

Shear Transformation Zones: State Determined or Protocol Dependent?

Oleg Gendelman¹, Prabhat K. Jaiswal², Itamar Procaccia², Bhaskar Sen Gupta², and Jacques Zylberg²

¹ Faculty of Mechanical Engineering, Technion, Haifa 32000, Israel

² Weizmann Institute of Science, Rehovot 76100, Israel

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 is it 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 considers plasticity 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 (STZ) and their introduction to rheological models of amorphous solids goes back to the work of Argon, Spaepen, and Langer [4–7]. The second school 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 will result in a major change in the plastic event that may take place. Then it would be argued that it were not possible to predict where plasticity should appear. The aim of the present Letter is to propose simple numerical simulations that can decide between the two possibility, with the proposed result that the second way of thinking should prevail.

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. 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 σ_{AB} and ϵ_{AB} . The potential is truncated at $r_{co} = 2.5$ and goes smoothly to zero (with two derivatives). 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. Secondly, the system is quenched to temperature $T = 0.001$ at constant volume by molecular dynamics. Lastly, the system is energy minimized to $T = 0$. At this point we build from the given configuration a sub-system with circular symmetry using the following protocol: we discard all the particles outside a circle of radius R , fixing the positions of particles in an annulus (wall) of width $dR = 2r_{co} = 5.0$. An example of the resulting system with $N = 20,000$ is shown in Fig. 1. Needless to say, once we fix the wall the periodic boundary conditions are lost.

Having constructed a system with circular symmetry we can now follow its response to external loading. We load the system athermally and quasi-statically, pulling along the x -axis and compressing along the y -axis such as to conserve the area. Thus, the circular system that

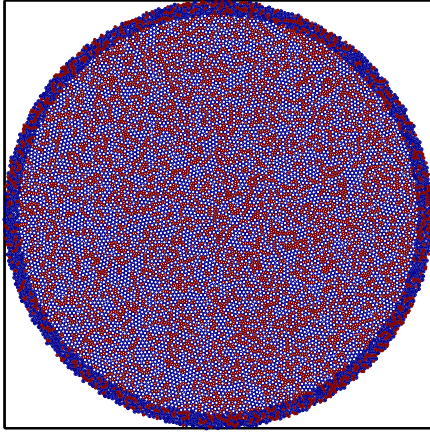


FIG. 1: The system with circular symmetry constructed as described in the text. In this example the total number of particles is $N = 20,000$.

begins with $L_x = L_y = R$ deforms to an ellipse with principal axes $L_x \neq L_y$. The affine step is area preserving, written as

$$x' = x(1 + \delta\gamma), \quad (1)$$

$$y' = \frac{y}{1 + \delta\gamma}. \quad (2)$$

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 annul 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 responds reversibly. The mechanical stability of the system is determined by the Hessian matrix \mathbf{H} :

$$H_{ij} \equiv \frac{\partial^2 U}{\partial \mathbf{r}_i \partial \mathbf{r}_j}, \quad (3)$$

where $U(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ is the total potential energy of the system as a function of the particle positions $\{\mathbf{r}_i\}_{i=1}^N$. 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 \mathbf{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 λ_P approaches zero via a square-root singularity

$$\lambda_P \sim \sqrt{\gamma_P - \gamma}. \quad (4)$$

An example of this scaling law is presented in Fig. 2.

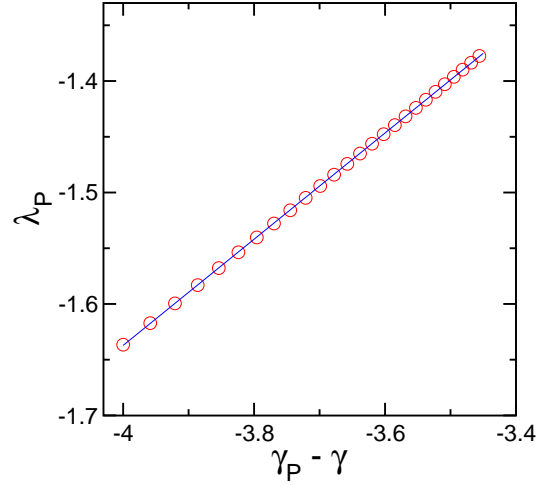


FIG. 2: A log-log plot of λ_P vs. $\gamma_P - \gamma$. The measured slope is 0.48 ± 0.0004 .

