Evolution of displacements and strains in sheared amorphous solids

Craig E Maloney\(^1,2\) and Mark O Robbins\(^2\)

\(^1\) Department of Civil and Environmental Engineering, Carnegie Mellon University, Pittsburgh, PA, USA
\(^2\) Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD, USA

E-mail: craigmaloney@cmu.edu and mr@pha.jhu.edu

Received 5 February 2008, in final form 22 February 2008
Published 29 May 2008
Online at stacks.iop.org/JPhysCM/20/244128

Abstract
The local deformation of two-dimensional Lennard-Jones glasses under imposed shear strain is studied via computer simulations. Both the mean squared displacement and mean squared strain rise linearly with the length of the strain interval \( \Delta \gamma \) over which they are measured. However, the increase in displacement does not represent single-particle diffusion. There are long-range spatial correlations in displacement associated with slip lines with an amplitude of order the particle size. Strong dependence on system size is also observed. The probability distributions of displacement and strain are very different. For small \( \Delta \gamma \) the distribution of displacement has a plateau followed by an exponential tail. The distribution becomes Gaussian as \( \Delta \gamma \) increases to about 0.03. The strain distributions consist of sharp central peaks associated with elastic regions, and long exponential tails associated with plastic regions. The latter persist to the largest \( \Delta \gamma \) studied.

(Some figures in this article are in colour only in the electronic version)

1. Introduction
The mechanical properties of amorphous materials are important in many structural applications and the microscopic mechanisms underlying plastic deformation have been the subject of great theoretical interest [1–3]. While deformation of crystalline materials can be understood through the generation and propagation of dislocations, no analogous defect has been identified in disordered materials. This has a direct impact on their mechanical properties, since dislocation motion reduces the yield stress of crystals by orders of magnitude. In the last decade, it has also been realized that amorphous materials share many features with colloids, granular media and other systems where motion is jammed or arrested by packing constraints [4–6]. Common features are observed in the onset of motion under external forces in such systems, and understanding their behavior represents a fundamental problem in nonequilibrium statistical mechanics.

Recent simulations and experiments have followed the motion of individual atoms or particles to understand how disordered solids deform under shear [2, 5–30]. One of the most studied quantities has been the van Hove function \( P(\Delta r; \Delta t) \), which describes the probability distribution of the displacements \( \Delta r \) of atoms as a function of time interval \( \Delta t \). Here \( \Delta r \) is defined relative to a uniformly (affinely) sheared system. In equilibrium systems, \( P(\Delta r) \) has been used to determine the timescale on which particles escape from local cages [5, 6, 31] and its long time behavior gives the diffusion constant. Studies of sheared systems have examined the changes in \( P(\Delta r) \) to determine the effect of strain rate on caging times and diffusion [14, 15, 22, 24, 32]. These studies have generally found \( \langle \Delta r^2 \rangle \propto \Delta t \) as expected for single-particle diffusion. In some cases the associated nonequilibrium diffusion constant obeys a generalized fluctuation dissipation theorem with an effective temperature [14, 15, 24].

In this work, we use molecular dynamics (MD) simulations to examine the spatio-temporal correlations in \( \Delta r \) in athermal systems that are driven by steady shear. This models the low temperature behavior of amorphous atomic systems as well as disordered granular or colloidal systems where thermal fluctuations are small. As in most studies of similar systems [22, 24, 32], we find that the long time evolution of \( P(\Delta r; \Delta t) \) is consistent with the diffusion equation. However, the displacement shows strong spatial correlations that span the entire system. Thus \( P \) does not describe single-particle diffusion and the diffusion constant...
There are \( N \) value of the damping constant was set to 0. Each other which are proportional to their relative velocity. The Neighboring particles exert equal and opposite drag forces on undergoing single-particle diffusion. The distributions of \( \omega \) more isotropic and converges to a Gaussian at strain intervals of order 3%. The distribution of \( \omega \) retains an exponential tail out to much larger strains, indicating that particles are still not critically damped and damping decreases at longer lengths. The long-range spatial correlations in \( \Delta r \) reflect the fact that large regions deform elastically. To measure the local magnitude of non-affine deformations, we evaluate the vorticity in the displacement field \( \omega = \nabla \Delta r \). Other measures of the relative particle displacement have been considered in previous work, but \( \omega \) has the advantage that it allows both the magnitude and direction of the displacements to be quantified. This allows strong directional, spatial and temporal correlations in strain to be identified.

The distributions of \( \Delta r \) and \( \omega \) provide additional information about correlations. Over short intervals, both distributions show exponential tails covering up to eight orders of magnitude. The strain characterizing the exponential decay for \( \omega \) is close to the macroscopic yield strain of the material. As the interval of time or strain increases, \( P(\Delta r) \) becomes more isotropic and converges to a Gaussian at strain intervals of order 3%. The distribution of \( \omega \) retains an exponential tail out to much larger strains, indicating that particles are still not undergoing single-particle diffusion.

