Shear Transformation Zones: State determined or protocol dependent?

OLEG GENDELMAN1, PRABHAT K. JAISWAL2, ITAMAR PROCACCIA2(a), BHASKAR SEN GUPTA2 and JACQUES ZYLBERG2

1 Faculty of Mechanical Engineering - Technion, Haifa 32000, Israel
2 Department of Chemical Physics, Weizmann Institute of Science - Rehovot 76100, Israel

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Abstract – The concept of a Shear Transformation Zone (STZ) refers to a region in an amorphous solid that undergoes a plastic event when the material is put under an external mechanical load. An important question that had accompanied the development of the theory of plasticity in amorphous solids for many years now is whether an STZ is a region existing in the material (which can be predicted by analyzing the unloaded material), or it is an event that depends on the loading protocol (i.e., the event cannot be predicted without following the protocol itself). In this letter we present strong evidence that the latter is the case. Infinitesimal changes of protocol result in macroscopically big jumps in the positions of plastic events, meaning that these can never be predicted from considering the unloaded material.

The origin of plastic responses to external mechanical loads in crystalline solids is understood: topological defects, and in particular dislocations, glide under the action of external stresses or strains, and this glide is irreversible, dissipating energy as it is taking place [1–3]. Of course, when the density of such defects increases, the situation becomes hairy, and proper theories are still under active research. The fundamental mechanism of plasticity in amorphous solids is, on the other hand, still not fully resolved. In essence there are two schools of thought. The first is phenomenological, considering plasticity as resulting from the existence of some regions in the material that are more sensitive to external load. These regions are referred to as Shear Transformation Zones (STZs) and their introduction to rheological models of amorphous solids goes back to the work of Argon, Spaepen, and Langer [4–7]. The second school pursues a microscopic approach and considers plasticity as an instability of the amorphous solids [8–10] resulting from a protocol of an increase in the external load. This instability can be understood by focusing on the Hessian matrix of the material (and see below for more details) with an eigenvalue that goes to zero following a saddle-node bifurcation [11–13]. Both schools of thought agree that until the appearance of system spanning plastic events (shear bands) at high values of the external load, the plastic events that one is discussing are localized. In the instability way of thinking this is explained by the localization of the eigenfunction associated with the eigenvalue that is going to zero.

The difference in thought is not only in choosing words to describe plasticity in amorphous solids. If the STZ approach is valid, one should be able to predict, by a judicious analysis of the unstrained system, where a plastic event is likely to take place. If indeed there are some regions that are more sensitive than others to external loads, they should be identifiable and marked prior to exercising the external load. On the other hand, if the protocol dependence of an instability is the right way of thinking, then one should be able to show that even minute changes in protocol may result in a major change in the plastic event that takes place. If an infinitesimal change in the loading protocol were sufficient to induce an uncorrelated plastic event then the picture of a random distribution of structure-determined STZ’s would be less compelling. It would be argued that it were not possible to predict where plasticity should appear without detailed knowledge of the precise loading protocol. The aim of the present letter is to propose simple numerical simulations that can decide between the two possibilities, with the proposed result that the second way of thinking should prevail. We note that

(a)E-mail: itamar.procaccia@gmail.com
when loading is exercised the system may undergo a series of affine and non-affine (reversible) transformations before the appearance of the first plastic event, indicating why the position of this event is unpredictable from the virgin random structure.

In our simulations we construct a 2-dimensional glass-forming system in the usual way [14], selecting a binary mixture of \( N \) particles, 50% particles \( A \) and 50% particles \( B \), interacting via Lennard-Jones potentials

\[
U_{ij}(r_{ij}) = 4\epsilon_{ij} \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{6} + A_0 + A_1 \left( \frac{r_{ij}}{\sigma_{ij}} \right) + A_2 \left( \frac{r_{ij}}{\sigma_{ij}} \right)^2, \tag{1}
\]