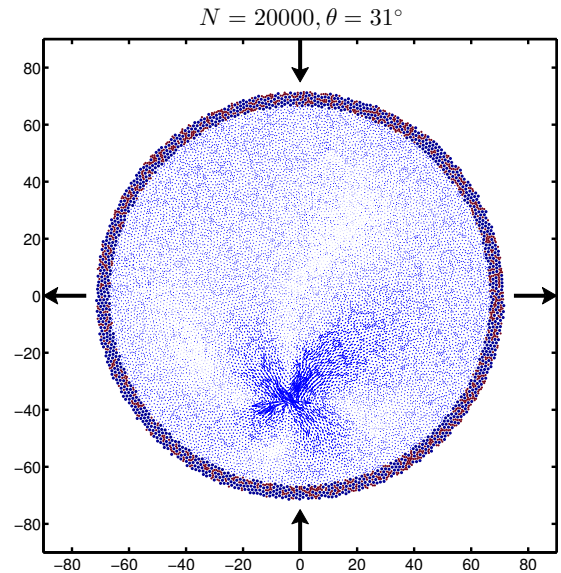


FIG. 3: The first plastic event that occurs as a result of choosing the x -axis to be in 31° with respect to the horizontal direction of the original square box. In this example $N = 20,000$.

In the unloaded state all the eigenfunctions of the Hessian matrix which are associated with low lying eigenvalues are delocalized. Upon the approach of the lowest eigenvalue to zero, the associated wave-function Ψ_P localizes on a typical quadrupolar structure which is identical with 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. (2) to be at 31° with respect to the horizontal direction of the original square box from which we constructed the circularly symmetric system. The plastic event is shown as the quadrupolar displace-

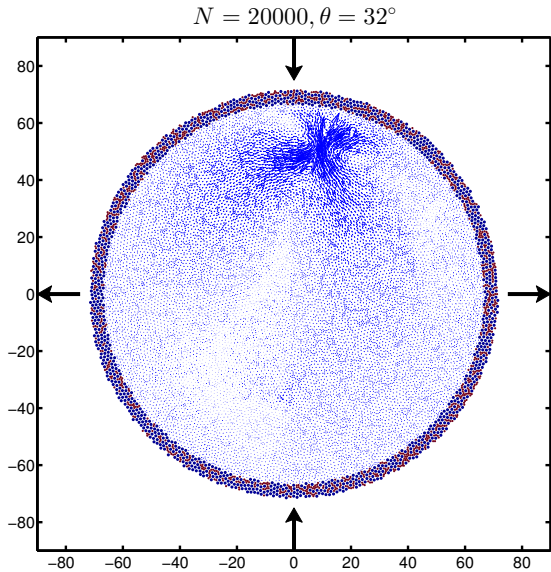


FIG. 4: Same as in Fig. 3 but with choosing the x -axis to be in 32° with respect to the horizontal direction of the original square box.

ment field near the bottom of the system. One can at all call it an STZ, but consider what happens if we change the x -axis to be at 32° 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 in 1° in the chosen direction 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 $N = 5,000 - 100,000$. 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 γ_P where it appears. In a second step of this exercise we change the x -axis to have an angle θ with respect to the original horizontal direction. We then determine, for each realization, the first angle θ for which *the first plastic event is different*, as seen in Figs. 3 and 4. Finally, we average the angle θ 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

