

# Relaxation dynamics in amorphous alloys under asymmetric cyclic shear deformation

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## ABSTRACT

The influence of cyclic loading and glass stability on structural relaxation and yielding transition in amorphous alloys was investigated using molecular dynamics simulations. We considered a binary mixture cooled deep into the glass phase and subjected to cyclic shear deformation where strain varies periodically but remains positive. We found that rapidly cooled glasses under asymmetric cyclic shear gradually evolve towards states with lower potential energy and finite stress at zero strain. At the strain amplitude just below a critical value, the rescaled distributions of nonaffine displacements converge to a power-law decay with an exponent of about -2 upon increasing number of cycles. By contrast, more stable glasses yield at lower strain amplitudes, and the yielding transition can be delayed for hundreds of cycles when the strain amplitude is near a critical value. These results can be useful for the design of novel thermo-mechanical processing methods to improve mechanical and physical properties of metallic glasses.

## 1. Introduction

The development and optimization of bulk metallic glasses is important for various structural and biomedical applications including wear-resistant gears [1] and biocompatible implants [2]. It is well known that due to their amorphous structure, metallic glasses possess advantageous properties such as high strength, large elastic strain limit, and high corrosion resistance [3]. Under applied strain, the elementary plastic deformation in such amorphous alloys involve swift rearrangement of a small group of atoms or shear transformations [4,5]. Upon further loading, well annealed glasses typically yield via the formation of narrow shear bands where strain is localized [6]. It was shown that the ductile behavior can be restored by relocating glasses to higher energy states [7]. Such rejuvenation can be achieved via high-pressure torsion, cold rolling, wire drawing, irradiation, elastostatic loading, and other thermo-mechanical processing methods [7, 8]. A particularly elegant method involves cryogenic thermal cycling that can rejuvenate metallic glasses due to plastic deformation under internal stresses arising during spatially heterogeneous thermal expansion [9–21]. Moreover, the process of rejuvenation during elastostatic compression can be accelerated when stress is temporarily applied along alternating directions [22,23]. In addition, it was also recently demonstrated experimentally and by means of molecular dynamics (MD) simulations that higher energy states can be realized via rapid freezing of a glass former under applied stress [24,25]. However, in

spite of the progress made, the design of novel strategies for thermo-mechanical processing of metallic glasses is required to access a broader range of energy states and improved mechanical properties.

In the last decade, the dynamic response of amorphous materials to cyclic loading was extensively investigated using atomistic simulations [26–58]. Interestingly, it was demonstrated that in a broad range of energy states, athermal glasses under oscillatory quasistatic shear deformation exhibit a sharply defined yielding transition; and, in general, cyclic shear provides a better characterization of the yielding transition than uniform loading [34]. Moreover, the yielding transition in well annealed binary glasses can be delayed for thousands of cycles when temperature is well below  $T_g$  [48], whereas at about half  $T_g$ , the critical strain amplitude remains the same for stable glasses with initially different energy levels [55]. It was further shown that under small-amplitude cyclic loading, rapidly quenched glasses undergo structural relaxation, termed as ‘mechanical annealing’, and gradually evolve towards low-energy steady states [28,37,40,41,45]. In some cases, mechanically induced annealing can be accelerated when the shear orientation is periodically alternated in two or three spatial dimensions [41,50] or if the strain amplitude of cyclic loading is occasionally increased above a critical value [51]. More recently, it was found that the yielding behavior in binary glasses under asymmetric cyclic shear deformation is markedly different from the case of symmetric loading,

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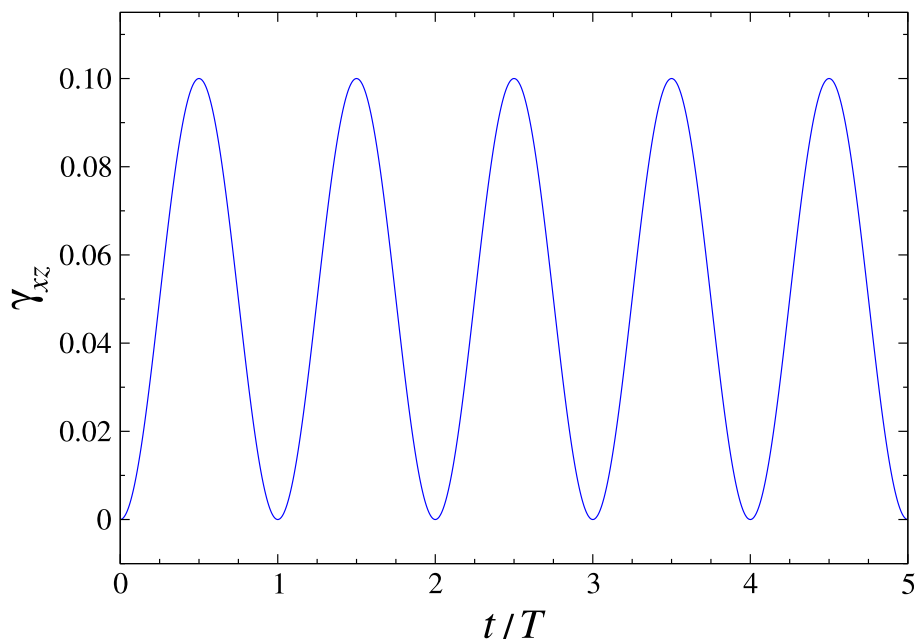


Fig. 1. The applied shear strain,  $\gamma_{xz}$ , as a function of time,  $t/T$ , specified by Eq. (2) for the strain amplitude  $\gamma_0 = 0.10$ . The oscillation period is  $T = 5000 \tau$ .

