Predicting plastic flow events in athermal shear-strained amorphous solids

Smarajit Karmakar¹, Anaël Lemaitre², Edan Lerner¹ and Itamar Procaccia¹
¹ Department of Chemical Physics, The Weizmann Institute of Science, Rehovot 76100, Israel
² UMR Navier, 2 allé Képler, 77420 Champs-sur-Marne, France

We propose a method to predict the value of the external strain where a generic amorphous solid will fail by a plastic response (i.e. an irreversible deformation), solely on the basis of measurements of the nonlinear elastic moduli. While usually considered fundamentally different, with the elastic properties describing reversible phenomena and plastic failure epitomizing irreversible behavior, we show that the knowledge of some nonlinear elastic moduli is enough to predict where plasticity sets in.

Introduction: Studies of plasticity in amorphous solids have always been hampered by the lack of any method to identify a-priori the locations of dissipative (plastic) events. This is in sharp contrast with crystals, where plasticity can be assigned to the motion of identifiable, topological defects like dislocations, the discovery of which has triggered tremendous theoretical breakthroughs. In the absence of any clear-cut definition of “shear transformation zones”, studies of amorphous systems are thus still in search for reliable predictors of yielding. Obvious observables such as local stress or density have proven unreliable [1, 2]. More promising are studies of local elastic fluctuations [3–6]. It appeared that plastic softening regions with strain at larger scales.

“Softening” regions with strain at larger scales. A small strain...
which implies
\[
\frac{\partial^2 U}{\partial \gamma \partial u_i} + \frac{\partial^2 U}{\partial u_j \partial u_i} \frac{d u_j}{d \gamma} = \Xi i + H_{ij} \frac{d u_j}{d \gamma} = 0 . \tag{3}
\]
This condition introduces the all-important Hessian matrix \( H_{ij} \) and the ‘non-affine field’ \( \Xi \), which can both be computed from the interparticle interactions. We rewrite this condition as
\[
\frac{d u_i}{d \gamma} = -H_{ij}^{-1} \Xi j = -\sum_k \frac{\psi_{ij}^{(k)} : \Xi j_k}{\lambda_k} \psi_{ij}^{(k)} \approx -\frac{\psi_{ij}^{(p)}}{\lambda_p} \Xi j \psi_{ij}^{(p)} , \tag{4}
\]
where the second equation results from expanding in the eigenfunctions of \( H, H_{ij} \psi_{ij}^{(k)} = \lambda_k \psi_{ij}^{(k)} \); the last estimate stems from our knowledge that in finite systems the plastic event is associated with a single eigenvalue going through zero when the systems slides over a saddle. Denote the critical eigenvalue as \( \lambda_p \). Eq. \( \boxed{4} \) integrates to provide the distance of the non-affine field \( u_i \) from its value at \( \gamma_p, u_i(\gamma) - u_i(\gamma_p) = X(\gamma) \psi_{ij}^{(p)} \), where \( X(\gamma) \) is a function of \( \gamma \) only, satisfying \( \lambda_p \approx 0 \) and
\[
\frac{d X(\gamma)}{d \gamma} \approx -\frac{\psi_{ij}^{(p)} : \Xi j}{\lambda_p} . \tag{5}
\]
Finally, we use the crucial assumption \( \boxed{3} \) that the eigenvalue \( \lambda_p \) crosses zero with a finite slope in the \( X \)-coordinate system itself, where distances are measured along the unstable direction:
\[
\lambda_p \approx A X + O(X^2) \tag{6},
\]
Together with Eq. \( \boxed{6} \) and asserting that \( \Xi j \) is not singular (it is a combination of derivatives of the potential function \( \boxed{1} \)), implies that
\[
X(\gamma) \propto \sqrt{\gamma_p - \gamma} . \tag{7}
\]
These results are now used to determine the singularity of the stress at \( \gamma_p \). We start with the exact result for the shear modulus \( \boxed{3, 11} \)
\[
\mu = \mu_B - \Xi \cdot H^{-1} \cdot \Xi \cdot V , \tag{8}
\]
where \( \mu_B \) is the Born term. Using Eqs. \( \boxed{8} \) and \( \boxed{7} \) we conclude that near \( \gamma_p \) we can write the shear modulus as a sum of a regular and a singular term,
\[
\mu \approx \mu_B - \frac{a/2}{\sqrt{\gamma_p - \gamma}} + O(\sqrt{\gamma_p - \gamma}) . \tag{9}
\]
We thus assert that in the vicinity of \( \gamma_p \):
\[
\sigma_{xy} \sim \sigma_p + a\sqrt{\gamma_p - \gamma} + b(\gamma_p - \gamma)^{3/2} + \cdots , \quad \gamma < \gamma_p . \tag{10}
\]
Indeed, the stress begins to go down before the plastic even takes place, but this is not seen in Fig. \( 11 \) since this happens very sharply. We can now come back to the question of predicting plasticity by looking at derivatives at any given point \( \gamma_0 < \gamma_p \). Near \( \gamma_0 \), we know that \( \sigma_{xy} \sim \mu(\gamma - \gamma_0) + \cdots \). Using \( \boxed{10} \) we write the ansatz
\[
\sigma_{xy}(\gamma) = \sigma_0 + \mu(\gamma - \gamma_0) + a\sqrt{\gamma_p - \gamma} + b(\gamma_p - \gamma)^{3/2} , \tag{11}
\]
from which we can recalculate the derivatives at \( \gamma = \gamma_0 \):
\[
B_2 = \frac{1}{4\sqrt{\gamma_p - \gamma_0}} \left[ 3b - \frac{a}{\gamma_p - \gamma_0} \right] , \tag{12}
\]
\[
B_3 = \frac{3}{8(\gamma_p - \gamma_0)^{3/2}} \left[ b - \frac{a}{\gamma_p - \gamma_0} \right] , \tag{13}
\]
\[
B_4 = \frac{3}{16(\gamma_p - \gamma_0)^{3/2}} \left[ 3b - \frac{5a}{\gamma_p - \gamma_0} \right] . \tag{14}
\]
Note that the shear modulus has disappeared from these expressions, becoming irrelevant for the subsequent prediction of the instability threshold. By measuring these three derivatives at \( \gamma_0 \) we can determine all the unknowns in Eq. \( \boxed{11} \). \( \gamma_p \) solves a 4th order polynomial, and
\[
\gamma_p = \gamma_0 + \frac{3B_4 - \sqrt{9B_4^2 - 2B_2B_4}}{2B_4} \tag{15}
\]
is the only physical solution among the four available ones. Next we test these results in a specific model.

