# Supplemental Material for "Glass stability changes the nature of yielding under oscillatory shear"

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# S-1. THE MEASUREMENT OF RHEOLOGICAL PROPERTIES

The shear stress  $\sigma$  is defined by [1]

$$\sigma = \frac{1}{L^3} \sum_{i>j} \left( \frac{\partial U(r_{ij})}{\partial \mathbf{r}_{ij}} \cdot \hat{\mathbf{x}} \right) (\mathbf{r}_{ij} \cdot \hat{\mathbf{y}}), \tag{1}$$

where  $U(r_{ij})$  is the pair interaction potential defined in the main text,  $\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$ ,  $\mathbf{r}_i$  is the position of the *i*-th particle,  $\hat{\mathbf{x}}$  and  $\hat{\mathbf{y}}$  are the unit vectors in the *x* and *y* directions, and *L* is the linear box length.

In the finite strain-rate protocol, the shear strain given by  $\gamma(t) = \gamma_0 \sin(2\pi t/T_{\rm cyc})$  with an oscillation period  $T_{\rm cyc}$  and a strain amplitude  $\gamma_0$  is applied to the system. We calculate the leading order coefficients of the nonlinear stress-strain relation [2] by fitting the instantaneous shear stress  $\sigma(t)$  to  $\sigma_0 \sin(2\pi t/T_{\rm cyc} + \delta_0)$ , where  $\sigma_0$  is the stress magnitude and  $\delta_0$  is the phase lag between stress and strain. Using  $\sigma_0$  and  $\delta_0$ , we calculate the storage modulus G' and loss modulus G'' from the relation  $G' + iG'' = \sigma_0 e^{i\delta_0}/\gamma_0$ . We measure  $\sigma_0$ ,  $\delta_0$ , G', and G''at each cycle. The steady-state values are obtained by performing a long time average after the system reaches a steady state.

In the athermal quasi-static (AQS) protocol, on the other hand, we employ the accumulated strain defined by  $\gamma_{\rm accu} \equiv \int_0 |d\gamma|$  as a substitute for the time scale. After each cycle,  $\gamma_{\rm accu}$  is increased by  $4\gamma_0$  which is equivalent to the oscillation period. Figs. S1(a) and (c) are typical  $\sigma$  and  $\gamma$  as a function of  $\gamma_{\rm accu}/4\gamma_0$  in AQS simulation. Note that  $\gamma_{\rm accu} = 4\gamma_0(n + 0.25)$  and  $4\gamma_0(n + 0.75)$  with  $n = 0, 1, 2, \cdots$  are the positions at which the shear direction is reversed.

In order to extract  $\sigma_0$  and  $\delta_0$  from the AQS data, we convert  $\gamma$  to a time  $t^*$  using  $\gamma = \gamma_0 \sin(2\pi t^*)$ . We then transform  $\sigma = \sigma(\gamma_{accu})$  to  $\sigma = \sigma(t^*)$ , from which  $\sigma_0$  and  $\delta_0$  are obtained by fitting the relation  $\sigma = \sigma_0 \sin(2\pi t^* + \delta_0)$ . G' and G'' are obtained consequently. Figs. S1(b) and (d) are  $\gamma(t^*)$  and  $\sigma(t^*)$  mapped from Figs. S1(a) and (c) obtained using this procedure.

#### S-2. NON-AFFINE DEFORMATION

For amorphous solids under shear deformation, the displacement of the particles are often non-affine [3]. In



FIG. S1. Typical profiles of the strain (a) and stress (c) in the AQS protocol as a function of the accumulated strain  $\gamma_{\rm accu}$  scaled by the period  $4\gamma_0$ . The right panels are replots of the strain (b) and stress (d) using the scaled time  $t^*$  defined by  $\gamma = \gamma_0 \sin(2\pi t^*)$  (see the text). The red dashed curve in (d) represents the best fit of  $\sigma$  by  $\sigma_0 \sin(2\pi t^* + \delta_0)$ . In these figures, the strain amplitude is  $\gamma_0 = 0.13$  and the system size N = 48000.