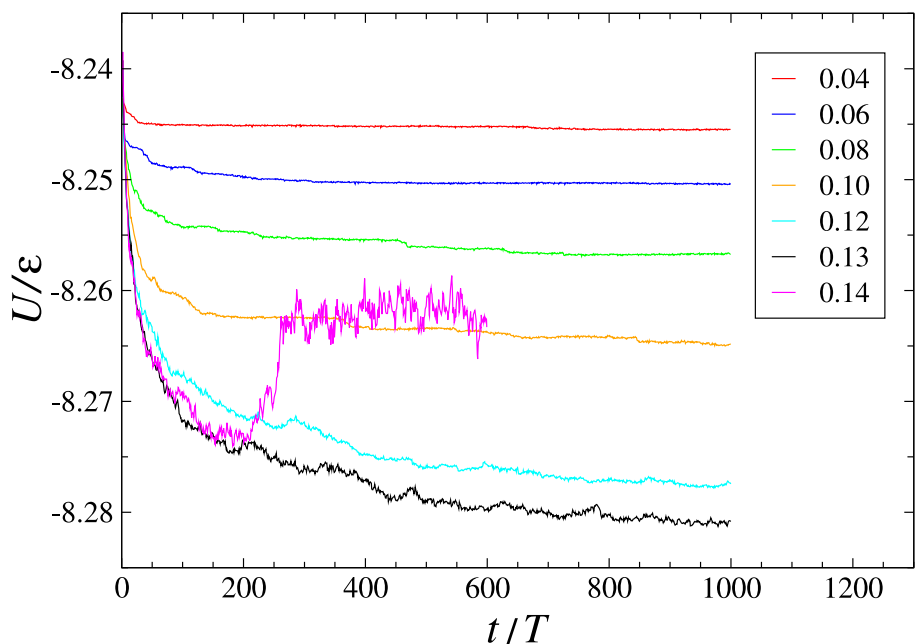


Fig. 2. (Color online) The potential energy minima as a function of the number of shear cycles for the indicated values of strain amplitude  $\gamma_0$  in Eq. (2). The period of oscillation is  $T = 5000 \tau$ . The glass was initially prepared by cooling across the glass transition temperature with the rate of  $10^{-2} \epsilon/k_B \tau$  to  $T_{LJ} = 0.01 \epsilon/k_B$  at  $\rho = 1.2 \sigma^{-3}$ .

and, in particular, better annealed glasses under asymmetric shear yield at a smaller strain amplitude and exhibit an enhanced plastic activity at strain amplitudes below a critical value [56]. Despite extensive modeling efforts, however, the influence of the deformation protocol and preparation history on the yielding transition and mechanical annealing remain not fully understood.

In this paper, we present results of molecular dynamics simulations of binary glasses subjected to asymmetric oscillatory deformation where shear strain varies periodically but remains positive. It will be shown that rapidly cooled glasses under cyclic loading at strain amplitudes below a critical value evolve towards progressively lower energy states with a finite stress at zero strain. This relaxation process

proceeds via irreversible rearrangements of atoms whose nonaffine displacements become power-law distributed. We also find that stable glasses undergo a yielding transition at smaller strain amplitudes and the onset of yielding is delayed for hundreds of shear cycles near the critical strain amplitude.

The rest of this paper is organized as follows. We describe the details of molecular dynamics simulations and the asymmetric deformation protocol in the next section. The analysis of the potential energy, nonaffine displacements, and stress-strain response is presented in Section 3. The results are briefly summarized in the last section.

