = 2.5\sigma_{\alpha\beta}$ to improve computational efficiency. All physical quantities are expressed in the reduced LJ units of length, mass, energy, and time, which are defined as $\sigma = \sigma_{AA}$, $m = m_A$, $\varepsilon = \varepsilon_{AA}$, and $\tau = \sigma\sqrt{m/\varepsilon}$, respectively. The total number of atoms throughout the study is $N_{tot} = 40,000$. The equations of motion were integrated using the velocity Verlet algorithm [36] with the time step $\triangle t_{MD} = 0.005\tau$ using the LAMMPS numerical code [37].

We next describe the preparation procedure and the stress-controlled deformation protocol at constant pressure. The system was initially equilibrated at the temperature $1.1\varepsilon/k_B$ and constant volume, which corresponds to the atomic density $\rho = \rho_A + \rho_B = 1.2\sigma^{-3}$. Here, k_B denotes the Boltzmann constant. This temperature is well above the glass transition temperature of the KA model at the density $\rho = 1.2\sigma^{-3}$ [34]. In the next step, the temperature was instantaneously reduced to $T_{LJ} = 0.1\varepsilon/k_B$ below the glass transition, and the pressure along the $\hat{x}$ and $\hat{y}$ directions was set to zero. In contrast, the normal stress along the $\hat{z}$ direction was varied periodically with the period of oscillations $T = 500\tau$. More specifically, the normal stress σ_{zz} was changed piecewise linearly as follows: from 0 to σ_{zz}^{max} during $T/4$, from σ_{zz}^{max} to $-\sigma_{zz}^{max}$ during $T/2$, and from $-\sigma_{zz}^{max}$ back to 0 during $T/4$. Thus, the average of σ_{zz} over the oscillation period is zero, and the system was subjected to 5000 stress-controlled, tension-compression cycles. In all simulations, periodic boundary conditions were applied along the $\hat{x}$, $\hat{y}$, and $\hat{z}$ directions. The data for the potential energy, stresses, system dimensions, and atomic configurations were collected in one sample for the post-processing analysis (see Fig. 1).

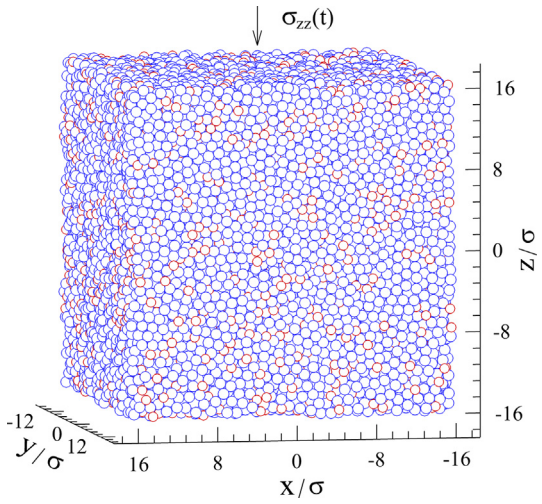

Fig. 1. A snapshot of the Lennard-Jones binary glass ($N_{tot} = 40,000$) after the quench to the temperature $T_{LJ} = 0.1\varepsilon/k_B$. The time-dependent stress $\sigma_{zz}(t)$ is applied along the $\hat{z}$ direction, while the normal stresses along the $\hat{x}$ and $\hat{y}$ directions are kept constant (see text for details). Note that atoms of types *A* and *B* (indicated by blue and red circles) are now shown to scale. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

3. Results

As described in the previous section, the normal stress in the $\hat{z}$ direction was applied piecewise linearly in time with the oscillation period $T = 500\tau$. As an example, the actual stress σ_{zz} measured in MD simulations during the first 5 cycles after the thermal quench to the temperature $T_{LJ} = 0.1\varepsilon/k_B$ is presented in Fig. 2 for two values of the stress amplitude. As expected, it can be seen that the stress variation is linear with superimposed fluctuations during the consecutive time intervals. Note also that in the case $\sigma_{zz}^{max} = 0.8\varepsilon\sigma^{-3}$, the stress becomes slightly smaller than the value $-0.8\varepsilon\sigma^{-3}$, when the sample is at maximum tension. It should be emphasized that due to periodic boundary conditions in the transverse directions, it is expected that a shear band

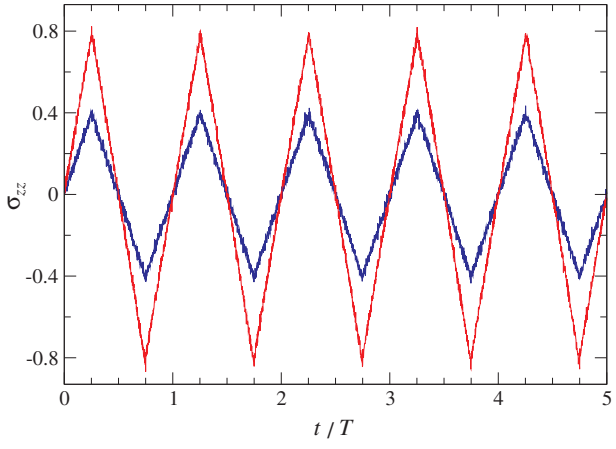

Fig. 2. The time series of the normal stress σ_{zz} (in units of $\varepsilon\sigma^{-3}$) during the first 5 periods after the thermal quench to the temperature $T_{LJ} = 0.1\varepsilon/k_B$. The stress amplitude is $\sigma_{zz}^{max} = 0.4\varepsilon\sigma^{-3}$ (blue lines) and $\sigma_{zz}^{max} = 0.8\varepsilon\sigma^{-3}$ (red lines). The oscillation period is $T = 500\tau$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)