



# The yielding transition in periodically sheared binary glasses at finite temperature



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## ABSTRACT

Non-equilibrium molecular dynamics simulations are performed to investigate the dynamic behavior of three-dimensional binary glasses prepared via an instantaneous quench across the glass transition. We found that with increasing strain amplitude up to a critical value, the potential energy approaches lower minima in steady state, whereas the amplitude of shear stress oscillations becomes larger. Below the yielding transition, the storage modulus dominates the mechanical response, and the gradual decay of the potential energy over consecutive cycles is accompanied by reduction in size of transient clusters of atoms with large nonaffine displacements. In contrast, above the yield strain, the loss modulus increases and the system settles at a higher level of potential energy due to formation of a system-spanning shear band after a number of transient cycles.

## 1. Introduction

The deformation and flow dynamics of yield stress materials, which include foams, gels and glasses, generally depend on physical aging processes, shear-induced rejuvenation, and shear banding, as well as wall slip and finite-size effects [1]. At the microscopic scale, the elementary plastic deformation in disordered materials occurs in a small volume occupied by a group of particles undergoing irreversible rearrangements, sometimes referred to as the shear transformation zone [2–4]. Thus, it was recently shown that during tension–compression cyclic loading of metallic glasses, the initiation of a shear band takes place at the sample surface when aggregates of shear transformation zones reach a critical size [5]. In addition, the results of cyclic nanoindentation tests on metallic glasses have revealed that hardening occurs due to irreversible particle displacements in small volumes beneath the indenter and stiffening of the preferred yielding path [6–10]. Despite significant experimental and computational efforts, the combined effect of microplasticity and confined geometry on the mechanical properties of disordered solids remains not fully understood.

In the last few years, the mechanical response of disordered solids to oscillatory shear deformation was investigated by a number of groups using molecular dynamics simulations [11–24]. It was found that in the elastic range of deformation at zero temperature, particles with large amplitudes of repetitive displacements are organized into clusters [15], while at finite temperatures some trajectories become irreversible [11,16,17]. When the thermal fluctuations are not important, the

yielding transition is accompanied by a sharp increase of the irreversible particle diffusion, whereas the static structure remains unaffected [18,25]. Interestingly, it was recently shown for five model glasses that the loss modulus exhibits a characteristic peak in the high-frequency regime that overlaps with the range of natural vibrational frequencies, while at low frequencies, persistent damping arises from long time-scale local, irreversible deformation [23]. Furthermore, cyclic loading with the strain amplitude below (above) the yield point results in the formation of transient clusters (a permanent shear band) of atoms with large nonaffine displacements [19]. With increasing strain amplitude, the thickness of the shear band increases until it becomes comparable to the linear system size [19,20]. However, the exact mechanism of shear band formation in periodically driven disordered solids has not yet been determined.

In the recent study, the periodic deformation of binary glasses, prepared via instantaneous quench from a liquid phase to temperatures of about two to six orders of magnitude smaller than the glass transition temperature, was examined using atomistic simulations [24]. In particular, it was shown that the number of cycles required to reach a state with minimum potential energy is larger at higher temperatures and/or larger strain amplitudes. Moreover, the gradual decrease in potential energy was found to correlate with the size of clusters of atoms with large nonaffine displacements. On the other hand, the amplitude of shear stress oscillations in the elastic regime reaches a maximum value when a large part of the system starts to deform reversibly [24].

In this paper, we use non-equilibrium molecular dynamics

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simulations to study the dynamic response of poorly annealed binary glasses to periodic shear at a temperature approximately one quarter of the glass transition temperature. In agreement with the results of the previous study [24], we find that below the yielding transition, the potential energy gradually decreases to a level that is deeper for larger strain amplitudes. Above the yield strain, the potential energy approaches a higher value, and the amplitude of shear stress oscillations is reduced in the steady state, which is characterized by a system-spanning shear band and enhanced diffusion of particles. It will be shown that the transition from transient clusters to a permanent shear band is reflected in the shape of the probability distribution function of non-affine displacements.