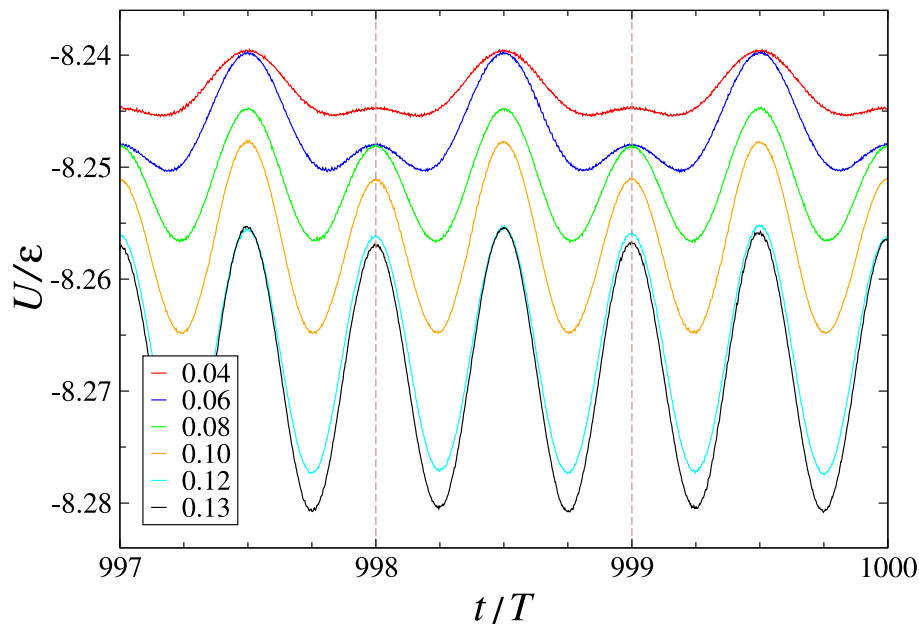


Fig. 3. (Color online) The variation of the potential energy during the last three loading cycles for the indicated strain amplitudes  $\gamma_0$ . The oscillation period is  $T = 5000\tau$ . The same data as in Fig. 2. The vertical dashed lines are plotted for reference.

## 2. Molecular dynamics simulations

In our study, the amorphous alloy was represented by means of the binary (80:20) Lennard-Jones (LJ) mixture model originally proposed by Kob and Andersen (KA) over twenty years ago [59]. In the KA model, the interaction between atoms of types  $\alpha, \beta = A, B$  is specified via the LJ potential, as follows:

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

where the parameters are set to  $\varepsilon_{AA} = 1.0$ ,  $\varepsilon_{AB} = 1.5$ ,  $\varepsilon_{BB} = 0.5$ ,  $\sigma_{AA} = 1.0$ ,  $\sigma_{AB} = 0.8$ ,  $\sigma_{BB} = 0.88$ , and  $m_A = m_B$  [59]. A similar parameters were employed by Weber and Stillinger to study the amorphous metal-metalloid alloy  $\text{Ni}_{80}\text{P}_{20}$  [60]. In the present study, the results are reported in terms of the reduced units of length, mass, energy, and time, as follows:  $\sigma = \sigma_{AA}$ ,  $m = m_A$ ,  $\varepsilon = \varepsilon_{AA}$ , and  $\tau = \sigma\sqrt{m/\varepsilon}$ . The total number of atoms is  $N = 60000$  and the cutoff radius is  $r_{c,\alpha\beta} = 2.5\sigma_{\alpha\beta}$ . The MD simulations were performed using the LAMMPS code with the integration time step  $\Delta t_{MD} = 0.005\tau$  [61,62].

The sample preparation procedure involved the following steps. First, the binary mixture was placed in a cubic box of size  $L = 36.84\sigma$  and equilibrated at the temperature  $T_{LJ} = 1.0\varepsilon/k_B$  and density  $\rho = \rho_A + \rho_B = 1.2\sigma^{-3}$ . Here,  $k_B$  is the Boltzmann constant. This temperature is well above the critical temperature  $T_g = 0.435\varepsilon/k_B$  of the KA model at the density  $\rho = 1.2\sigma^{-3}$  [59]. In all simulations, the temperature was controlled via the Nosé–Hoover thermostat [61,62] and periodic boundary conditions were applied along the  $\hat{x}$ ,  $\hat{y}$ , and  $\hat{z}$  directions. Second, the system was rapidly cooled from the temperature  $T_{LJ} = 1.0\varepsilon/k_B$  to  $0.01\varepsilon/k_B$  with the rate of  $10^{-2}\varepsilon/k_B\tau$  at constant density  $\rho = 1.2\sigma^{-3}$ . After the thermal quench, the binary glass was subjected to time periodic shear deformation along the  $xz$  plane, as follows:

$$\gamma_{xz}(t) = \gamma_0 [1 + \sin(2\pi t/T - \pi/2)]/2, \quad (2)$$

where  $\gamma_0$  is the strain amplitude,  $T = 5000\tau$  is the oscillation period, and the strain  $\gamma_{xz}$  varies from zero to  $\gamma_0$  and then back to zero during one period. The example of the imposed shear strain for the strain amplitude  $\gamma_0 = 0.10$  during five oscillation periods is shown in Fig. 1. The production run involved 1000 shear cycles for each value of  $\gamma_0$  in the range from 0.04 to 0.13 at  $T_{LJ} = 0.01\varepsilon/k_B$  and  $\rho = 1.2\sigma^{-3}$ . The simulations were performed for one sample due to computational limitations, and the potential energy, stress components, and atomic configurations were periodically saved for post-processing analysis.

## 3. Results

It has long been realized that mechanical and physical properties of metallic glasses depend sensitively on the rate of cooling from the liquid state [7]. In particular, more slowly cooled glasses typically settle at lower energy states and upon large enough deformation might exhibit brittle yielding via strain localization along narrow bands. By contrast, rapid cooling across the glass transition temperature generally results in higher energy states and ductile behavior [7]. Moreover, metallic glasses can be further relaxed to lower energy states via oscillatory deformation when the strain amplitude is below a critical value [28, 37,41]. In what follows, we consider rapidly and slowly cooled binary glasses under asymmetric cyclic deformation, where the imposed shear strain is varied periodically but remains positive, and compare the simulation results with the case of symmetric deformation with respect to zero strain.