other words, the particle displacements are not simply described by the affine transformation of the coordinate by shear even when the macroscopic strain is very small [4]. This non-affine contribution of the particle displacements plays an essential role in determining the rheological properties. In our study, we decomposed the displacement  $\Delta \mathbf{r}_i$  of the *i*-th particle during a small time increment into the affine and non-affine contributions as

$$\Delta \mathbf{r}_i = \Delta \mathbf{r}_i^{(\text{aff})} + \Delta \mathbf{r}_i^{(\text{na})}, \qquad (2)$$

where

$$\Delta \mathbf{r}_{i}^{(\text{aff})} = \Delta \gamma \cdot (\mathbf{r}_{i} \cdot \hat{\mathbf{y}}) \cdot \hat{\mathbf{x}}, \qquad (3)$$

is the affine displacement due to the background shear transformation. In the finite strain-rate protocol,  $\Delta \gamma = \dot{\gamma}(t)\Delta t$  is the strain change during period  $[t, t+\Delta t]$ . In order to quantify the non-affine contribution, we introduce the one-cycle non-affine deformation of the *i*-th particle



FIG. S2. Typical profile of the coarse-grained one-cycle nonaffine deformation  $\bar{d}_{na}^{(y)}$  as a function of y/L for the system with horizontal shear-band shown in Fig. S4(c), where L is the linear box length. Three typical trajectories for particles located in y/L = 0, 0.3, and 0.5 are plotted in Fig. S5. The error bar of each data point represents the standard deviation inside the slice which we use to coarse-grain the system.

defined by

$$d_{\mathrm{na},i}(n) \equiv \int_{(n-1)T_{\mathrm{cyc}}}^{nT_{\mathrm{cyc}}} \left| \frac{d\mathbf{r}_{i}^{(\mathrm{na})}(t)}{dt} \right| dt, \qquad (4)$$

where we have used non-affine trajectories  $\mathbf{r}_{i}^{(\mathrm{na})}(t)$  which is defined by [5]

$$\mathbf{r}_{i}^{(\mathrm{na})}(t) \equiv \int_{0}^{t} \left( \lim_{\Delta t \to 0} \frac{\Delta \mathbf{r}_{i}(t') - \Delta \mathbf{r}_{i}^{(\mathrm{aff})}(t')}{\Delta t} \right) dt'.$$
(5)

 $d_{\mathrm{na},i}(n)$  characterizes the arc length of the non-affine trajectory of the *i*-th particle in the *n*-th oscillatory cycle, and its physical meaning is similar to the atomic strain obtained from the particle movement relative to its nearest neighbor particles [6, 7]. In the AQS protocol, Eq. (4) should be modified as

$$d_{\mathrm{na},i}(n) \equiv \int_{4(n-1)\gamma_0}^{4n\gamma_0} \left| \frac{d\mathbf{r}_i^{(\mathrm{na})}}{d\gamma_{\mathrm{accu}}} \right| d\gamma_{\mathrm{accu}},\tag{6}$$

and  $\Delta \gamma$  in Eq. (3) is a strain increment. Typical nonaffine trajectories under oscillatory shear and their associated  $d_{\text{na},i}$  values are shown in Sec. S-6 B.

# S-3. THE ORDER PARAMETER OF SHEAR-BAND

For amorphous solids under shear, the shear-bands are often observed. The shear-band can be most easily visualized using the spatial distribution of non-affine deformation  $d_{na,i}$  defined in Eqs. (4) and (6). Shear-band can be either horizontal or vertical to the flow direction [8, 9]. Typical horizontal shear-band is shown in Fig. S4(c) in which the spatial distribution of  $d_{\text{na},i}$  is represented by color map.

To quantify the inhomogeneity of the shear-band, we introduce a shear-band order parameter defined in the following way. First we divide the system into  $N_s$  slices along the x direction (we choose  $N_s = 50$  for all system sizes N we studied. We have checked that the results are insensitive to  $N_s$  if  $N_s \ge 50$ ). Then, we coarse-grain  $d_{\text{na},i}$  by taking average inside the slices as

$$\bar{d}_{\mathrm{na}}^{(x)}(x_k) \equiv \frac{1}{N_k} \sum_{i}^{\prime} d_{\mathrm{na},i} \tag{7}$$

for the x-direction. Here  $k = 1, ..., N_s$  is the index of slice,  $x_k = (k - 0.5)L/N_s$  is the center position of the slice k, L is the linear box length,  $N_k$  is the number of particle in the slice k, and  $\sum'$  is the summation over all the particles located in the k-th slice. We also divide the system into  $N_s$  slices along the y direction and define  $\bar{d}_{na}^{(y)}(y_k)$  in a similar way. Typical  $\bar{d}_{na}^{(y)}(y_k)$  for a shear-band formed parallel to the x-direction is shown in Fig. S2. Finally, from  $\bar{d}_{na}^{(x)}(x_k)$  and  $\bar{d}_{na}^{(y)}(\alpha_k)$ , we define the normalized distributions  $p_k^{(\alpha)} \equiv \bar{d}_{na}^{(\alpha)}(\alpha_k) / \sum_{l=1}^{N_s} \bar{d}_{na}^{(\alpha)}(\alpha_l)$ for  $k = 1, ..., N_s$  and  $\alpha \in \{x, y\}$ , and then we calculate the corresponding Shannon entropy

$$H^{(\alpha)} \equiv -\sum_{k=1}^{N_s} p_k^{(\alpha)} \ln p_k^{(\alpha)}.$$
 (8)