**Model and numerical procedures**: Below we employ a model system with point particles of two ‘sizes’ but of equal mass \( m \) in two-dimensions, interacting via a pairwise potential of the form
\[
\phi \left( \frac{r_{ij}}{\lambda_{ij}} \right) = \varepsilon \left[ \left( \frac{\lambda_{ij}}{r_{ij}} \right)^k + \sum_{\ell=0}^q c_{2\ell} \left( \frac{\lambda_{ij}}{r_{ij}} \right)^{2\ell} \right] , \quad \frac{r_{ij}}{\lambda_{ij}} \leq x_c , \tag{15}
\]
\[
\frac{r_{ij}}{\lambda_{ij}} > x_c ,
\]
where \( r_{ij} \) is the distance between particle \( i \) and \( j \), \( \varepsilon \) is the energy scale, and \( x_c \) is the dimensionless length for which the potential will vanish continuously up to \( q \) derivatives. The interaction lengthscale \( \lambda_{ij} \) between any two particles \( i \) and \( j \) is \( \lambda_{ij} = 1.0\lambda \), \( \lambda_{ij} = 1.18\lambda \) and \( \lambda_{ij} = 1.4\lambda \) for two ‘small’ particles, one ‘large’ and one ‘small’ particle and two ‘large’ particle respectively. The coefficients \( c_{2\ell} \) are given by
\[
c_{2\ell} = \frac{(-1)^{\ell+1} \ell!!}{(2q-2\ell)!(2\ell)!!} \left( \frac{k+2q}{k-2} \right)!!(k+2\ell)^{-(k+2\ell)} . \tag{16}
\]
We chose the parameters \( x_c = 7/4, k = 10 \) and \( q = 6 \). The unit of length \( \lambda \) is set to be the interaction length scale of two small particles, and \( \varepsilon \) is the unit of energy. The density for all systems is set to be \( N/V = 0.85\lambda^{-2} \). We employ an athermal quasi-static scheme which consists of imposing an affine transformation to each particle of a configuration, followed by a potential energy minimization under Lees-Edwards boundary conditions \( \boxed{13} \). In this scheme one can obtain purely elastic trajectories of stress vs strain \( \boxed{12} \), which allows for the calculation of the total derivatives of stress with respect to strain using finite differences; we choose the stopping criterion
for the minimizations to be $|\nabla_i U| < 10^{-25}$ for every coordinate $x_i$, and select the strain increment for taking derivatives to be $\delta \gamma = 5 \times 10^{-7}$.