In our analysis, a rapidly quenched binary glass was repeatedly loaded for 1000 cycles using the asymmetric shear deformation protocol given by Eq. (2). The potential energy minima during each cycle are shown in Fig. 2 for the indicated values of the strain amplitude. As is evident, the glass is relocated to lower energy states upon increasing strain amplitude. Note that, as loading continues, the potential energy levels off to a plateau for  $\gamma_0 \leq 0.10$ , whereas progressively lower energy states are attained for  $0.12 \leq \gamma_0 \leq 0.13$ . These conclusions are consistent with the results of the previous study of rapidly quenched glasses under symmetric cyclic shear deformation [41,51]. For example, the asymmetric loading at  $\gamma_0 = 0.12$  results in the same energy level,  $U \approx -8.277\varepsilon$ , as the symmetric cyclic shear deformation at the strain amplitude of 0.06 for the same operating conditions [41]. As shown in Fig. 2, mechanically induced annealing at  $\gamma_0 = 0.14$  proceeds for about 200 cycles, followed by the yielding transition via the formation of a shear band with a higher energy. Similar yielding behavior was reported for symmetric cyclic shear deformation of rapidly quenched binary glasses at the strain amplitude of 0.07 [47].

The main difference between symmetric and asymmetric cyclic shear deformation of rapidly quenched glasses is that in the latter case the potential energy minima as well as zero stress are attained at nonzero strain. For example, the variation of the potential energy during the last three cycles is shown in Fig. 3 for the strain amplitudes  $\gamma_0 \leq 0.13$ . It can be seen that for  $0.08 \leq \gamma_0 \leq 0.13$ , the potential energy

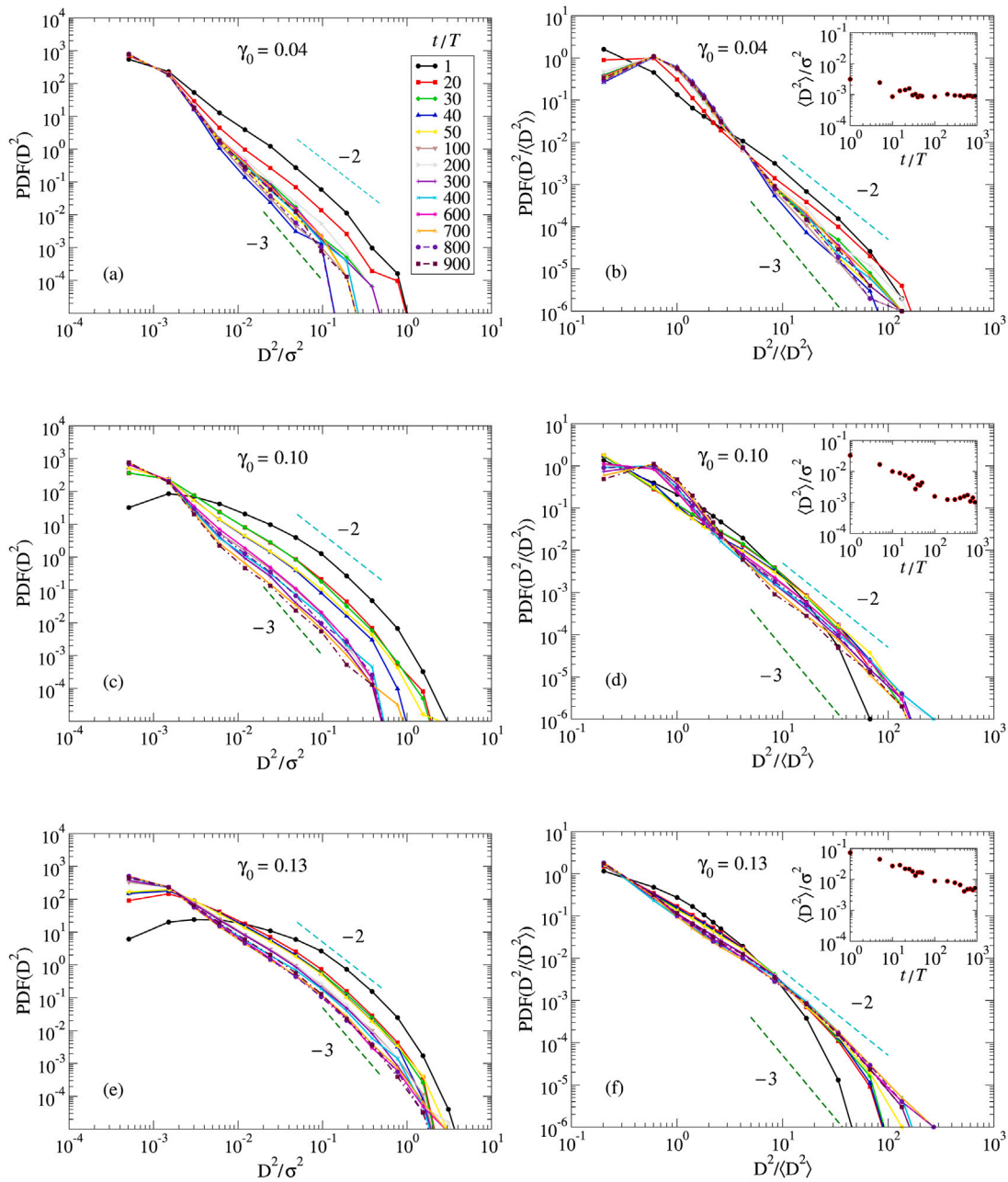


Fig. 4. The probability distributions of the nonaffine quantity,  $D^2(t, \Delta t = T)$ , (left panels) and the corresponding rescaled distributions (right panels) for (a, b)  $\gamma_0 = 0.04$ , (c, d) 0.10, and (e, f) 0.13. The cycle numbers,  $t/T$ , are listed in the legend. The insets show the average values of  $D^2$  as a function of  $t/T$ . The dashed lines with the slopes of  $-2$  and  $-3$  are plotted for reference.