2. Protocol and definitions

We perform classical 2D molecular dynamics simulations of a bi-disperse mixture that is chosen to inhibit crystallization [29]. There are \( N_L \) large (L) particles and \( N_S \) small (S) particles with \( N_L/N_S = (1 + \sqrt{5})/4 \). The interaction between particles of type I and J is a Lennard-Jones (LJ) potential: \( U_{IJ} = 4\epsilon[(r/\sigma_{IJ})^{-6} - (r/\sigma_{IJ})^{-12}] \) where \( \epsilon \) sets the characteristic energy scale and \( \sigma_{IJ} \) reflects the size of I and J. We set \( \sigma_{LL} = 1.0\sigma_0, \sigma_{SS} = 0.6\sigma_0, \) and \( \sigma_{LS} = 0.5(\sigma_{LL} + \sigma_{SS}) = 0.8\sigma_0 \) and measure all lengths in units of \( \sigma_0 \). To speed calculations, the potential is truncated smoothly using a fourth order polynomial that matches the LJ potential and force at \( r_{cut} = 1.2\sigma_{IJ} \) and takes both to zero at \( r_{cut} = 1.5\sigma_{IJ} \). All particles have mass \( m \) and the characteristic time is \( \tau = \sqrt{m\sigma_0^2/\epsilon} \).

The equations of motion are integrated using the parallel MD code LAMMPS [33] with time step \( \delta t = 0.0056\tau \). The system temperature is maintained at zero by applying a locally Galilean-invariant Kelvin damping mechanism [34]. Neighboring particles exert equal and opposite drag forces on each other which are proportional to their relative velocity. The value of the damping constant was set to 0.45 m/\( \tau \). With this choice, modes with wavelengths at the particle scale are nearly critically damped and damping decreases at longer lengths. The limit of zero temperature is of fundamental interest in atomic systems and thermal motion can generally be ignored in systems where the particles represent larger entities such as grains or colloids.

An amorphous state of the system is prepared following the protocol in previous studies [30]. Periodic boundary conditions with periods \( L_x \) and \( L_y \) are used. A random configuration with a particle area fraction of 0.85 is equilibrated for 20,000 time steps using a soft repulsive potential to ensure particles do not overlap. The interaction is then switched to the LJ potential, and the damped system is run for 10,000 timesteps with fixed area. The system is next allowed to expand toward a zero pressure state under an isotropic Nose–Hoover barostat [33] with a time constant of 220\( \tau \) and a damping parameter of 45 \( \tau^{-1} \) for 10,000 timesteps. A final quench is run for 10,000 timesteps with a fixed cell size prior to shearing.

Equilibrated systems are compressed along the y direction at constant true strain rate \( \dot{\gamma} \) and expanded along x to maintain constant area: \( L_x = L_{0x} e^{\dot{\gamma} t}, L_y = L_{0y} e^{-\dot{\gamma} t} \). Unless noted, the results below are for about 1.6 \times 10^6 particles with \( L_{0x} = L_{0y} \approx 1000\sigma_0 \), and \( \dot{\gamma} = 0.45 \times 10^{-5} \tau^{-1} \). Studies showed that this strain rate was slow enough to be in a quasistatic regime where results are rate-independent. For this reason, results will be expressed in terms of the interval of strain \( \Delta \gamma \) over which they were obtained, rather than in terms of time interval. For small strains the rate of plastic deformation increases with strain and may be sensitive to initial conditions [18, 20, 35]. For strains greater than 6% the behavior becomes independent of strain and initial state. Data presented below are all from this steady state regime.

The non-affine component \( \tilde{v} \) of a particle’s velocity \( v \) is the deviation from the velocity associated with a uniform strain:

\[
\tilde{v}_x = v_x - \dot{\gamma} x(\tau) \\
\tilde{v}_y = v_y + \dot{\gamma} y(\tau).
\]

Integrating over time gives the net non-affine displacement \( \Delta r = (\Delta x, \Delta y) \) over any finite strain interval. Note that this is not the same as taking the difference between the final position of a particle and the position corresponding to an affine displacement. The reason is that a small non-affine displacement at the beginning of a time interval is amplified by subsequent affine flow and would have the same impact as a much larger non-affine motion at the end of the interval. A similar effect produces an extra Taylor diffusion in sheared fluids [36]. From now on we shall refer to the non-affine displacement simply as ‘displacement’ and use ‘total displacement’ when the affine component is not subtracted. Note that the non-affine displacement averaged over the periodic cell is zero. This follows because the equations of motion in the deforming cell [33] conserve the sum over particles of the peculiar momentum \( m\tilde{v} \) and all particles have the same mass.

The results presented below show that the displacement field has long-range spatial correlations. A more local measure of deformation is provided by the spatial derivatives of \( \Delta r \), which are obtained in the following way. A Delaunay triangulation is found for an initial reference configuration, with vertices at the center of all particles. The derivatives \( \partial_i \Delta r_j \) on each triangle are then calculated from the finite difference between displacement vectors at the three vertices.
To make plots and evaluate probability distributions, the derivatives are sampled on a fine, rectilinear grid with spacing $\delta$. An important property of this piece-wise constant definition of $\delta_r$ is that its integral along an arbitrary path connecting any two particles gives the exact difference between the displacement vectors of the two particles. This guarantees that mean strains on large scales are equal to the spatial average of local values.