It is useful to compare our prediction with a simple failure criterion which uses a naive Taylor series of the form $\sigma_{xy}(\gamma) = \sigma_0 + \mu(\gamma - \gamma_0) + \frac{1}{2} B_2 (\gamma - \gamma_0)^2 + \frac{1}{6} B_3 (\gamma - \gamma_0)^3$. From here $\gamma_P$ is estimated as the point at which $\left( \frac{\partial \sigma_{xy}}{\partial \gamma} \right)_{\gamma = \gamma_P} = 0$—the difference between this point and the actual yield point is negligible compared to all other strain scales entering the problem [14]. This is the solution of the equation:

$$
\mu + B_2(\gamma_P - \gamma_0) + \frac{1}{2} B_3 (\gamma_P - \gamma_0)^2 + \frac{1}{6} B_4 (\gamma_P - \gamma_0)^3 = 0.
$$

\hspace{1cm} (17)

**Predictions:** Fig. 2 in the upper panel demonstrates the quality of our predictor for a typical initial condition taken in the elasto-plastic steady state in a system with $N = 484$. Here, $\gamma_0$ corresponds to the strain at which the elastic branch was reached via a prior plastic event. The total length of the branch on the stress-strain curve is thus exactly $\gamma_P - \gamma_0$. We show the stress vs. strain curve in (symbols) and the values of $\gamma_P$ predicted using either Eq. (14) or (17) at each value of the external strain. We see that the naive Taylor expansion fails except right at $\gamma_P$, whereas our accelerated method works very well over nearly the whole length of the elastic branch. Of course, in the elasto-plastic steady state the strain range between plastic events is rather limited—as reflected by the scale of abscissa. But our data shows that the transition between one plastic event and the next in entirely controlled by a single mode, i.e. by a single soft zone. We will shortly come back on this issue.

We also test our predictor starting from an equilibrium isotropic state obtained by thermal annealing. Here we need to predict the first plastic event which occurs upon increasing the external strain. This situation could be expected to be more tricky since at $\gamma = \gamma_0 = 0$ all the even derivatives $\frac{\partial^n \sigma_{xy}}{\partial \gamma^{2n}}$ vanish on the average. We could expect that, upon straining, these derivatives must build up before predictability of plasticity is achieved. In fact, as illustrated on the lower panel of Fig. 2 predictability is often achieved rapidly, even though the strain range is considerably larger than in the upper panel. In steady state the vast majority of the elastic branches end up in a plastic event whose onset can be predicted as demonstrated here. In contradistinction, the elastic branch emanating from the isotropic equilibrium state may exhibit large non-affine elastic events which resemble a typical precursor to a plastic failure but avoids it by eventually stabilizing. Our derivatives will pick up these elastic events and will incorrectly predict a plastic failure before landing on the right prediction. This scenario is shown in Fig. 3 in which two non-affine large events occur before the first plastic event. All three derivatives undergo huge changes at the non-affine events and then dive to $-\infty$ at the true plastic event. This seems to be a trace of the typical presence of several interacting eigenmodes, not necessarily well-aligned with the direction of shear.

We stress that this phenomenon is quite rare and the normal situation is the one that is exhibited in Fig. 2 lower panel.