reaches minima at about  $0.25T$  and  $0.75T$  when strain is  $\gamma_0/2$ , while for smaller strain amplitudes,  $\gamma_0 = 0.04$  and  $0.06$ , the energy minima become less pronounced and occur at lower strain. These results imply that for sufficiently large strain amplitudes, rapidly quenched glasses under asymmetric cyclic shear deformation evolve towards symmetric deformation with respect to  $\gamma_0/2$ .

The spatial and temporal distribution of local plastic events in amorphous alloys can be quantified via the analysis of the so-called nonaffine displacements of atoms [63]. By definition, the nonaffine measure for the  $i$ th atom is calculated using the transformation matrix  $\mathbf{J}_i$ , which linearly transforms a group of neighboring atoms and, at the same time, minimizes the following expression:

$$D^2(t, \Delta t) = \frac{1}{N_i} \sum_{j=1}^{N_i} \left\{ \mathbf{r}_j(t + \Delta t) - \mathbf{r}_i(t + \Delta t) - \mathbf{J}_i [\mathbf{r}_j(t) - \mathbf{r}_i(t)] \right\}^2, \quad (3)$$

where the sum is taken over  $N_i$  neighbors that are located within  $1.5\sigma$  from the position of the  $i$ th atom,  $\mathbf{r}_i(t)$ , and  $\Delta t$  is the time interval between two configurations of atoms. The local plastic rearrangement is typically associated with the values of the nonaffine measure  $D^2(t, \Delta t)$  greater than the cage size, which for the KA model at  $\rho = 1.2\sigma^{-3}$  is about  $0.1\sigma^2$  [59]. It was recently shown, however, that during cyclic shear deformation below the yielding transition, a fraction of atoms undergo reversible nonaffine displacements with amplitudes that are approximately power-law distributed [31,33].

The probability distribution functions of the nonaffine measure are presented in Figs. 4a, 4c, and 4e for the strain amplitudes  $\gamma_0 = 0.04$ , 0.10, and 0.13, respectively. The nonaffine quantity  $D^2(t, \Delta t)$  in Eq. (3) was computed for atomic configurations at zero strain at the beginning and end of a cycle, i.e.,  $\Delta t = T$ , for the tabulated values of the cycle number  $t/T$  shown in Fig. 4a. Note also that the data in Fig. 4 are

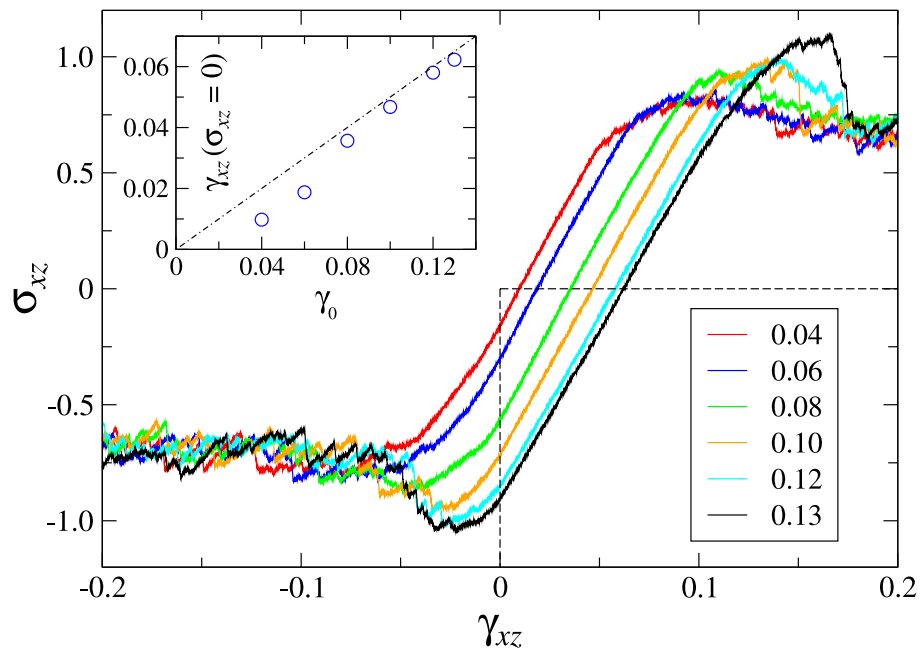


Fig. 5. (Color online) The shear stress,  $\sigma_{xz}$  (in units of  $\epsilon\sigma^{-3}$ ), as a function of strain,  $\gamma_{xz}$ , during steady loading with the rate of  $10^{-5}\tau^{-1}$ . The values of the strain amplitude,  $\gamma_0$ , used for mechanical annealing are listed in the legend. The dashed lines indicate  $\gamma_{xz} = 0$  and  $\sigma_{xz} = 0$ . The inset shows shear strain as zero stress versus the strain amplitude. The dash-dotted line  $y = 0.5x$  is plotted for reference.