Because the area is fixed and the system is densely packed, changes in density are small. As a result, we find that the local divergence of the displacement field is negligible. Most of the deformation takes the form of local shear strains that are quantified by the curl of the displacement field or vorticity: $\omega = \partial_x \Delta y - \partial_y \Delta x$, which represents the antisymmetric part of the derivative tensor. For two-dimensional systems the curl is a vector perpendicular to the plane and thus invariant under rotations within the plane. Note that it is conventional to associate the magnitude of shear with a symmetric scalar component proportional to $\delta_y \Delta x - \delta_x \Delta y$, while the antisymmetric part is dominated by a region of strong gradient extended roughly along $y = -x$ while the $\Delta x + \Delta y$ component has a few smaller features extended along $y = x$ and centered roughly about the large feature in $\Delta x - \Delta y$. The displacements $\Delta x$ and $\Delta y$ show a superposition of all these features. Note that some of the features extend around the periodic boundary conditions.

### 3. Spatial variation of displacement and strain

In figure 1, we plot projections of a typical displacement field for $\Delta y = 0.002$ onto horizontal, vertical and diagonal directions: $\Delta x$, $\Delta y$, $(\Delta x + \Delta y)/\sqrt{2}$, and $(\Delta x - \Delta y)/\sqrt{2}$. All projections show strong spatial correlations over scales comparable to the system size, but different projections highlight different features. For example, the plot for the component proportional to $\Delta x - \Delta y$ is dominated by a region of strong gradient extended roughly along $y = -x$ while the $\Delta x + \Delta y$ component has a few smaller features extended along $y = x$ and centered roughly about the large feature in $\Delta x - \Delta y$. The displacements $\Delta x$ and $\Delta y$ show a superposition of all these features. Note that some of the features extend around the periodic boundary conditions.

The strong spatial correlations evident in figure 1 show that most of the displacements of atoms that contribute to $P(\Delta r; \Delta y)$ are very far from independent random walks by each particle. The correlations result from shear along spatially extended slip lines. The slip lines show up as lines of rapid gradients in figure 1. Because they reflect a shear displacement, the amplitude of the displacements is largest for the projection

---

**Figure 1.** Grayscale plots of the projections of a typical non-affine displacement field $\Delta r$ onto different directions. Top left: $\Delta x$. Top right: $\Delta y$. Bottom left: $(\Delta x + \Delta y)/\sqrt{2}$. Bottom right: $(\Delta x - \Delta y)/\sqrt{2}$. Here $\Delta y = 0.002$, the $x$-axis is horizontal, and the gray scale is linear, ranging from $-\sigma_0$ (black) to $+\sigma_0$ (white).
along the slip line. Thus the slip line that spans the entire system along \( \hat{x} \) shows up most clearly in \( \Delta x - \Delta y \), while a number of smaller slip lines along \( \hat{x} + \hat{y} \) are emphasized in \( \Delta x + \Delta y \). The reason that slip lines are at an angle of roughly \( 45^\circ \) from the compressive axis is that the stress tensor has the largest shear (off-diagonal) components for these orientations.

Put another way, shear along these lines is most efficient in simultaneously contracting the system along the compressive direction and expanding it in the tensile direction.

Figure 2 illustrates (top) the total displacement and (bottom) the non-affine displacement along a slip line as a function of the distance away from the slip line. The change \( a \) in the total displacement across the periodic cell is accommodated in a plastic zone of width \( h \) where the displacement changes rapidly, \( \omega \approx a/h \). The total displacement in the surrounding elastic regions is nearly constant. Subtracting the affine displacement associated with a strain \( \Delta \gamma \) leads to a small gradient, \( \omega \approx \Delta \gamma \), in the elastic regions of plots of the non-affine displacement.

The form of plots like figure 1 depends on strain, strain interval and system size. At very small strains, the entire system responds elastically and the displacements are small. As the strain increases, the stress and rate of plasticity rise. For strains of 6% and greater we find that the system is in a nearly steady state. In this regime, plastic deformation tends to occur in a series of rapid ‘avalanches’ with a wide range of sizes that will be discussed further in future work [37]. Between these avalanches the displacement field may be small, but the strain interval between avalanches decreases rapidly with system size. For the system size considered here, plastic zones that span a large fraction of the system are always observed for \( \Delta \gamma \gg 0.002 \) and this is the reason we focus on intervals of this order. Many avalanches occur during this strain interval and they cluster spatially to produce the slip lines evident in figure 1.

The evolution of the spatial organization of plastically deformed regions is illustrated in figure 3. The left-hand side shows the magnitude of the non-affine displacement, \( \Delta r \), rather than individual components. It is these magnitudes that are used to construct the widely studied \( P(\Delta r; \Delta \gamma) \). The right-hand side shows \( \omega \), which quantifies the amount and direction of local shear. The successive panels moving downwards in figure 3 show the changes over progressively longer strain windows starting from the same initial configuration as in figure 1.