The remainder of the paper is organized as follows. In the next section, the molecular dynamics simulation method is described. The simulation results for the potential energy, shear stress, mechanical properties, and nonaffine displacements of atoms as a function of the strain amplitude are presented in Section 3. A brief summary of the results is given in the last section.

## 2. Molecular dynamics simulations

The model glass is represented by the three-dimensional (80:20) binary mixture originally introduced by Kob and Andersen [26] to describe the amorphous metal alloy  $\text{Ni}_{80}\text{P}_{20}$  [27]. In the Kob-Andersen (KA) model, the interaction between neighboring atoms of types  $\alpha, \beta = A, B$  is specified via the truncated Lennard-Jones (LJ) potential:

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

with the following parametrization  $\varepsilon_{AA} = 1.0$ ,  $\varepsilon_{AB} = 1.5$ ,  $\varepsilon_{BB} = 0.5$ ,  $\sigma_{AB} = 0.8$ ,  $\sigma_{BB} = 0.88$ , and  $m_A = m_B$  [26]. This choice of interaction parameters prevents crystallization below the glass transition temperature [26]. The cutoff radius is fixed  $r_{c,\alpha\beta} = 2.5\sigma_{\alpha\beta}$  to reduce computational cost. All results are reported in the reduced LJ units of length, mass, energy, and time, which are set to  $\sigma = \sigma_{AA}$ ,  $m = m_A$ ,  $\varepsilon = \varepsilon_{AA}$ , and  $\tau = \sigma\sqrt{m/\varepsilon}$ , respectively. The integration of the equations of motion was performed using the velocity Verlet algorithm [28] with the time step [29].

The equilibration was first performed at the high temperature of  $1.1\varepsilon/k_B$ , which is well above the critical temperature  $T_c \approx 0.435\varepsilon/k_B$  of the KA model [26]. Here,  $k_B$  denotes the Boltzmann constant. All simulations were carried out at a constant volume and the atomic density  $\rho = \rho_A + \rho_B = 1.2\sigma^{-3}$ . The total number of atoms is  $N = 60000$  and the linear size of the periodic cubic cell is  $L = 36.84\sigma$ . Next, following an instantaneous quench across the glass transition to the temperature  $T_{LJ} = 0.1\varepsilon/k_B$ , the system was subjected to time periodic shear deformation as follows:

$$\gamma(t) = \gamma_0 \sin(2\pi t/T), \quad (2)$$

where  $\gamma_0$  is the strain amplitude and  $T$  is the period of oscillation. The shear deformation was applied parallel to the  $xz$  plane (see Fig. 1) by using the Lees-Edwards periodic boundary conditions and the SLLD algorithm [30]. In addition, the temperature  $T_{LJ} = 0.1\varepsilon/k_B$  was maintained by the dissipative particle dynamics (DPD) thermostat, which ensures that the particle dynamics is not coupled to the imposed flow profile [31]. In the present study, the oscillation period was fixed to  $T = 5000\tau$  and the strain amplitude was varied in the range  $0.03 \leq \gamma_0 \leq 0.07$ . The data for the shear stress, potential energy, and atom positions were collected during 600 shear cycles for each value of the strain amplitude. The postprocessing analysis was performed only in one sample due to computational restrictions.