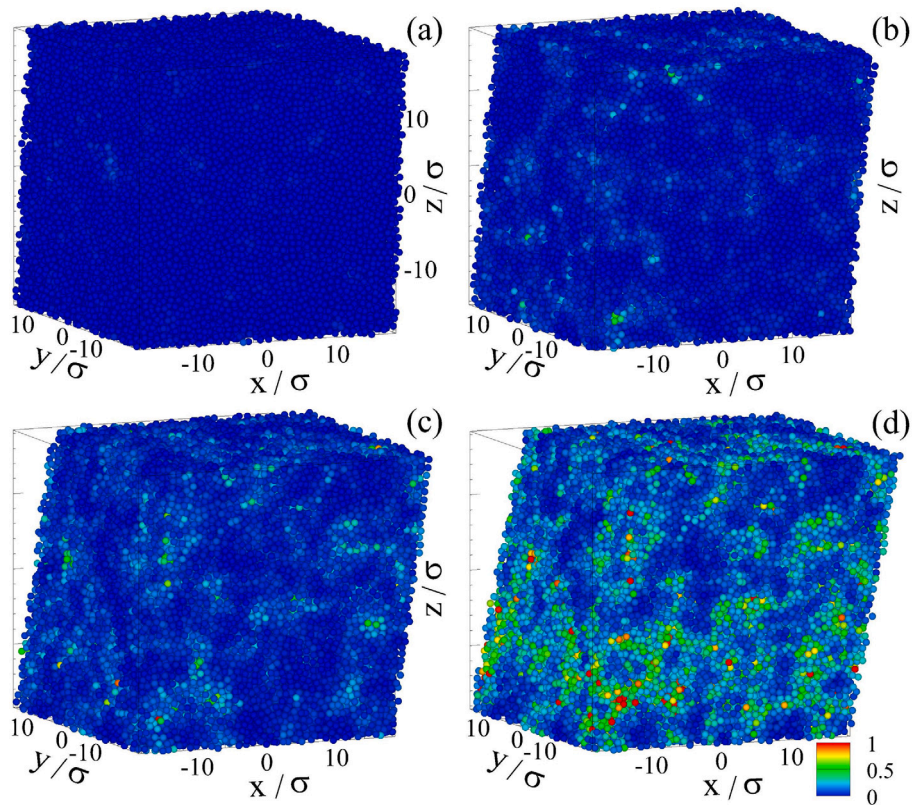


Fig. 6. The atomic configurations of the binary glass strained along the  $xz$  plane with the strain rate of  $10^{-5}\tau^{-1}$ . The shear strain is (a) 0.05, (b) 0.10, (c) 0.15, and (d) 0.20. The colorcode indicates values of  $D^2$  computed with respect to the atomic configuration at zero strain. The glass was initially cooled across  $T_g$  with the rate of  $10^{-2}\epsilon/k_B\tau$  and periodically deformed for 1000 shear cycles with  $\gamma_0 = 0.04$  in Eq. (2).

presented on the log-log scale using logarithmic bin widths to avoid noise at large values of  $D^2$ . It can be clearly seen that distributions for  $t/T = 1$  are relatively wide and extend up to  $D^2 \approx 1.0\sigma^2$ , indicating

enhanced plastic activity at the beginning of the loading process. With increasing cycle number, the distributions of  $D^2$  tend to become more narrow but remain approximately power-law distributed. Notice,