The families of slip systems along both diagonals contribute equally to \( \Delta r \) and are visible in the left-hand panels. However, taking the magnitude of the displacement obscures the nature of the atomic rearrangements. The slip lines that appeared as sharp steps in \( \Delta x - \Delta y \) and \( \Delta x + \Delta y \) appear now as regions of low \( \Delta \gamma \) surrounded by halos of higher \( \Delta \gamma \). The origin of this behavior is evident from figure 2. The peak displacements occur at the outer edges of the plastic zone at a distance of order \( h/2 \) from the center of the slip line. The magnitude drops rapidly to zero at the slip line and much more slowly in the elastic region outside.

A better measure of the local plastic response is provided by \( \omega \). The \( \omega \) field is clearly localized on the regions of strong shear and much smaller away from these regions. From figure 2 we expect the shear strain to be of order \( \Delta \gamma \) in the elastic regions and much higher in the plastic regions that accommodate almost all the deformation of the cell. The numerical values of \( \omega \) are consistent with this expectation. Note that the sign of \( \omega \) carries important information about the direction of slip. In particular, the two families of slip planes produce opposite signs, with a clockwise rotation along lines running parallel to \( \hat{x} - \hat{y} \) and a counterclockwise rotation on perpendicular slip lines. Thus plots of \( \omega \) highlight the correlations among individual slip lines.

The successive panels moving down figure 3 show how displacements add as the strain interval increases. Over short intervals \( \Delta \gamma \leq 0.002 \) we find that the displacements tend to organize along system spanning lines. This allows the entire displacement to be accommodated in plastic zones with minimal energy stored in deformation of elastic regions.
Subsequent slip lines appear to occur at random locations rather than continuing to nucleate along the same path to produce a persistent shear band (e.g. as in [38]). One way of quantifying this is through the autocorrelation function for displacements over successive intervals. We find that this correlation function drops rapidly. By $\Delta \gamma = 0.003$ the correlations have dropped by about 2 orders of magnitude and are comparable to the noise. This is consistent with figure 3 where we see a growing number of independent slip lines for $\Delta \gamma \geq 0.004$. A superposition of randomly located slip lines is consistent with the diffusive growth in $\Delta r$ and $\omega$ discussed in the next section.

The strain interval over which deformations are correlated depends on system size and seems to be related to a characteristic amplitude of the slip across plastic zones. Examination of many plots like figure 1 shows that $a$ varies from about the mean particle diameter $0.8\sigma_0$ in the central region of shorter slip lines to about twice this value in a system spanning slip line like that in the bottom right of figure 1. It is perhaps not surprising that once $a$ is of order a particle size it is energetically favorable to have plastic deformation everywhere along the slip line rather elastic deformation. Note that the strain interval needed to produce a displacement $a$ is of order $a/L$. This implies that throughgoing faults should occur over $\Delta \gamma \sim 0.001$ to 0.002 in our systems. Our observations are consistent with this and analysis of the avalanche size distribution also shows that the largest events are spaced by $\Delta \gamma \sim 0.002$. 
The plastic regions in figure 1 and on the left of figure 3 have a significant width $h \sim 50\sigma$. Thus the mean shear strain across these regions is only of order $a/h \sim 0.02$–0.04 for $\Delta\gamma = 0.002$. While this is an order of magnitude larger than the mean strain $\Delta\gamma$, the peak strains on the right of figure 3 are higher still. Each broad slip zone contains a number of much sharper features with strains that are an order of magnitude higher ($|\omega| = 0.2$–0.4). The width of these smaller features is only a few particle diameters. More detailed studies of the time dependence show that the slip zones are formed by a large number of avalanches that are spatially correlated to produce the system spanning lines in the figures. The long-range spatial correlations in the strain field are analyzed in [39] and we will focus below on the temporal evolution of the probability distribution of displacement magnitudes and $\omega$.

Comparing results for different system sizes, $L_0$, indicates that $h$ increases roughly linearly with $L_0$ while the width of the high strain regions remains of order the particle diameter. It is interesting to note that the width of fault regions in earthquake systems also tends to scale in rough proportion to the length [40]. Studies of different system sizes also indicate that the slip amplitude along throughgoing slip lines is always of order one to two particle diameters. If $a$ is independent of system size, then the strain interval needed to produce a slip line should be inversely proportional to system size. There should also be a slower decay with $\Delta\gamma$ in the displacement autocorrelation function. Results for smaller systems ($L_0 = 250$ and 500) are consistent with these predictions.

4. Probability distributions of displacement and strain

Figure 4 shows the probability distribution for finding a given displacement over successive strain intervals with $\Delta\gamma = 0.002$. The distribution $P(\Delta r)$ is normalized so that the integral over all vectors $\Delta r$ is unity. With this definition the distribution goes to a constant as $\Delta r \to 0$. Note that the distribution varies significantly from interval to interval. This reflects the large scale structure of the slip lines discussed above. In contrast, the distribution of the more local variable $\omega$ is nearly the same for all intervals. Its average behavior is discussed below.