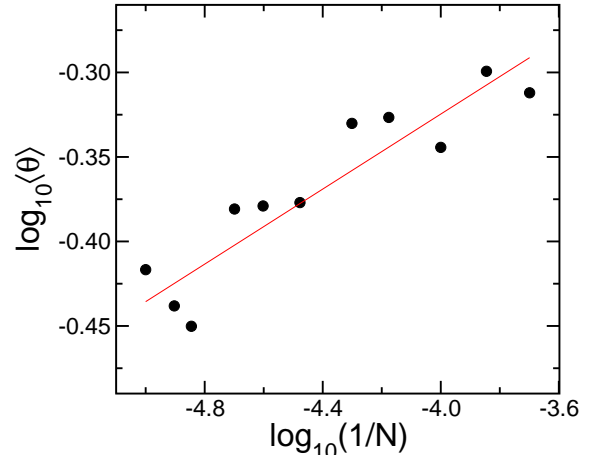


FIG. 5: The average angle required to observe a major change in the position of the first plastic event as a function of the system size. Note the logarithmic scale used that supports the power-law dependence Eq. (5). The systems studied here spanned the sizes $N = 5,000$ to $N = 100,000$, all quenched at rate of 10^{-1} .

data shown in Fig. 5 supports a power law of the form

$$\langle \theta \rangle(N) \sim N^{-\alpha}, \quad \alpha \approx 0.11 \pm 0.02. \quad (5)$$

Clearly, in the thermodynamic limit $N \rightarrow \infty$, this result strongly indicates that indeed any infinitesimal change in angle should result in a macroscopic change in the position of the plastic event. 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 the similar data top those shown in Fig. 5 were also obtained with other quench rates with identical conclusions.

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. (5). This and related findings are however beyond the scope of this Letter which aims specifically to sharpen

the difference in the current approaches to plasticity in amorphous solids.

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- [1] “Mechanics of Solids”, Ed. C. Truesdell (Encyclopedia of Physics. Chief Editor S. Flugge, Vol. YIa/1): J. F. Bell, “The Experimental Foundations of Solid Mechanics” (Springer-Verlag, Berlin-Heidelberg-New York, 1973).
- [2] A. H. Cottrell, “Dislocations and plastic flow in crystals”, (Oxford University Press, 1953).
- [3] J.-C. Toldano, “Physical Basis of Plasticity in Solids”, (World Scientific, 2011).
- [4] A. S. Argon and H. Y. Kuo, *Mater. Sci. Eng.* **39**, 101 (1979); A. S. Argon, *Acta Metall.* **27**, 47 (1979); A. S. Argon and L. T. Shi, *Philos. Mag. A* **46**, 275 (1982).
- [5] A.I Taub and F Spaepen, *Acta Metall.* **28**, 1781 (1980).
- [6] M. L. Falk and J. S. Langer, *Phys. Rev. E* **57**, 7192-7205 (1998).
- [7] E. Bouchbinder, J.S. Langer and I. Procaccia, *Phys. Rev. E*, **75**, 036107 (2007); **75**, 036108 (2007).
- [8] D. L. Malandro and D. J. Lacks, *Phys. Rev. Lett.* **81**, 5576 (1998).
- [9] C. Maloney and A. Lemaître, *Phys. Rev. Lett.* **93**, 195501 (2004).
- [10] S. Karmakar, A. Lemaître, E. Lerner, I. Procaccia, *Phys. Rev. Lett.* **104**, 215502 (2010).
- [11] E. Lerner and I. Procaccia *Phys Rev E*, **79**, 066109 (2009).
- [12] R. Dasgupta, S. Karmakar and I. Procaccia, *Phys. Rev. Lett.* **108**, 075701 (2012).
- [13] H.G.E. Hentschel, S. Karmakar, E. Lerner and I. Procaccia, *Phys. Rev. E* **83**, 061101 (2011).
- [14] W. Kob and H. C. Andersen, *Phys. Rev. Lett.* **73** 1376-1379 (1994).