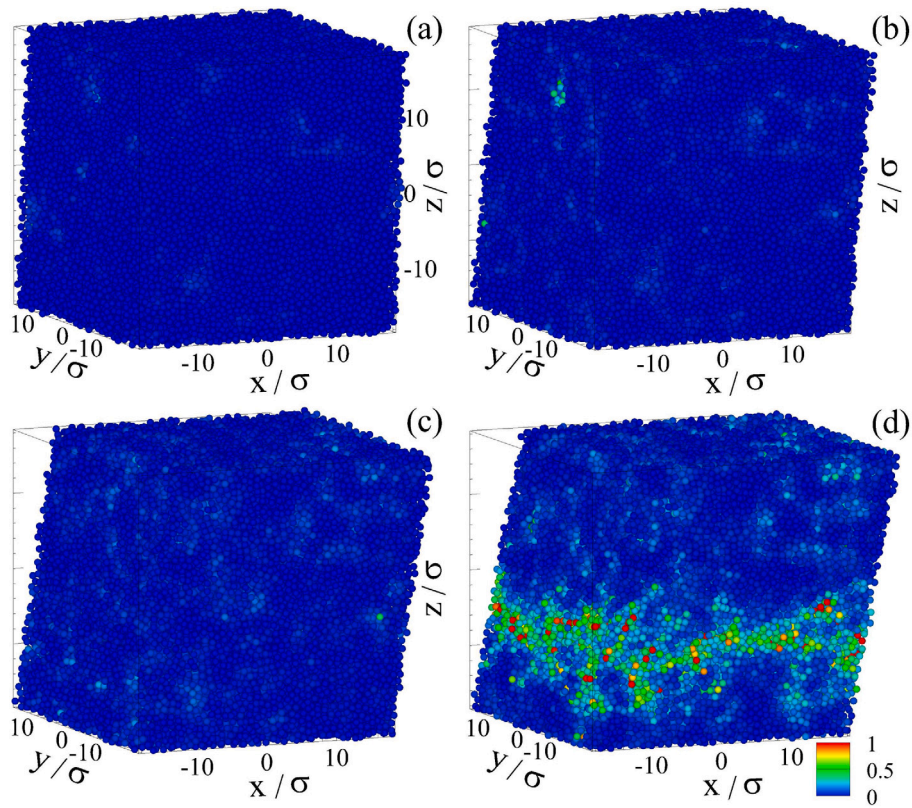


Fig. 7. The snapshots of strained glass along the  $xz$  plane with the rate of  $10^{-5}\tau^{-1}$ . The strain is (a) 0.05, (b) 0.10, (c) 0.15, and (d) 0.20. The nonaffine measure  $D^2$  is indicated by the color in the legend. The sample was initially cooled with the rate of  $10^{-2}\epsilon/k_B\tau$  and loaded for 1000 shear cycles with the strain amplitude  $\gamma_0 = 0.13$ .

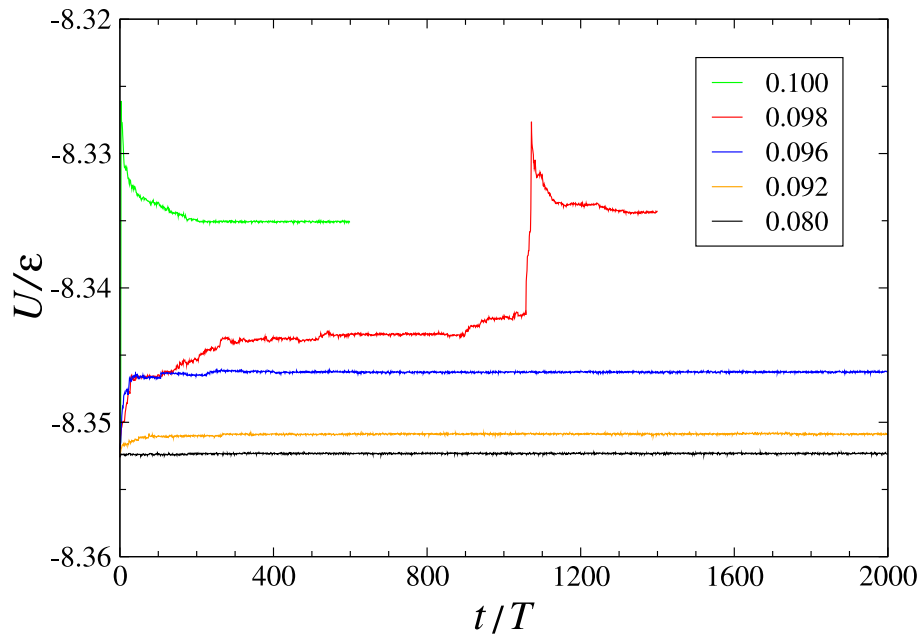


Fig. 8. The potential energy minima in periodically deformed stable glasses for the tabulated values of the strain amplitude  $\gamma_0$  in Eq. (2). The oscillation period is  $T = 5000\tau$ .

however, that in some cases, more narrow distributions correspond to smaller number of loading cycles, e.g.,  $t/T = 40$  in Fig. 4a, which can

be attributed to fluctuations in the average of  $D^2$  as a function of the cycle number (see insets in the right panels of Fig. 4).

Further, the corresponding rescaled distributions of  $D^2/\langle D^2 \rangle$  are presented in Figs. 4b, 4d, and 4f for the same strain amplitudes  $\gamma_0 = 0.04, 0.10, \text{ and } 0.13$ . It can be seen in Fig. 4f that for the largest strain amplitude  $\gamma_0 = 0.13$ , the distributions of  $D^2/\langle D^2 \rangle$  converge to a single curve with the power-law exponent of about  $-2$  upon increasing number of cycles. This behavior might be related to a continued structural relaxation at  $\gamma_0 = 0.13$  during 1000 cycles, which is reflected in the fast decay of the potential energy reported in Fig. 2 and relatively large values of  $\langle D^2 \rangle$  shown in the inset of Fig. 4f. The accelerated relaxation at  $\gamma_0 = 0.13$  involves a large number of plastic events and thus results in broad distributions of  $D^2$  during 1000 cycles. By contrast, for the lower strain amplitudes,  $\gamma_0 = 0.04$  and  $0.10$ , the deformation becomes nearly reversible after a number of transient cycles (see Fig. 2). As a result, the average of  $D^2$  is much smaller than the typical cage size, and the distributions of  $D^2/\langle D^2 \rangle$  become weakly dependent on the cycle number due to relatively large scatter in  $\langle D^2 \rangle$ , as shown in Figs. 4b and 4d.