For an ideal system spanning slip line with a constant magnitude $a$ and $h \ll L$, traces like figure 2 (bottom) would consist of two straight segments of constant slope $\Delta\gamma$ and $a/h$, respectively. The distribution $P(\Delta r)$ would be constant from 0 to $a/2$ and zero for larger displacements. Given the range of $a$ discussed above, one would expect plateaus extending to $\Delta r \sim 0.4\sigma_0$ to $0.8\sigma_0$ in figure 4. The curves show a crossover from gradual to rapid decrease at $\Delta r$ in this range, but do not show true plateaus. Analysis of displacement fields like those in figures 1 and 3 show that $a$ varies along the slip line. As discussed above, there is also smearing along the edge of the plastic region that rounds the peaks in traces like figure 2. Interactions between the two families of slip planes also alter the distribution. Together these effects lead to a reduction in the range of $\Delta r$ where the distribution for each interval is constant, and an exponential tail in the probability distribution at large magnitudes. Averaging over all intervals between 12% and 24% produces the thick solid line. The crossover to the exponential tail is broadened by averaging over intervals with different values of $a$ and the exponential tail becomes more pronounced.

Figure 5 shows how the mean-squared displacement and strain increase with $\Delta\gamma$. All results are averaged over strains between 12% and 24%. As would be expected for a diffusive process, both $\langle \Delta r^2 \rangle$ and $\langle \omega^2 \rangle$ rise linearly with $\Delta\gamma$. The fit lines have a small negative offset at $\Delta\gamma = 0$. This reflects the correlation in the increase in both quantities at small strains, which cause them to rise quadratically with $\Delta\gamma$ at small strain intervals ($\Delta\gamma \leq 0.001$). While the linear rise of $\langle \Delta r^2 \rangle$ at large $\Delta\gamma$ is consistent with diffusion, this only implies that the displacements of any given particle in successive strain intervals are uncorrelated. As shown above, there are strong spatial correlations that imply one should not view the slope of figure 5 (left) as a single-particle diffusion constant. A detailed examination of the probability distributions also reveals some subtle longer-lived correlations in displacement.

Figure 6 shows the probability distribution of displacements averaged over initial states and scaled by $\sqrt{100\Delta\gamma}$ to remove the mean increase in magnitude shown in figure 5. For
the smallest interval, the distribution has an exponential tail that extends over eight orders of magnitude. It is interesting to note that the displacement distributions following individual plastic events or avalanches have also been found to be exponential [22, 32]. If successive events were strictly decorrelated, the distributions for longer intervals would be given by autoconvolving the distributions for short intervals and would converge to a Gaussian. The distributions do seem to become more Gaussian as $\Delta \gamma$ increases, but there is a systematic decrease in the probability of large events for $\Delta \gamma = 0.008$. This suggests that the behavior is still correlated, with large displacements less likely to occur in the same location as in previous intervals. By $\Delta \gamma = 0.032$ these correlations have nearly disappeared and the data are consistent with a Gaussian distribution. It is interesting to note that at this point the product of the number of throughgoing faults ($\sim 0.032/0.002 = 16$) and the fraction of the system affected by each ($h/L \sim 50/1000$) is of order one, implying that slip lines must revisit the same regions of space.

Figure 7 shows the time averaged $\omega$ distributions for various $\Delta \gamma$. The distributions consist of central peaks that cross over to exponential tails. The exponential tails persist even at the largest $\Delta \gamma$. Roughly speaking, regions of the material with small strains away from any shear zones (the gray regions in the right column of figure 3) contribute to the ‘elastic’ central peaks, while the strongly sheared material in the core of the shear zones (the black and white regions in the right column of figure 3) contributes to the ‘plastic’ exponential tails. To first order, weight is removed from the central peak and redistributed to the tails as the amount of plastic strain increases.

To test this picture quantitatively, the $\omega$ distributions are scaled by $\Delta \gamma$ and replotted in figure 8. This rescaling comes close to collapsing the data in the tails for the smallest $\Delta \gamma$, but becomes less satisfactory for increasing $\Delta \gamma$. Direct convolution of data from small intervals shows similar deviations from probabilities for larger intervals. This implies that there is some additional correlation over the range of $\Delta \gamma$ considered here. Fits to an exponential decay, $P(\omega) \sim \exp(\omega/\omega^\ast)$, show a slight increase in $\omega^\ast$ with $\Delta \gamma$ (inset). This increase implies that increasing $\Delta \gamma$ does not merely increase the size of the plastic region and thus the total weight in the tails. In addition, there is a slight increase in the relative weight of large magnitude regions that must reflect a correlated increase in strain in regions of large strain.

It is interesting to note that the value of $\omega^\ast$ has a natural physical interpretation. The vorticity $\omega = \partial_x \Delta \gamma - \partial_y \Delta \gamma$ while the shear strain is $0.5 \ast [\partial_x \Delta \gamma + \partial_y \Delta \gamma]$. Thus $\omega^\ast = 0.1$ corresponds to a shear strain of about $5\%$, which is close to the yield strain [19]. As noted above, the regions of large $\omega$ have strains much bigger than the mean strain in the plastic region ($\alpha/h)$ but small enough that there are several in the plastic zone that combine to produce the total displacement. The probability distribution suggests that the yield strain sets the characteristic scale for these high strain regions.