where the parameters \( A_0, A_1 \) and \( A_2 \) are added to smooth the potential at a scaled cut-off of \( r_{co}/\sigma_{AB} = 2.5 \) (up to the second derivative). The difference between the particles is in the positions and the depths of the minima of the potentials; we choose the positions of the minima such that \( \sigma_{AA} = 1.17557, \sigma_{AB} = 1.0, \) and \( \sigma_{BB} = 0.618034 \). The depths of the potentials are \( \epsilon_{AA} = \epsilon_{BB} = 0.5 \) and \( \epsilon_{AB} = 1.0 \). Below lengths and energies are measured in units of \( \sigma_{AB} \) and \( \epsilon_{AB} \). These parameters are known to guarantee good glass formation and the avoidance of crystallization.

The system is first equilibrated in a square box of length \( 2R \) at a high temperature \( T = 0.8 \) with periodic boundary conditions. Next the system is quenched to temperature \( T = 0.001 \) at constant volume by molecular dynamics. Lastly, the system is energy minimized to guarantee good glass formation and the avoidance of crystallization.

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Having constructed a system of circular shape we can now follow its response to external loading. We load the system athermally and quasi-statically, pulling along the \( x \)-axis such as to conserve the wall the periodic boundary conditions are lost. The affine step is area preserving, written as

\[
x' = x(1 + \delta \gamma), \tag{2}
\]
\[
y' = \frac{y}{1 + \delta \gamma}. \tag{3}
\]

Note that in this affine steps also the wall particles are participating, to hold the system as desired. After every affine step of loading we annihil the forces between the bulk particles (excluding the wall particles) using gradient energy minimization. The system then undergoes a non-affine step that brings the system back to mechanical equilibrium. This quasi-static loading is continued as long as the system responses reversibly. The mechanical stability of the system is determined by the Hessian matrix \( H \):

\[
H_{ij} \equiv \frac{\partial^2 U}{\partial r_i \partial r_j}, \tag{4}
\]

where \( U(r_1, r_2, \ldots, r_N) \) is the total potential energy of the system as a function of the particle positions \( \{r_i\}_{i=1}^N \). The Hessian matrix is real, symmetric, and positive definite as long as the system is mechanically stable, the first plastic event occurs when the lowest eigenvalue of \( H \) approaches zero. It is well known that this happens via a saddle-node bifurcation, meaning that as a function of \( \gamma = \sum \delta \gamma \) there exists a value \( \gamma = \gamma_p \) where the lowest eigenvalue \( \lambda_p \) approaches zero via a square-root singularity

\[
\lambda_p \sim \sqrt{\gamma_p - \gamma}. \tag{5}
\]

An example of this scaling law obtained from the present system is displayed in fig. 2.

In the unloaded state all the eigenfunctions of the Hessian matrix which are associated with low lying eigenvalues are delocalized. As the lowest eigenvalue attains zero, the associated wave function \( \Psi_p \) localizes on a typical quadrupolar structure. This structure is identical to the non-affine irreversible displacement associated with the plastic instability. An example of this phenomenon is shown in fig. 3 which is obtained by selecting the \( x \)-axis in eq. (3) to be at 31º with respect to the horizontal direction of the original square box from which we extracted the circular system. The plastic event is shown as the quadrupolar displacement field near the bottom of the system. One can at will call it an STZ, but consider what happens if we change the \( x \)-axis to be at 32º with respect to the horizontal direction. This is shown in fig. 4. We see that a relatively small change in the chosen strain protocol, in this case by a variation of 1º in the chosen direction.
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-4.0 -3.8 -3.6 -3.4 $\gamma_P - \gamma$

Fig. 2: (Colour on-line) A log-log plot of $\lambda_P$ vs. $\gamma_P - \gamma$. The measured slope is 0.48 ± 0.0004.

Fig. 3: (Colour on-line) The first plastic event that occurs as a result of choosing the $x$-axis to be at 31° with respect to the horizontal direction of the original square box. Here and below the arrows represent the non-affine displacements of each particle. In this example $N = 20000$.

Fig. 4: (Colour on-line) Same as in fig. 3 but with choosing the $x$-axis to be at 32° with respect to the horizontal direction of the original square box.