Finally, the shear-band order parameter H is defined by

$$H \equiv \frac{H^{(y)} - H^{(x)}}{H_{\max}},\tag{9}$$

where  $H_{\text{max}} \equiv \ln N_s$  is a normalized factor defined by the Shannon entropy for a uniform distribution. If the deformation is homogeneous, *i.e.*, no shear-band, then  $H^{(x)} = H^{(y)} = H_{\text{max}}$ , and thus we obtain H = 0. On the other hand, if there is a horizontal (vertical) shear-band, then  $H^{(y)} \ll H^{(x)}$  ( $H^{(y)} \gg H^{(x)}$ ), and thus we obtain Hwith finite and negative (positive) value. The strength of shear-band is captured by the absolute value of H. A typical value of |H| when the clear shear-band is formed is in the order of  $10^{-2}$ . In this study, we define that the shear-band is formed when |H| exceeds numerical criteria of 0.08 for all system sizes we studied.

### S-4. ESTIMATION OF THE CRITICAL TEMPERATURE

In the main text, we found that there exists a critical temperature  $T_c$  separating the nonequilibrium phase diagram into the mechanical annealing (MA) and thermal annealing (TA) regimes. Its value can be estimated by the power-law fitting of the yield strain amplitude  $\gamma_{\rm Y}$  versus  $T_{\rm init}^{-1}$  relation in the TA regime (see



FIG. S3. The energy-strain  $(E-\gamma)$  curves for systems at  $T_{\text{init}} = 0.5$  (a) and 0.085 (b) for several strain amplitudes  $\gamma_0$ . The gray curves represent the trajectories of E from the initial configurations marked by the red dots. The black curves are the averaged trajectories in the steady states. For  $\gamma_0 = 0.104$  of (b), one observes the coexistence of the "initial branch" where the system stay near the ground energy state and the "yielded branch" at high energy. Note that this coexistence is not observed in the poorly annealed system (a). In these figures, the system size is N = 12000 and the finite strain-rate protocol with  $\dot{\gamma}_0 = 6.2832 \times 10^{-4}$ . is used. The yield strain amplitudes are  $\gamma_{\rm Y} \approx 0.078$  for  $T_{\rm init} = 0.5$  and  $\gamma_{\rm Y} \approx 0.101$  for  $T_{\rm init} = 0.085$ .

Fig. 2(b) of the main text). To be specific, we fit  $\gamma_{\rm Y}$  with  $\gamma_{\rm c} + A_0 |T_{\rm init}^{-1} - T_c^{-1}|^{\beta}$ , where  $\gamma_{\rm c} = 0.078$  representing the yield strain amplitude in the MA regime. The best fit shown as the black solid line in the TA regime of Fig. 2(b) of the main text gives  $A_0 \approx 0.017$ ,  $T_c \approx 0.101$ , and  $\beta \approx 0.542$ .

## S-5. THE DEFINITION OF YIELD STRAIN AMPLITUDE AND THE ASSOCIATED DISCONTINUOUS CHANGES

In this section, we present the definition of yield strain amplitude  $\gamma_{\rm Y}$  (shown in Fig. 2(b) of the main text) and the discontinuous change of rheological quantities above yielding, such as  $\Delta \sigma_0$ ,  $\Delta \delta_0$ , and  $\Delta G'$  (shown in Fig. 1(d) of the main text).

## A. Bistability in the TA regime

In the main text, we have shown that the oscillatory shear brings the system in the MA regime into a deeper energy state before yielding, up to the deepest energy at  $\gamma_0 \rightarrow \gamma_{\rm Y}^-$ . On the other hand, for systems in the TA regime, the mechanical training by oscillatory shear does not stabilize the system and the system's initial memories are kept until yielding. Fig. S3 demonstrates the evolution of the instantaneous average energy  $E \equiv (1/N) \sum_{i>j} U(r_{ij})$  as a function of the strain  $\gamma$  for typical MA and TA systems under several strain amplitude  $\gamma_0$  across the yielding point.