Another important parameter is the strain interval required to produce plastic deformation throughout the entire system. One can estimate this from the integral under the exponential tails in $P(\omega)$ at small strains, and the assumption that the weight grows approximately linearly with $\Delta \gamma$ as in figure 8. The result is that the regions of plastic strain should cover the system after a strain of about $10\%$. This is larger than the estimate of $3\%$ strain required for plastic zones to cover the system, but as noted above, only a fraction of the plastic zones has the large strains indicative of local plasticity.
5. Discussion

Although ours is, to our knowledge, the first study of strain distributions in simulations of sheared systems, several studies have looked at displacement distributions in athermal systems. All considered simple shear, \( v_y = \dot{\gamma} y \), rather than the pure shear strain studied here. Some simulations used quasistatic protocols with small strain steps [22, 24, 32], while others used a constant slow shear rate as in our simulations [14, 15, 41]. The quasistatic studies all employed Lennard-Jones potentials and imposed simple shear with Lees-Edwards periodic boundary conditions [24, 32] or rigid walls parallel to the flow direction [22].

Ono and co-workers [14, 15] simulated steady shear of wet foams using Durian’s bubble model [42], while Radjai and Roux simulated granular media with dissipation entering through friction at particle contacts [41]. Only the latter work and our simulations include inertia. Despite the wide range of protocols and interactions, almost all studies find diffusive behavior for the non-affine displacement\(^4\). The only exception is the work of Radjai and Roux [41] who found \( (\Delta \gamma)^2 \propto \Delta \gamma \). It seems very important to determine the cause of this striking difference. The only unique feature of these simulations appears to be the incorporation of friction forces, which are not generally thought to lead to such qualitative changes in behavior.

The value of the effective diffusion constant \( D_{\text{eff}} \equiv \sigma^2 / \Delta \gamma \) can be estimated from our observations of slip lines and the simple model in figure 2. This displacement field gives a constant distribution of displacements from \(-a/2\) to \(a/2\), implying a mean-squared displacement of \( a^2 / 12 \). If system spanning slip lines produce independent displacements at strain intervals of \( a/L \), then \( \langle \Delta x^2 \rangle \approx \langle \Delta \gamma \rangle / (a/L) a^2 / 12 \) or \( D_{\text{eff}} = L a / 12 \). Using the value of \( D_{\text{eff}} = 57 \sigma_0^2 \) from figure 5, one finds \( a \approx 0.7 \sigma_0 \).

Improving the estimate of the mean-squared displacement from each slip line leads to larger values of \( a \) since the actual distribution of displacements (figure 4) is cut off before \( a/2 \). We conclude that the measured diffusion is consistent with the direct observation that slip lines have amplitudes of one to two particle diameters and contribute independently to the displacement.

This model for the effective diffusion constant implies a linear scaling with system size. Our simulations for \( L = 250 \sigma \) and 1000\( \sigma \) are consistent with this linear scaling. Recent studies of a similar model by Lemaitre and Caroli [32] also showed a pronounced increase in \( D_{\text{eff}} \) with system size. Data for the two largest systems, \( L = 20 \) and 40, appear consistent with linear scaling with \( L \). Results for \( L = 10 \) are larger than expected, but there may be significant finite size effects in such small systems. Note that we find \( h/L \sim 1/20 \), so system sizes with \( L < 20 \) could not have the plastic zone occupying the same fraction of the system. Extrapolating Lemaitre and Caroli’s result\(^5\) for \( L = 40 \), \( D_{\text{eff}} = (2.2 \pm 1) \sigma_0^2 \) to \( L = 1000 \) yields \( D_{\text{eff}} \approx (55 \pm 2.5) \sigma_0^2 \), which is consistent with our measured value of \( 57 \sigma_0^2 \). The magnitude of \( \Delta \gamma \) needed to observe diffusive behavior is also roughly a factor of 25 smaller in our systems. These results provide a dramatic check of the linear scaling with system size in diffusion, although we caution that the different shearing geometry in [32] could affect the comparison.

Lemaitre and Caroli discuss the system-size dependence of their results in terms of displacements produced by independent avalanches rather than independent slip lines. Earlier studies of individual plastic events showed that the rate of large avalanches scales with the system length [27, 29]. Based on the assumption that the total strain \( \Delta \gamma \) was accommodated by these avalanches, Maloney and Lemaitre concluded that the displacement \( a_0 \) associated with each avalanche was independent of system size and of order 0.1\( \sigma_0 \). Extrapolating their results [27, 29] for \( L \sim 50 \) to our system sizes would give large avalanches spaced by \( \Delta \gamma = 0.0002 \), an order of magnitude more frequent than the rate of system spanning slip lines in our simulations. This is consistent with our conclusion that the slip lines in figures 1 and 3 are not the result of individual avalanches, but the correlated displacement produced by multiple avalanches. Assuming that each avalanche contributes independently to the displacement would give too small a value of \( D_{\text{eff}} \).