After periodic deformation for 1000 shear cycles, the binary glass was sheared at a constant strain rate of  $10^{-5}\tau^{-1}$  from zero strain to  $0.2$  and to  $-0.2$ . The results for the shear stress as a function of strain are displayed in Fig. 5 for the indicated values of the strain amplitude used for cyclic loading. It can be seen that with increasing  $\gamma_0$  (lower energy glasses), the magnitude of stress at zero strain as well as the peak value of the stress overshoot increase. The maximum value of the yielding peak is  $\sigma_y \approx 1.1 \epsilon \sigma^{-3}$  for the better annealed sample at  $\gamma_0 = 0.13$ . In turn, the inset in Fig. 5 shows the shear strain at zero stress as a function of the strain amplitude of cyclic loading. Note that except for the cases  $\gamma_0 = 0.04$  and  $0.06$ , the shear strain  $\gamma_{xz}(\sigma_{xz} = 0)$  is about half the strain amplitude, indicating that during cyclic loading, the oscillation of shear stress becomes nearly symmetric with respect to  $\gamma_0/2$ . For all values of  $\gamma_0$ , the relative strain  $\gamma_{xz}(\sigma_{xz} = 0)/\gamma_0$  correlates well with the locations of minima in the potential energy reported in Fig. 3. These results are in agreement with a recent MD study on binary glasses under asymmetric cyclic deformation using athermal quasistatic shear protocol [56].

The shear stress response to the applied strain shown in Fig. 5 indicates that a glass undergoes a transition from ductile to brittle failure upon increasing strain amplitude of cyclic loading. To illustrate microscopic details of plastic deformation, we presented a series of snapshots at shear strain ranging from  $0.05$  to  $0.2$  in Fig. 6 for the glass initially annealed at the strain amplitude  $\gamma_0 = 0.04$  and in Fig. 7 for  $\gamma_0 = 0.13$ . In each panel, the nonaffine measure was computed with respect to an atomic configuration at zero strain. It can be clearly observed in Fig. 6 that the yielding transition in the poorly annealed sample is associated with homogeneous distribution of atoms with large nonaffine displacements. In contrast, the yielding transition in the more stable glass annealed at  $\gamma_0 = 0.13$  proceeds via the formation of a shear band, as shown in Fig. 7. Interestingly, nonaffine displacements in the better annealed glass remain relatively small when strain is varied in the range  $0 \leq \gamma_{xz} \leq 0.15$ , despite a large variation in shear stress of about twice the yielding peak (see the black curve in Fig. 5).

Lastly, we include a comment about the yielding transition in stable glasses under asymmetric cycle shear deformation. In this case, the binary mixture was first slowly cooled from  $T_{LJ} = 1.0 \epsilon/k_B$  to  $0.3 \epsilon/k_B$  with the rate of  $10^{-5} \epsilon/k_B \tau$  at  $\rho = 1.2 \sigma^{-3}$ , then periodically deformed for 5000 cycles, and finally cooled to  $T_{LJ} = 0.01 \epsilon/k_B$  at  $\rho = 1.2 \sigma^{-3}$ . In the previous study [53], it was shown that this preparation procedure leads to a relatively stable glass with the potential energy  $U \approx -8.352 \epsilon$  in the undeformed state. Fig. 8 shows the energy minima during each cycle in the stable glass loaded at the selected strain amplitudes. It can be seen that the yielding transition, which is reflected in an abrupt energy change, occurs after loading is applied at  $\gamma_0 = 0.100$ , while at  $\gamma_0 \leq 0.096$ , after about 300 cycles, the potential energy remains nearly constant for 2000 cycles, indicating reversible deformation. For  $\gamma_0 = 0.092$  and  $0.096$ , the energy increase during the first 300 cycles is associated with plastic deformation, similar to the results reported for athermal glasses under asymmetric shear [56]. Furthermore, loading at  $\gamma_0 = 0.098$  results

in a stepwise increase of the potential energy during 1000 cycles and the yielding transition after 1057 cycles (see the red curve in Fig. 8). This behavior is consistent with the delayed yielding transition in stable glasses sinusoidally deformed at a finite temperature [48]. Altogether, the results in Figs. 2 and 8 demonstrate that the yielding transition in more stable glasses under the deformation protocol given by Eq. (2) occurs at lower strain amplitudes and the transition can be significantly delayed when the strain amplitude is in the vicinity of the critical value.

#### 4. Conclusions

In summary, we investigated the effects of asymmetric cyclic shear deformation and preparation history of amorphous alloys on mechanical annealing and yielding transition using molecular dynamics simulations. We considered a binary mixture rapidly cooled deep into the glass phase and applied periodic deformation where shear strain varied sinusoidally but remained positive. Similar to the symmetric case, we demonstrated that cyclic deformation induced structural relaxation and resulted in a gradual decay of the potential energy upon continued loading. It was further shown that rescaled distributions of nonaffine displacements during one cycle followed a power-law decay when the strain amplitude is below a critical value. In agreement with the recent results for athermal glasses under asymmetric cyclic shear [56], we found that the yielding transition in more stable glasses occurs at lower strain amplitudes. In the presence of thermal fluctuations, the yielding transition can be delayed for hundreds of shear cycles in a relatively large system when periodically deformed at strain amplitudes near a critical value.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Both the authors contributed equally to this work.

#### Data availability

Data will be made available on request.

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