Interestingly, in the TA regime, we observe a bistable or coexistence phase in the vicinity of yielding,  $\gamma_0 \approx \gamma_{\rm Y}$ ; Look at Fig. S3(b), where  $\gamma_0 = 0.104$  (>  $\gamma_Y \approx 0.101$ , whose exact definition will be given below). We clearly observe that some trajectories stay in the initial ground state (the initial branch) where the trajectory is parabolic whereas the others reach the higher energy state with loop-shaped trajectories signaling that the system is in the yielded branch. For a finite system size simulation, the initial and yielded branches can coexist over a finite region of the strain amplitude. This coexistence region is too narrow to recognize in Figs. 1(a)-(c) and 2(a) in the main text. Larger system size makes this coexistence region even narrower (data not shown), which is consistent with the observation that yielding transition of a well-annealed system under uniform shear is sharper for larger systems [10].

We emphasize that this bistable coexistence of the initial and yielded branches is an unique feature of TA regime, which is strongly related to the abrupt and discontinuous changes of the physical observables such as  $\sigma_0$  and  $\delta_0$  at the yielding point (see Fig. 1(d) of the main text). In the MA regime, where  $\Delta \sigma$ ,  $\Delta \delta_0$ , and  $\Delta G'$  are negligibly small (see also Sec. S-6 E for more discussion), one does not observe such a coexistence region even for a larger system (N = 48000).

#### B. The definition of yield strain amplitude

We use the different methods to determine the yielding transition point  $\gamma_{\rm Y}$  depending on whether the system is in the MA or TA regimes. In the MA regime, we can simply define  $\gamma_{\rm Y}$  as the point beyond which  $E_{\rm IS}$  starts increasing. On the other hand, in the TA regime, due to the coexistence region over which the initial and yielded branches are overlapped, we define  $\gamma_{\rm Y}$  as the geometrical average of the endpoint of both branches. In other words,  $\gamma_{\rm Y} \equiv (\gamma_1 + \gamma_2)/2$ , where  $\gamma_1$  and  $\gamma_2$  are the smallest and largest values of the yielded and initial brunches, respectively. Note that the error of the estimated  $\gamma_{\rm Y}$ 's has different origins in the MA and TA regimes. In the MA regime, it is merely due to the finite discretization of the data point. In the TA regime, it is due to the finite system size, and the corresponding error is expected to disappear in the thermodynamic limit.

$\dot{\gamma}_0$ N	1500	3000	6000	12000	48000
0 (AQS)	Ν	Ν	Ν	Т	Y
$6.2832 \times 10^{-4}$	Ν	Ν	Ν	Т	Y
$5.2360 \times 10^{-3}$	Ν	Ν	Ν	N	N
$3.1416 \times 10^{-2}$	Ν	Ν	Ν	Ν	Ν

TABLE I. The existence condition for the persistent shearband in the steady state after yielding. Several different combinations of the system size N and the strain rate  $\dot{\gamma}_0$  are explored. In this table, 'Y' and 'N' represent the cases that the shear-band is observed and is not observed, respectively. 'T' represents the case where the metastable shear-band is found.

$\gamma_0$ Setup	0.085	0.09	0.11	0.12	0.125	0.13	0.15
N = 12000 (AQS)	Т	Ν	Ν	Ν	Ν	Ν	Ν
N = 48000 (AQS)	Y	Y	Y	Y	Т	Ν	Ν

TABLE II. The existence condition for the persistent shearband in the steady state after yielding. The dependence on the strain amplitude  $\gamma_0$  for N = 12000 and 48000 systems in the AQS limit are explored. Note that the yield strain amplitude  $\gamma_Y$  for these two cases is about 0.08 (see Fig. S10(b) for details). The notations are the same as Table I.

#### C. The discontinuous changes above yielding

In Fig. 1(d) of the main text, we plot the height of the discontinuous jump of several rheological observables at the yielding transition point. Due to i) the presence of the coexistence of the initial and yielded brunches and ii) the small but finite discontinuity even in the MA regime (see Sec. S-6 E for details), special care is required to define these jumps. A precise definition of  $\Delta \sigma_0$ ,  $\Delta \delta_0$ , and  $\Delta G'$  is

$$\Delta A \equiv \left| \frac{A_Y(\gamma_0 = \gamma_Y) - A_{\rm ini}(\gamma_0 = \gamma_Y)}{A_{\rm ini}(\gamma_0 = \gamma_Y)} \right|, \qquad (10)$$

where  $A \in \{\sigma_0, \delta_0, G'\}$ .  $A_{\text{ini}}(\gamma_0)$  and  $A_Y(\gamma_0)$  are the observables in the initial and yielded branches, respectively. In the MA regime, this definition naturally leads to  $\Delta A = 0$  since there is no bistability.

