Avalanches and Structural Change in Cyclically Sheared Silica Glass

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We investigate avalanches associated with plastic rearrangements and the nature of structural change in the prototypical strong glass, silica, computationally. Although qualitative aspects of yielding in silica are similar to other glasses, we find that the statistics of avalanches exhibits non-trivial behaviour. Investigating the statistics of avalanches and clusters in detail, we propose and verify a new relation between exponents characterizing the size distribution of avalanches and clusters. Across the yielding transition, anomalous structural change and densification, associated with a suppression of tetrahedral order, is observed to accompany strain localisation.

The mechanical response of amorphous solids such as metallic glasses, window glass, foams, emulsions, colloidal suspension etc., to external deformation or applied stress is of central importance to characterise their behaviour and determining their utility [1, 3]. The response for large enough deformations involves plastic rearrangements, leading eventually to yielding. The yielding transition in amorphous solids has been investigated actively in recent years through experiments [4–8], numerical simulations [9–19] and theoretical investigations including analysis of elasto-plastic and other models [20–30]. Yielding has been observed to be a discontinuous transition for sufficiently well annealed glasses under uniform shear [17] and for cyclic shear [15, 18, 31], accompanied by a discontinuous drop in energy and stress, and by localisation of strain in shear bands [18, 32–34].

Plasticity in amorphous solids is distinguished from that in crystalline solids [35] by the absence of well defined structural defects with which it can be associated. Thus, the structural aspects of plastic rearrangements [18, 36–40] have been a subject of investigation, to understand the structural motifs associated with plastic rearrangements below yielding, and to investigate the structural features that distinguish the regions in which plasticity is concentrated.

Another aspect of the approach to yielding and steady state flow that has received considerable attention is the distribution of avalanches corresponding to plastic rearrangements [41, 45, 21, 31, 32], of interest also in a wide variety of phenomena exhibiting crackling noise [43]. The avalanche distribution is expected to have a power-law form, with a characteristic cutoff that is finite below yielding, with a mean field prediction of $\tau = 3/2$ for the power law exponent. The scaling form has been rationalised by several elasto-plastic models and mean-field theories constructed to pin down the scaling properties of avalanches [21, 44, 48]. In numerical simulations, the avalanche distribution is found to be different across the yielding transition for cyclic shear [15], and to depend on factors such as the inertia of the system [49], shear rate [15], and the quantification of avalanche size (in terms of energy drops, or the size of the connected clusters of active particles) [15]. The dependence of the characteristic size of the avalanches on system size have been analysed [10, 15, 17], with an observed $N^{1/3}$ scaling with the number of particles $N$. The implication of long range interactions on the break up of avalanches into clusters, and their statistics have been investigated for crack propagation [50, 51], but not, to our knowledge, in the context of yielding of glasses. Performing such analysis, in addition to confirming key results in [51], we propose and verify a new relation between exponents characterising avalanches and clusters.

Computational investigations of yielding in amorphous solids described above have largely been performed for solids with particles interacting with spherically symmetric, short ranged interactions. In particular, relatively few studies [52, 53, 54] have addressed the archetypal glass, silica, which is characterised by an open, tetrahedral, local geometry, and whose interaction potential includes long range Coulomb interactions (or silicon [57–60], which shares several geometric and thermodynamic characteristics). In the liquid state, the tetrahedral network structure of silica entails a rich spectrum of novel behavior, including density maxima [61, 62], a liquid-liquid phase transition [63, 64] and a strong-to-fragile transition [65, 66]. It is of interest to investigate the role of such directional, tetrahedral local geometry, and of long range interactions in the yielding behavior of silica and, in particular, the nature of avalanches and the structural changes involved in plasticity and strain localisation. The yielding behavior of silica under cyclic shear has been shown to be broadly similar to that for the Kob-Andersen binary Lennard-Jones mixture (KA-BMLJ) [31], characterised by a qualitative change across a threshold temperature of $T_{th} = 3100 K$ (see Fig. S1 in Supplemental Material (SM) for illustration). In contrast, we show in this letter that the nature of avalanches and structural change associated with yielding display unusual features in the case of silica.

We study a version of the BKS model introduced by Saika-Voivod [65, 69] (see SM for details). We prepared several equilibrated samples by performing constant temperature (NVT) molecular dynamics simula-
Avalanche properties display significant size dependence and, for this reason, we also simulate sizes ranging from \( N = 1728\) to \( N = 74088\). All the samples are equilibrated for at least \( 20 \tau_\alpha\), \( \tau_\alpha\) being the structural relaxation time obtained from the self intermediate scattering function \( F_0(k, t)\). Inherent structures (energy minimum configurations) obtained from instantaneous quenches of equilibrated liquid configurations are then subjected to an athermal quasi-static shearing (AQS) protocol involving two steps: (i) affine deformation by a small strain increments of \( d\gamma = 2 \times 10^{-4}\) in the \( xy\)-plane \((x' \rightarrow x + d\gamma y, y' \rightarrow y, z' \rightarrow z)\) and (ii) energy minimization. The procedure is then repeated and the strain \( \gamma \) is varied cyclically as : \( 0 \rightarrow \gamma_{\text{max}} \rightarrow -\gamma_{\text{max}} \rightarrow 0\). Repeating the deformation cycle for a fixed strain amplitude \( \gamma_{\text{max}}\), the glasses are driven to the steady state wherein properties of the system remain stable with further cycles of strain.