System-size dependence of \( D_{\text{eff}} \) could be crucial in analyses which invoking the notion of an effective temperature based on an effective Stokes–Einstein relationship between \( D_{\text{eff}} \) and the viscosity \( \eta \) [15, 24]. The product of diffusion and viscosity is related to the temperature in equilibrium systems. In systems with a yield stress, the viscosity diverges like the inverse strain rate, \( \eta \sim \Delta t / \Delta \gamma \), at low strain rates where the stress reaches a plateau. As we have seen here, one also expects the effective diffusion constant to grow linearly with the strain rate: \( \Delta x^2 / \Delta t = \langle \Delta \gamma \rangle \sigma / L \). This means that the product of the viscosity and diffusivity should become constant at small enough strain rate: \( (\Delta x^2 / \Delta t) \eta \sim \sigma^2 \). However, our results imply that this constant should have a dramatic size dependence, and one must proceed with caution to utilize it as an effective temperature.

The scaling of \( D_{\text{eff}} \) would be very different if the correlations in displacement did not span the system. There is some evidence that system spanning slip lines are suppressed by increasing temperature [18, 20]. They may also be suppressed by the surrounding fluid in experiments on colloidal systems [43]. Dissipation through flow in the fluid is reduced by maintaining a linear flow profile that may inhibit localization of the plastic deformation. Studies of both effects would be of interest.

Correlated atomic motions have also been observed in unsheared systems. In particular, several studies reveal spatial correlations that grow in extent as the temperature is decreased to the glass transition temperature \( T_g \) [5, 44-48]. Large displacements are associated with strings of particles whose displacement is directed along the string [47, 48]. Such displacement fields are very different than the thick, system spanning slip zones described above. Rather than producing a net shear displacement, the strings allow the total displacement...
of surrounding regions to remain small. A plot like figure 2 would have the form of a sharp peak, rather than a step. It seems clear that shear is responsible for producing the long-range correlations and striking size-dependent diffusion in our systems.

The most important message in our results is that one must go beyond the second moments of the displacement and strain distributions to get insight into the microscopic processes at play in sheared systems. Displacement distributions may be nearly Gaussian, scaling with $\sqrt{\Delta t}$, while at the same time, there may be strong spatial correlations and heterogeneities in the system. The strain distributions can remain far from Gaussian, even while the displacement distributions become nearly Gaussian. Such behavior provides a clear signature of spatial organization. Furthermore, while individual particle trajectories may seem jerky, with smooth motion interrupted by abrupt jumps, these jumps should not necessarily be interpreted as a particle escaping the cage formed by its neighbors (as is often assumed to be the case), but could just as easily correspond to coherent displacement of the neighborhood with very little relative motion of particles. In the future, it will be interesting to repeat the strain analysis here for thermal (e.g. super-cooled liquids) or Brownian (colloidal suspensions) systems on approach to the jamming transition. This kind of measurement could serve as an important probe of the cooperative nature of the dynamics.

Acknowledgments

This material is based on work supported by the National Science Foundation under Grant No. DMR-0454947, CTS-0320907 and PHY-99-07949.