## S-6. THE EFFECTS OF FINITE SIZE AND FINITE STRAIN RATE

#### A. The existence condition of shear-bands

In the main text, we argued that a persistent shearband might form in the steady state for the system under oscillatory shear after yielding. In this subsection, we systematically examine the effects of the system-size N, strain rate  $\dot{\gamma}_0$ , and strain amplitude  $\gamma_0$  on the existence of the shear-bands.

Table I summarizes our simulation results for various N and  $\dot{\gamma}_0$ . We found that persistent shear-bands are

$\dot{\gamma}_0$ N	1500	3000	6000	12000	48000
0 (AQS)	Y	Y	Y	Y	Y
$6.2832 \times 10^{-4}$	Y	Y	Y	Y	Y
$5.2360 \times 10^{-3}$	Y	Y	Y	Y	Y
$3.1416 \times 10^{-2}$	Ν	Ν	Ν	Ν	Ν

TABLE III. The existence condition for the initial shear-band for well annealed system ( $T_{\text{init}} = 0.085$ ) during the relaxation process after yielding ( $\gamma_0 = 0.11 > \gamma_{\text{Y}}$ ). Several different combinations of the system size N and maximum strain rate  $\dot{\gamma}_0$  are explored. The notations are the same as Table I.

observed only if N is large and  $\dot{\gamma}_0$  is small enough. Interestingly, in an intermediate region where N = 12000and  $\dot{\gamma}_0 \geq 6.3 \times 10^{-4}$ , we found that the system is in a metastable regime and the shear-bands are repeatedly created and annihilated in the steady state. The existence of the persistent shear-band also sensitively depends on  $\gamma_0$ . In Table II, we examine the effect of  $\gamma_0$  on the shear-band formation. We find that both the persistent and metastable shear-band can be observed only when  $\gamma_0$  is close to the yield strain amplitude  $\gamma_{\rm Y}$ . For large  $\gamma_0$ , say  $\gamma_0 \geq 0.13$ , the shear-band in the steady state does not exist even for N = 48000 in the AQS limit.

We found that the persistent shear-band is observed for both MA and TA regime, irrespective of the preparation temperature  $T_{\text{init}}$ , as long as N is large and  $\dot{\gamma}_0$  is small. We emphasize that the persistent shear-band is observed in the steady state, hence it is naturally independent of  $T_{\text{init}}$ .

On the contrary, the initiation of the shear-band formation during the transient region on the way to the steady state after yielding is sensitively affected by  $T_{\text{init}}$ . As we show in the main text, exactly when the wellannealed system with  $T_{\rm init} < T_{\rm c}$  yields, a strong shearband concomitantly appears, which gradually weakens during the transient period. We refer to this as the "initial shear-band". In Table III, we list the existence condition of the initial shear-band for various N and  $\dot{\gamma}_0$ . Interestingly, the initial shear-band formation is less sensitive to N and  $\dot{\gamma}_0$  than that of the persistent shearband (see Table. I). The initial shear-band exists even when the persistent shear-band is absent in the steady state. If  $\dot{\gamma}_0$  is too large, even the initial shear-band disappears. Fig. S4 demonstrates this  $\dot{\gamma}_0$ -dependence. Fig. S4(a) shows that the energy at the end of each cycle  $E_0(n) \equiv E(t = nT_{cyc})$  increases with time, as the system evolves towards the yielding. Fig. S4(b) shows the *n*dependence of the shear-band order parameter |H|. The initial shear-band can form only for small  $\dot{\gamma}_0$  (see the red squares in Fig. S4(b)) where the shear-band develops at the transient period  $n \approx 2$  but fades away eventually in the long time limit, since the  $\gamma_0$  we used for demonstration ( $\gamma_0 = 0.15$ ) is larger than the maximum value for the existence of persistent shear band ( $\approx 0.13$ , see Table I). These observations suggest that the mechanism of the