We consider 12 samples for \( N = 1728\), 4 samples for \( N = 5832\) and 3824, and one sample for \( N = 27000\) and \( N = 74088\) to perform the cyclic shear. We employ the conjugate-gradient algorithm for energy minimization and execute all the numerical simulations in LAMMPS [70].

We investigate avalanches by computing the statistics of avalanche size \((S)\), cluster size \((s)\), and the number of clusters \((n_c)\). The size of the avalanches is computed as the total number of active particles during a plastic rearrangement, identified by computing the deviatoric strain \( \epsilon_d \) for each particle. Active particles are identified as those for which \( \epsilon_d > 0.22\), following the procedure introduced in [71] (see SM). We further obtain the sizes of clusters of connected active particles. Distributions of avalanche size and cluster size for several \( \gamma_{\text{max}}\) are shown in Fig. 1(a) and follow power laws with exponents close to \( \tau_c = 1.1\) for avalanches and \( \tau_c = 2\) for clusters, with \( \gamma_{\text{max}}\) dependent cut-offs in each case. Strikingly, the cluster size exponent \( (\tau_c)\) is significantly greater than the mean field value, 3/2 [35], whereas \( \tau_c\) is significantly smaller. The distributions of energy drops, however, follow a power-law with exponent \( \approx -1.25\) (see SM) as also observed for the KA-BMLJ [15] for which \( \tau_c = 3/2\).

In order to confirm these exponents, we perform a finite scaling analysis of the distributions of \( S, s_c\) and \( n_c\), for \( \gamma_{\text{max}} = 0.25\) (consistent results for other \( \gamma_{\text{max}}\) are shown in the SM). We assume a scaling form for cluster size

\[
P(s_c) \approx N^{-\beta_c} f \left[ s_c / N^{\beta_c / \tau_c} \right],
\]

where the scaling function \( f(x) \rightarrow x^{-\tau_c} \) for \( x \rightarrow 0\), and \( f(x) \rightarrow 0 \) for \( x \rightarrow 1\). This scaling form implies that the moments \( \langle s_c^n \rangle \sim N^{\alpha(m)}\), where \( \alpha(m) = \beta(m + 1 - \tau_c) / \tau_c\) is the moment exponent [72] [73] (see SM for details). In the inset of Fig. 1(b), we show a log-log plot of \( \langle s_c^n \rangle\) against \( N\) for \( m = 1, 2, 3\), and 4, from which we obtain \( \alpha(m)\). In Fig. 1(b), we present \( \alpha(m)\) and the corresponding derivative \( \partial \alpha(m) / \partial m\) (which must equal \( \beta_c / \tau_c\) for large \( m\) as a function \( m\). By a linear fit of \( \alpha(m)\) in the large \( m\) range, we determine \( \beta_c / \tau_c = 0.79 \pm 0.02\) and \( \beta_c = 1.70 \pm 0.10\). Fig. 1(c) shows the scaled distribution \( P(s_c, N) N^{\beta_c / \tau_c}\) plotted against the scaled variable \( s_c / N^{\beta_c / \tau_c}\), using these values, for different system size \( N\) to obtain the data collapse which supports the validity of the assumed scaling function. However, the collapsed data is best described by \( \tau_c = 2\) (close to, but slightly smaller than, \( \tau_c = 2.15 \pm 0.07\) obtained from \( \beta_c / \tau_c\) above) which we treat as our estimate below (see SM, Fig. S7, that further supports the value \( \tau_c = 2\). Assuming similar scaling forms for \( S\) and \( n_c\), we estimate
tem. While the former analysis for silica yields deviatoric local strain for analysing the KA-BMLJ systems as reported in [15] for KA-BMLJ, and employ the active by identifying to these systems may provide an explanation. We speculate that the open framework structure common model [75]. Although the details in these systems differ, and in preliminary results for a short ranged silica-like such consistent analysis within the framework of [51], the Such consistency is also obtained for a two dimensional is surprising. Similar values have been with that does not vary with \( \gamma_{\text{max}} \), and the structure is indistinguishable from that of the initial undeformed samples. Beyond yielding, the distributions evolve and become broader with increasing amplitude \( \gamma_{\text{max}} \). The high \( q_i \) peak value becomes less pronounced and shoulder around \( q_i \approx 0.4 \) appears. Interestingly, the variation of \( P(q_i) \) with increasing \( \gamma_{\text{max}} \) has a strong resemblance to what is observed in equilibrium when temperature is increased [76]. For \( T = 6000K \), Fig. 2(b), the behaviour is very different. Below yielding, a strong enhancement of the tetrahedral order upon increasing \( \gamma_{\text{max}} \) is observed, with the initial undeformed glass displaying very weak tetrahedral order. This effect is reflected in the growth of the high \( q_i \) peak which continues until the yielding amplitude is reached. Beyond yield, similarly to what is observed for the low temperature case, the peak value decreases with \( \gamma_{\text{max}} \).