## 3. Results

The structure and properties of metallic glasses depend strongly on

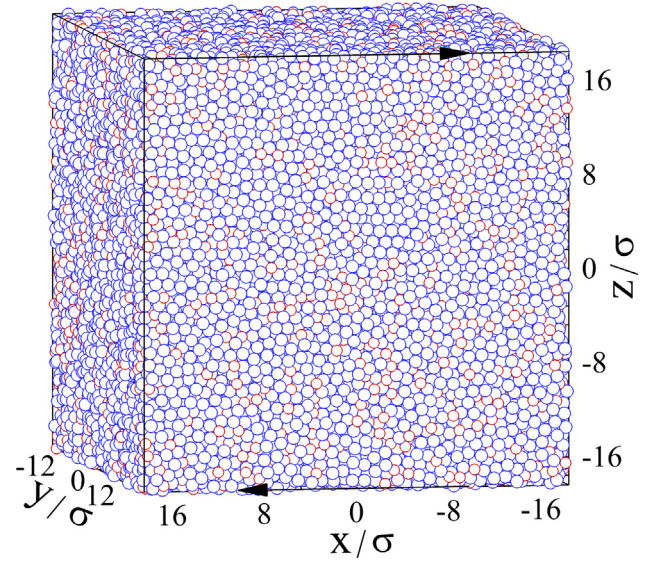


Fig. 1. A snapshot of the annealed Lennard-Jones binary glass after 600 shear cycles with the strain amplitude  $\gamma_0 = 0.05$ . The temperature is  $T_{LJ} = 0.1\varepsilon/k_B$  and the oscillation period is  $T = 5000\tau$ . The plane of shear is denoted by black arrows. Atoms of types A and B (blue and red circles) are now drawn to scale. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the details of the production and processing routes [32]. For example, it is well known that upon slower cooling, the glassy system can reach states with lower potential energy and smaller volume [32]. Moreover, under applied deformation, the system can further explore different regions of the potential energy landscape that are hardly accessible otherwise [33]. Thus, it was demonstrated that one shear cycle with large strain amplitude rejuvenates the glass by moving it to a state with shallower energy minima, whereas one small-strain cycle overages the glass by reaching a state with deeper energy minima [33]. Furthermore, it was recently shown that with increasing cooling rate, the strain-induced energy loss per strain (caused by particle rearrangements) increases and glasses become more ductile and less reversible [21]. In the present study, the binary mixture in a high-temperature liquid state is instantaneously quenched across the glass transition and then subjected to periodic deformation for hundreds of cycles with strain amplitudes above and below the yielding transition.

The variation of the potential energy,  $U/\varepsilon$ , during 600 shear cycles after the thermal quench to  $T_{LJ} = 0.1\varepsilon/k_B$  is shown in Fig. 2 for the strain amplitudes  $\gamma_0 = 0.03, 0.04, 0.05, 0.06$  and  $0.07$ . Note that the data for all strain amplitudes except for  $\gamma_0 = 0.05$  are displaced vertically for clarity (see caption to Fig. 2). It can be clearly seen that the potential energy decreases rapidly during the first few tens of shear cycles and then it gradually saturates to a nearly constant value for each strain amplitude. In the case  $\gamma_0 = 0.06$ , however, a markedly different behavior is observed; namely, the local minimum is developed at  $t \approx 80T$  (see Fig. 2). In other words, the system is first driven to a relatively deep energy minimum, where the amplitude of energy oscillations is enhanced, followed by a crossover to a steady state with a higher potential energy and reduced energy amplitude. For all cases presented in Fig. 2, the steady state with the lowest potential energy,  $U \approx -8.16\varepsilon$ , is achieved at  $\gamma_0 = 0.05$ , which suggests that the critical strain amplitude for the yielding transition is in the range between 0.05 and 0.06 at the temperature  $T_{LJ} = 0.1\varepsilon/k_B$ . For comparison, the cyclic loading with  $\gamma_0 = 0.05$  at lower temperatures,  $T_{LJ} \leq 10^{-2}\varepsilon/k_B$ , resulted in the states with the potential energy  $U \approx -8.26\varepsilon$ , and the critical strain amplitude was found to be greater than 0.07 [24]. We also comment that the potential energy saturates at  $U \approx -8.12\varepsilon$  when the system is instantaneously quenched to  $T_{LJ} = 0.1\varepsilon/k_B$  and evolves in the absence of

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