FIG. S4. Shear-band formation process of well-annealed systems with the system size N = 12000, strain amplitude  $\gamma_0 = 0.15 > \gamma_{\rm Y}$ , and preparation temperature  $T_{\rm init} = 0.085$ , varying the strain rate  $\dot{\gamma_0}$  (see the legend shown in (b). One realization is plotted for each  $\dot{\gamma_0}$ 's). We plot the energy at the end of each cycle  $E_0$  (a) and the shear-band order parameter |H| (b) versus the number of shearing cycle n. The arrows in (b) indicate the times when the value of |H| are maximized  $(n = 2 \text{ for } \dot{\gamma}_0 = 6.2832 \times 10^{-4} \text{ and } n = 250 \text{ for}$  $\dot{\gamma}_0 = 3.1416 \times 10^{-2}$ . Their corresponding spatial profile of the one-cycle non-affine deformation  $d_{na,i}$  are plotted in (c) and (d), respectively). It is worth to note that, even though  $E_0$ changes dramatically for the case  $\dot{\gamma}_0 = 3.1416 \times 10^{-2}$  indicating that yielding has actually happened, both the initial and persistent shear-bands are absent during the relaxation process.

formation of persistent shear-band and initial shear-band is fundamentally different. The latter originates from initial stability of the glass sample, or the initial memories, which is akin to the sharp shear-bands observed for well annealed glasses under uniform shear [10].



FIG. S5. Three typical non-affine trajectories on the x-y (a) and y-z (b) planes for the shear-band shown in Fig. S4(c) (the corresponding profile of coarse-grained  $d_{\mathrm{na},i}$  is shown in Fig. S2). Note that  $\hat{\mathbf{x}}$  is the flow direction,  $\hat{\mathbf{y}}$  is the shear-gradient direction, and  $\hat{\mathbf{z}}$  is the vorticity direction. The particles are chosen so that they are located at  $y_i/L \approx 0.5$ , 0, and 0.3, representing the positions inside, outside, and on the boundary of shear-band, respectively (see the legend shown in (a)). The trajectories are plotted within one shearing cycle (n = 2) and their corresponding  $d_{\mathrm{na},i}(n = 2)$  values are 12.39, 1.19, and 5.05. We shift all of the trajectories by  $\mathbf{r}_i^{(\mathrm{na})}(\mathrm{ref}) \equiv \mathbf{r}_i^{(\mathrm{na})}(t = T_{\mathrm{cyc}})$ , the end position of non-affine trajectory of the first cycle, for better comparison.

# B. The non-affine trajectories when a shear-band is present

In Figs. S2 and S4(c), we have shown that when an initial shear-band is formed (at cycle n = 2), its spatial distribution of  $d_{na,i}$  is highly inhomogeneous. Typically, for particles located in the center of the shear-band, one finds  $d_{na,i} \approx 13$  for some particles. To see why there are such large value of  $d_{na,i}$ , in Fig. S5, we plot three representative one-cycle non-affine trajectories  $\mathbf{r}_i^{(na)}(t)$  (defined in Sec. S-2) for particles located inside, outside, and on the boundary of shear-band, respectively. For the particle inside the shear-band, the trajectory winds around to form a large loop (see black curve in Figs. S5(a) and (b)). This leads to a large value of  $d_{na,i}$  even though the one-cycle end-to-end distance is very small (typically smaller than one particle diameter). On the other hand,



FIG. S6. (a) The steady state inherent structure  $E_{\rm IS}$  versus the strain amplitude  $\gamma_0$  for poorly annealed systems with several different strain rate  $\dot{\gamma}_0$ 's (see the legend shown in (a)).  $\dot{\gamma}_0 = 0$  represents the AQS limit. (b) The  $\dot{\gamma}_0$ -dependence on the yield strain amplitude  $\gamma_{\rm Y}$ . The system size is N = 12000 and the preparation temperature  $T_{\rm init} = 0.5$ . The error bars represent the standard deviation among samples in (a) and the uncertainty region to find  $\gamma_{\rm Y}$  in (b).

for the particles located away from the shear-band center, the  $\mathbf{r}_{i}^{(\mathrm{na})}(t)$  is relatively localized (red and green curves in Figs. S5(a) and (b)) and results in smaller  $d_{\mathrm{na},i}$ .

# C. Strain-rate dependence on the yielding transition

In this subsection, we study the effect of  $\dot{\gamma}_0$  on the yielding transition. For illustration, we focus on a poorly annealed system with  $T_{\text{init}} = 0.5$  and N = 12000. The results of the steady state inherent structure (Fig. S6(a)) and rheological properties (Fig. S7) reveal that the yield strain amplitude  $\gamma_{\rm Y}$  increases with  $\dot{\gamma}_0$ , which is consistent with the previous works in oscillatory shear [11] and uniform shear [12]. These results are natural because, if the strain rate is large, plastic activities would be suppressed due to shorter response time in each cycle, and this would



FIG. S7. The steady state rheological properties under oscillatory shear as a function of the strain amplitude  $\gamma_0$  for poorly annealed system with several different strain rate  $\dot{\gamma}_0$ 's (see the legend shown in (a)). (a) The stress amplitude  $\sigma_0$ , (b) phase lag between stress and strain  $\delta_0$ , (c) storage modulus G', and (d) loss modulus G''. In these figures, we use the system size N = 12000 and preparation temperature  $T_{\text{init}} = 0.5$ . The error bars represent the standard deviation among samples.

facilitate affine displacements [13, 14] and coordinated motions [15] of particles. As a result,  $\gamma_{\rm Y}$ , which marks the maximum strain amplitude where the particles can maintain their structure under oscillatory shear, should shift to a larger value. The dependence of  $\gamma_{\rm Y}$  on  $\dot{\gamma}_0$  is summarized in Fig. S6(b).