To further characterize the structural disorder induced by deformation, we study the mean and variance of \( q_i \) as a function of strain amplitude for different \( T \) as shown in Figs. 2(c) and 2(d) respectively. As expected, two very different trends are observed below and above yielding. Below yielding, we observe again two patterns. For \( T > T_{\text{th}} \), \( \langle q_i \rangle \) progressively increases with \( \gamma_{\text{max}} \) up to the the yield amplitude. Interestingly, the maximum orientational order is obtained at the yielding amplitude where, for all the cases with \( T \geq T_{\text{th}} \), it converges to 0.7 which is the value of \( \langle q_i \rangle \) for the undeformed samples at \( T_{\text{th}} \) (see Fig. S16 of SM). For \( T < T_{\text{th}} \), \( \langle q_i \rangle \) does not vary with \( \gamma_{\text{max}} \) until the yield point where it abruptly drops to the same values as for the high temperature case. Above yielding, all the curves collapse, indicating that the final structure depends only on the strain amplitude and not on the initial temperature. In this regime, \( \langle q_i \rangle \) decreases with \( \gamma_{\text{max}} \), indicating a progressively less tetrahe-
FIG. 2. Distributions $P(q_i)$ of the tetrahedrality parameter for zero strain configurations of cyclically deformed silica for different strain amplitude $\gamma_{\text{max}}$ for (a) $T = 2500\, \text{K}$ and (b) $T = 6000\, \text{K}$. (c) Averages $(q_i)$ and (d) Variances $\langle (\partial q_i)^2 \rangle = \gamma_i^2 - \langle q_i \rangle^2$, as a function of $\gamma_{\text{max}}$ for different temperatures $T$. Data are averaged over several configurations collected from different samples in the steady state for each $\gamma_{\text{max}}$. The vertical dashed line indicates the yield strain, dotted lines through data points are guide to the eyes and the arrows indicate the direction of increasing temperature.

We next investigate structural features associated with strain localization [18] above the yield strain amplitude. In Fig. 3(c) (inset), we show a snapshot of a zero strain configuration for the largest system size simulated ($N = 74088$) at a strain amplitude $\gamma_{\text{max}} = 0.23$. The color map corresponds to the deviatoric strain $\epsilon_d$, computed between two consecutive stroboscopic configurations, up to a cut-off value 1.25 (See SM for the discussion about this choice), highlighting the localisation of strain in a shear band. In Ref. 18 and 40 the density within the shear band was shown to be less than the average density. We compute and plot the slab-wise density $\langle \rho_x \rangle$ along $x$-direction in Fig. 3(b). Contrary to the observation in [18, 40], we find that $\langle \rho_x \rangle$ becomes progressively larger inside the shear band, with the number of cycles of shear. This reversal of trend is clearly a reflection of the fact that the energetically favorable tetrahedral structure of silica has lower density than more disordered structures, which leads to well-known density and other anomalies in silica [70]. In order to verify this expectation, we compute slab-wise averages of $q_i$, which are shown in Fig. 3(c). These results clearly demonstrate that the higher density structure within the shear band also has reduced orientational order, analogous to observations in [39, 77]. The suppressed tetrahedral order within the shear band is associated with the enhancement of the fraction of 5-coordinated defects (See Fig. S19 of SM). We compute the distributions of $q_i$ within and outside the shear band, and compare with the aggregate distribution in Fig. 3(d). These distributions reveal the structure within the shear band to be comparable to high temperature undeformed glasses, whereas outside, the are comparable to low temperature glasses.

In summary, we have investigated the statistics of avalanches and clusters in silica and obtained a satisfactory analysis of the relationship between exponents within a framework [51] that envisages the fragmentation of avalanches in the presence of long range interactions. We have further proposed and verified a new relation between avalanche and cluster exponents. How the microscopic structure may lead to the fragmentation of avalanches is an interesting question to investigate further. We have also investigated structural change across the yielding transition and differences in structure within and outside shear bands and have found that yielding and the formation of shear bands is accompanied by a reduction of tetrahedral order, which corresponds to an anomalous increase (rather than decrease) of density. Although the qualitative features of yielding in silica are analogous to other glass formers, the special features of local geometry in silica apparently lead to unusual avalanche
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