Fig. 5: (Colour on-line) The average angle required to observe a major change in the position of the first plastic event as a function of the system size. Note the logarithmic scale used that supports the power-law dependence eq. (6). The systems studied here spanned the sizes $N = 5000$ to $N = 50000$, all quenched at a rate of $10^{-1}$.

of the principal stress axes, results in a huge change in the position of the first plastic event. The aim of the rest of this Letter is to explain that this sensitivity increases indefinitely with the system size, such that for macroscopic systems, i.e., in the thermodynamic limit, any arbitrarily small change in protocol will result in a macroscopic change in the position of the first plastic event.

To this aim we prepare between 30 to 100 different realizations of our system for each system size, changing the number of particles in the range $N = 5000$–50000. Each realization is then strained as described above, choosing (arbitrarily) the $x$-axis to coincide with the original $x$-axis of the square box. For each realization we determine what is the first plastic event and what is the value of $\gamma_P$ where it appears. In a second step of this exercise we change the $x$-axis to have an angle $\theta$ with respect to the original horizontal direction. We then determine, for each realization, the first angle $\theta$ for which the first plastic event is different, as seen in figs. 3 and 4. Finally, we average the angle $\theta$ over the 100 realization to get $\langle \theta \rangle$ as a function of the system size $N$. The central result of this exercise is that $\langle \theta \rangle(N)$ is a decreasing function of $N$ as seen in fig. 5. A fit to the numerical data shown in fig. 5 supports a power law of the form

$$\langle \theta \rangle(N) \sim N^{-\alpha}, \quad \alpha \approx 0.29.$$  

Clearly, in the thermodynamic limit $N \to \infty$, this result strongly indicates that indeed any infinitesimal change in
angle should result in a macroscopic change in the position of the plastic event. We have checked that the actual positions in which the eigenfunction gets localized are uncorrelated; they are spread evenly in a seemingly random fashion in the system even when the change in \( \theta \) is minute. The observed high sensitivity is doubly stressed by examining the probability distribution function (pdf) of the angles \( \theta \). In fig. 6 we present these pdf for two system sizes, \( N = 5000 \) and \( N = 50000 \). We see that both pdf’s are peaked at low values of \( \theta \) but the sharpness of this peak increases rapidly with the system size. (This effect is systematic between \( N = 5000 \) and \( N = 50000 \) and there is no reason to expect that it would weaken or disappear for even larger systems.)

The results obtained indicate the interesting finding that there is a high sensitivity to small changes in straining angles. Moreover the positions of the first plastic events jump unpredictably to new uncorrelated positions. This effect increases notably with the system size. This evidently refutes any possibility to predict the position of the plastic event from the analysis of the system’s state in equilibrium, before straining. We should note that similar data to those shown in fig. 5 were also obtained with other quench rates with identical conclusions. Finally, we note the exponent \( \alpha \approx 0.29 \) in eq. (6). It is noteworthy that this exponent differs from unity. Any model that assumes a random distribution of STZs of comparable “weakness” would predict a scaling law with \( \alpha = 1 \).

In summary, we have presented very simple tests to decide between two deeply contrasting views of the nature of plastic events in amorphous solids. The evidence provided above indicates that in the thermodynamic limit it is impossible to predict where the first plastic event should appear in a stressed amorphous solid. The plastic events are protocol dependent, and any minute change in the protocol should result in a macroscopic change in the position of the first plastic event. We conclude that it would be futile to predict the position of the first plastic event from analyzing the structure of the amorphous solid at equilibrium, be the method of analysis as sophisticated as one might think of. It is important to stress at this point that our analysis also indicate that later plastic events are even more sensitive to the change in protocol, and the system size dependence of their sensitivity is more steep than the findings reported in eq. (6). This and related findings are however beyond the scope of this letter which aims specifically to underline the difference in the current approaches to plasticity in amorphous solids. In particular it would be interesting to develop a model of plasticity in amorphous solids that can explain in simple terms the results shown in figs. 5 and 6.

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