Another important message is that the result of  $\dot{\gamma}_0 = 6.2832 \times 10^{-4}$  almost overlaps with the results of the AQS limit, except at the very large  $\gamma_0$  (see black circles and red squares in Figs. S6(a) and S7(a)–(d)). This guarantees that our results which we obtained using the finite strain-rate protocol with  $\dot{\gamma}_0 = 6.2832 \times 10^{-4}$  in the main text, especially the phase diagram shown in Fig. 2(b) in the main text, agree with those of the AQS protocol.

#### D. The phase diagram in higher strain rate

In this subsection, we consider how the phase diagram is altered when the high strain rate  $\dot{\gamma}_0 = 3.1416 \times 10^{-2}$ is used. Recall that this strain rate is high enough to diminish both the initial shear-band and the persistent shear-band (see Tables I and III). We study the  $T_{\text{init}}$  dependence of the yielding transition. The result is shown in Fig. S8(a). Compared with Fig. 2(a) in the main text, we find that the results remain qualitatively unchanged. The major difference is a systematic shift of  $\gamma_{\rm Y}$  for all curves with different  $T_{\text{init}}$ . Most importantly, even in such a high strain rate, the critical temperature  $T_c$  can still be identified. In Fig. S8(b), we compare the dependence of  $\gamma_{\rm Y}$  on  $1/T_{\text{init}}$  for both low and high strain



FIG. S8. (a) The steady state inherent structure  $E_{\rm IS}$  as a function of the strain amplitude  $\gamma_0$  for the systems under higher strain rate  $\dot{\gamma}_0 = 3.1416 \times 10^{-2}$  with several different preparation temperature  $T_{\rm init}$ 's (see the legend shown in (a)). Dashed vertical lines represent the discontinuous jumps. (b) The yield strain amplitude  $\gamma_{\rm Y}$  versus  $1/T_{\rm init}$  for the systems with lower (black circles) and higher (blue triangles)  $\dot{\gamma}_0$ . Note that the  $E_{\rm IS}$  versus  $\gamma_0$  plot and the phase diagram of lower  $\dot{\gamma}_0$  are shown in Fig. 2 of the main text. The red dashed line in (b) represents the critical temperature  $T_c \approx 0.101$  (see the main text for details). In these figures, we use the systems under oscillatory shear with the system size N = 12000. The error bars represent the standard deviation among samples in (a) and the uncertainty region to find  $\gamma_{\rm Y}$  in (b).

rates. The critical temperature seems to be insensitive to  $\dot{\gamma}_0$ . Combined this result with the fact that there is no shear-band in the high strain rate, we conclude that the critical temperature is independent of both strain rate and the presence/absence of shear-banding. Instead, it more likely originates from the intrinsic characteristics of the initial glassy states.



FIG. S9. The relaxation process of (a) the energy  $E_0$  at the end of each cycle and (b) the one-cycle displacement  $\Delta r$  as a function of *n* with several different system size *N*'s (see the legend shown in (a)). (c) The average relaxation cycle  $\tau_{\rm L}$  as a function of *N*. In these figures, we use the AQS protocol with the strain amplitude  $\gamma_0 = 0.04$  ( $\langle \gamma_{\rm Y} \rangle$ ) and the preparation temperature  $T_{\rm init} = 0.5$  (a poorly annealed system). The error bars in (c) represent the standard deviation among samples.

# E. Effect of the system size and the influence of the persistent shear-band on the yielding transition

In this subsection, we shall consider whether the presence/absence of the persistent shear-band affects the yielding transition itself. In order to control the shearband formation, we change the system size N. Here, we shall consider a poorly annealed system ( $T_{\text{init}} = 0.5$ ) and use the AQS protocol to avoid the effect of the finite strain rate.