References

[1] Spaepen F 1977 Microscopic mechanism for steady-state inhomogeneous flow in metallic glasses Acta Metall. 25 407–15
[2] Falk M L and Langer J S 1998 Dynamics of visco-plastic deformation in amorphous solids Phys. Rev. E 57 7192–205
[3] Argon A S 1979 Plastic deformation in metallic glasses Acta Metall. 27 47–58
[4] Liu A J and Nagel S R 1998 Nonlinear dynamics—jamming is not just cool any more Nature 396 21–2
[5] Kob W, Donati C, Plimpton S J, Poole P H and Glotzer S C 1997 Dynamical heterogeneities in a supercooled Lennard-Jones liquid Phys. Rev. Lett. 79 2827–30
[6] Weeks E R, Crocker J C, Levitt A C, Schofield A and Weitz D A 2000 Three-dimensional direct imaging of structural relaxation near the colloidal glass transition Phys. Rev. Lett. 84 255501
[7] Argon A S and Kuo H Y 1979 Plastic-flow in a disordered bubble raft (an analog of a metallic glass) Mater. Sci. Eng. A 39 101–9
[8] Kobayashi S, Maeda K and Takeuchi S 1980 Computer-simulation of deformation of amorphous Cu57Zr43 Acta Metall. 28 1641–52
[9] Maeda K and Takeuchi S 1981 Atomic process of plastic-deformation in a model amorphous metal Phil. Mag. A 44 643–56
[10] Srolovitz D, Maeda K, Vitek V and Egami T 1981 Structural defects in amorphous solids statistical-analysis of a computer-model Phil. Mag. A 44 847–66
[11] Deng D, Argon A S and Yip S 1989 Simulation of plastic-deformation in a 2-dimensional atomic glass by molecular-dynamics. A Trans. R. Soc. (Lond.) A 329 613–40
[12] Lauridsen J, Twardos M and Dennin M 2002 Shear-induced stress relaxation in a two-dimensional wet foam Phys. Rev. Lett. 89 095703
[13] Shi Y F and Falk M L 2005 Strain localization and percolation of stable structure in amorphous solids Phys. Rev. Lett. 95 095502
[14] Ono I K, Tewari S, Langer S A and Liu A J 2003 Velocity fluctuations in a steadily sheared model foam Phys. Rev. E 67 061503
[15] Ono I K, O’Hern C S, Durian D J, Langer S A, Liu A J and Nagel S R 2002 Effective temperatures of a driven system near jamming Phys. Rev. Lett. 89 095703
[16] Utter B and Behringer R P 2004 Self-diffusion in dense granular shear flows Phys. Rev. E 69 031308
[17] Utter B and Behringer R P 2007 Experimental measurements of affine and non-affine deformation in granular shear Preprint cond-mat/0702334
[18] Rottler J and Robbins M O 2003 Shear yielding of amorphous glassy solids: effect of temperature and strain rate Phys. Rev. E 68 011507
[19] Rottler J and Robbins M O 2005 Unified description of aging and rate effects in yield of glassy solids Phys. Rev. Lett. 95 225504
[20] Varnik F, Bocquet L and Barrat J L 2004 A study of the static yield stress in a binary Lennard-Jones glass J. Chem. Phys. 120 2788–801
[21] Schall P, Weitz D A and Spaepen F 2007 Structural rearrangements that govern flow in colloidal glasses Science 318 1895–9
[22] Tanguy A, Leonforte F and Barrat J L 2006 Plastic response of a 2d Lennard-Jones amorphous solid: detailed analysis of the local rearrangements at very slow strain rate Eur. Phys. J. E 20 355–64
[23] Lacks D J and Osborne M J 2004 Energy landscape picture of overaging and rejuvenation in a sheared glass Phys. Rev. Lett. 93 255501
[24] Lacks D J 2002 Stokes–Einstein-like relation for athermal, quasistatic shear flow Phys. Rev. E 66 051202
[25] Malandro D L and Lacks D J 1998 Molecular-level mechanical instabilities and enhanced self-diffusion in flowing liquids Phys. Rev. Lett. 81 5576–9
[26] Lemaitre A and Maloney C 2006 Sum rules for the quasi-static and visco-elastic response of disordered solids at zero temperature J. Stat. Phys. 123 415–53
[27] Maloney C and Lemaitre A 2004 Subextensive scaling in the athermal, quasistatic limit of amorphous matter in plastic shear flow Phys. Rev. Lett. 93 016101
[28] Maloney C and Lemaitre A 2004 Universal breakdown of elasticity at the onset of material failure Phys. Rev. Lett. 93 195501
[29] Maloney C E and Lemaitre A 2006 Amorphous systems in athermal, quasistatic shear Phys. Rev. E 74 016118
[30] Maloney C E 2006 Correlations in the elastic response of dense random packings Phys. Rev. Lett. 97 035503
[31] Grest G S, Kremer K and Robbins M O 1987 Dynamics of supercooled liquids interacting with a repulsive Yukawa potential J. Phys. A: Math. Gen. 20 L181–7
[32] Lemaitre A and Caroli C 2007 Plastic response of a two-dimensional amorphous solid to quasistatic shear: transverse particle diffusion and phenomenology of dissipative events Phys. Rev. E 76 036104
[33] Plimpton S J 1995 Fast parallel algorithms for short-range molecular dynamics J. Comput. Phys. 117 1–19 http://www.cs.sandia.gov/sjplimp/lammps.html
[34] Hoogerbrugge P J and Koelman J M V A 1992 Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics *Europhys. Lett.* **19** 155

[35] Rottler J and Robbins M O 2005 Unified description of aging and rate effects in yield of glassy solids *Phys. Rev. E* **95** 225504

[36] Taylor G I 1953 Dispersion of soluble matter in solvent flowing slowly through a tube *Proc. R. Soc. A* **219** 186–203

[37] Salerno K *et al* 2008 in preparation

[38] Shi Y F and Falk M L 2006 Atomic-scale simulations of strain localization in three-dimensional model amorphous solids *Phys. Rev. B* **73** 214201

[39] Maloney C E *et al* 2008 in preparation

[40] Scholz C H 2002 *Mechanics of Earthquakes and Faulting* 2nd edn (Cambridge: Cambridge University Press)

[41] Radjai F and Roux S 2002 Turbulentlike fluctuations in quasistatic flow of granular media *Phys. Rev. Lett.* **89** 064302

[42] Durian D J 1997 Bubble-scale model of foam mechanics: melting, nonlinear behavior, and avalanches *Phys. Rev. E* **55** 1739–51

[43] Stevens M J and Robbins M O 1993 Simulations of shear-induced melting and ordering *Phys. Rev. E* **48** 3778–92

[44] Miyagawa H and Hiwatari Y 1991 Molecular-dynamics study of the glass transition in a binary soft-sphere model *Phys. Rev. A* **44** 8278–88

[45] Habasaki J and Hiwatari Y 2003 Fast and slow dynamics in single and mixed alkali silicate glasses *J. Non-Cryst. Solids* **320** 281–90

[46] Yamamoto R and Onuki A 1998 Dynamics of highly supercooled liquids: heterogeneity, rheology, and diffusion *Phys. Rev. E* **58** 3515–29

[47] Donati C, Douglas J F, Kob W, Plimpton S J, Poole P H and Glotzer S C 1998 Stringlike cooperative motion in a supercooled liquid *Phys. Rev. Lett.* **80** 2338–41

[48] Donati C, Glotzer S C, Poole P H, Kob W and Plimpton S J 1999 Spatial correlations of mobility and immobility in a glass-forming Lennard-Jones liquid *Phys. Rev. E* **60** 3107–19