Before we proceed, it is convenient to introduce another nonequilibrium phase transition known as the reversible-irreversible (RI) transition [16, 17], which is accompanied by the yielding transition under oscillatory shear: When  $\gamma_0 < \gamma_{\rm Y}$  and in the steady state, each particle comes back to the identical position after every cycle (or multiple cycles) of oscillatory shear, hence the sys-



FIG. S10. (a) The steady state inherent structure  $E_{\rm IS}$  as a function of the strain amplitude  $\gamma_0$  for poorly annealed systems under oscillatory shear in the AQS limit with several different system size N's (see the legend shown in (a)). The inset shows the zoom-in of the region in the vicinity of the yielding strain amplitude for N = 12000 and 48000 systems. The solid curves in the inset are guides for the eyes. (b) The yield strain amplitude  $\gamma_{\rm Y}$  versus N. In these figures, we use the systems with the preparation temperature  $T_{\rm init} = 0.5$ . The error bars represent the standard deviation among samples in (a) and the uncertainty region to find  $\gamma_{\rm Y}$  in (b).

tem is in a reversible state [18, 19]. If  $\gamma_0 > \gamma_Y$ , on the other hand, many particles do not meet the above condition and their trajectories become diffusive. It is the irreversible state. A typical order parameter of the RI transition is the one-cycle displacement  $\Delta r$  defined as the average end-to-end distance of particle trajectories per cycle;

$$\Delta r(n) \equiv \frac{1}{N} \sum_{i} \left| \mathbf{r}_{i}(n) - \mathbf{r}_{i}(n-1) \right|, \qquad (11)$$

where *n* is the number of cycles,  $\mathbf{r}_i(n)$  denotes the position of the *i*-th particle at the end of the *n*-th cycle. The steady-state value of  $\Delta r$  is zero in the reversible state and discontinuously jumps to a finite value at  $\gamma_0 = \gamma_{\rm Y}$ . Typical time (*n*) evolution of  $\Delta r$  towards a reversible state below yielding is shown together with that of the energy  $E_0$  in Figs. S9 (a) and (b).



FIG. S11. The steady state rheological properties under oscillatory shear in the AQS limit as a function of the strain amplitude  $\gamma_0$  for poorly annealed systems with several different system size N's (see the legend shown in (a)). (a) The stress amplitude  $\sigma_0$ , (b) phase lag between stress and strain  $\delta_0$ , (c) storage modulus G', and (d) loss modulus G''. In these figures, we use the systems with preparation temperature  $T_{\text{init}} = 0.5$ . The error bars in each figures represent the standard deviation among samples.

Figs. S9(c) shows that the relaxation time  $\tau_{\rm L}$  for the system to reach a reversible state increases with system size [16]. During the relaxation process towards a reversible state, the configuration of particles is optimized so that the number of plastic events is largely suppressed [18]. Therefore, it is natural to expect that a larger system should take a longer time to reach stationary state because there are more plastic events to be eliminated.

In Fig. S10(a), we show the steady state inherent structure  $E_{\rm IS}$  as a function of  $\gamma_0$  for three different system sizes (N = 3000, 12000, and 48000). It is clearly demonstrated that  $E_{\rm IS}$  decreases with increasing N below yielding. This trend can also be seen in Fig. S9(a). One possible explanation is that the larger system requires the longer  $\tau_{\rm L}$ , which in turn makes the system explore the potential energy landscape for a longer time and settle down in a deeper energy state before being trapped in a periodic trajectory. After yielding, one observes that  $E_{\rm IS}$  is less sensitive to N, except for the vicinity of yielding point, where  $\gamma_{\rm Y}$  sensitively depends on N as shown in Fig. S10(b) (see also Ref. [16]). As discussed in Sec. S-6 D, this is the only region where the persistent shear-band develops and it is natural to expect that the presence of the shear-band at large system sizes (see Table I) influences  $E_{\rm IS}$  near the yielding point. The inset of Fig. S10(a) shows that there is a small but distinct discontinuous change of  $E_{\rm IS}$  for N = 48000 at the yielding point, which is not clearly observed for smaller systems. A similar discontinuity has been reported in Ref. [9]. The reason why we do not clearly observe discontinuous jumps for smaller systems may be because i) the persistent shear-band is absent after yielding and ii) the systems are trapped to the reversible state easily before proper relaxation before yielding. We still have not fully confirmed these conclusions. Other studies showed a discontinuous, though less sharp, even for the small systems [20].

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Fig. S11 shows that rheological properties are also sensitive to N in the vicinity of the yielding point due to the presence of persistent shear-band of the large system. In particular, in the largest system we simulated (N = 48000), one observes very small but finite discontinuous changes of observables even though the system is poorly annealed.

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