**Dependence on system size:** The data shown in Figs. 2 and 3 pertain to a relatively small system of 484 particles. We therefore must raise the important question of how the predictability of the plastic failure depends on the system size. To study the size dependence of the
predictability we measured the distance $\Delta \gamma_p \equiv |\gamma - \gamma_p|$ for which the error in estimating $\gamma_p$, denoted as $\delta \gamma_p/\Delta \gamma_p$, satisfies $\delta \gamma_p/\Delta \gamma_p \leq 0.15$, for systems of varying sizes (see inset in Fig. 4). The results are shown in Fig. 4 indicating that the range of predictability reduces like a power law with the system size,

$$\Delta \gamma_p \sim N^\eta, \quad \eta \approx -0.61.$$  (18)

To estimate the exponent $\eta$ theoretically, we note that for predictability to be possible we need the divergent term of at least $B_2$ to be of the order of unity. The quantity $B_2$ (cf. Eq. (12)) has a coefficient $a$ which is of order of $1/N$ because there is only a single localized mode that becomes unstable [9], and the divergent term that goes like $(\gamma - \gamma_p)^{-3/2}$. Thus we expect predictability when $|\gamma - \gamma_p| \sim N^{-2/3}$, which estimates $\eta = -2/3$. Higher order derivatives are more singular and thus $\eta$ can only be smaller due to their effect. This estimate is very important, since it guarantees that predictability will not deteriorate in the elasto-plastic steady-state. To see this, we recall that the average distance between successive plastic events $\langle \Delta \gamma \rangle$ is known [12] to follow a scaling law with the system size $\langle \Delta \gamma \rangle \sim N^\beta$. The exponent $\beta$ was measured in a variety of systems in 2D, and was found to be always in the range $[-0.67, -0.63]$. In the present model system we measure $\beta \approx -0.65$. With the present accuracy we cannot exclude that $\eta \approx \beta$, leading to the realization that while the predictability is reduced with increasing $N$, the range of $\gamma$ over which we need to predict reduces almost at the same speed, if not slightly faster. Thus in effect the predictability in the elasto-plastic steady state does not deteriorate with $N$.

In summary, we showed that (i) the discussion of plasticity in amorphous solids calls for understanding the role of nonlinear elasticity, and (ii) for the elasto-plastic steady state the knowledge of a few nonlinear elastic constants suffices to predict where the next plastic event should occur. Finally, the analysis presented above is global, but it can be extended to local instability maps eliminating the system size dependence whatsoever. The first step toward a local analysis, which is the microscopic definition of the nonlinear elastic constants, has been already achieved and is available in Ref. [15]. The second step where it will be shown how to use these results in models of elasto-plasticity in both two and three dimensions will be discussed elsewhere [16].

Acknowledgments

This work had been supported in part by the Israel Science Foundation and the Ministry of Science under the French-Israeli collaboration.

[1] D. Srolovitz, Maeda, Takeuchi, Egami and Vitek et al., J Phys-F-Metal Phys 11, 2209 (1981).
[2] M. Tsamados, A. Tanguy, F. Leonforte, and J. L. Barrat, European Physical Journal E 26, 283 (2008).
[3] K. Yoshimoto, T. S. Jain, K. V. Workum, P. F. Nealey and J. Pablo, Phys. Rev. Lett. 93, 175501 (2004).
[4] K. Yoshimoto, G. J. Papakonstantopoulos, J. F. Lutsko, and J. J. de Pablo, Physical Review B 71, 184108 (2005).
[5] M. Tsamados, A. Tanguy, C. Goldenberg, and J. L. Barrat, Physical Review E 80, 026112 (2009).
[6] V. Iljin, I. Procaccia, I. Regev, and N. Schupper, Phys. Rev E 77, 061509 (2008).
[7] C. Maloney and A. Lemaître, Phys. Rev. Lett. 93, 195501 (2004).
[8] D. L. Malandro and D. J. Lacks, Phys. Rev. Lett. 81, 5576 (1998).
[9] C. Maloney and A. Lemaître, Phys. Rev. Lett. 93, 16001 (2004).
[10] See for example: C. Domb in Phase Transitions and Critical Phenomena vol 3 ed C Domb and M S Green (London: Academic Press) pp. 357458 (1974).
[11] A. Lemaître and C. Maloney, J. Stat. Phys. 123, 415 (2006).
[12] E. Lerner and I. Procaccia, Phys. Rev. E 79, 066109 (2009).
[13] M.P. Allen and D.J. Tildesley, Computer Simulations of Liquids (Oxford University Press, 1991).
[14] The difference is $O(10^{-4})$ for $N = 484$, and it decays like $N^{-2}$ for larger systems, following the same arguments leading to the estiamte of $\eta$ in Eq. (18).
[15] S. Karmakar, E. Lerner, and I. Procaccia, “Athermal Nonlinear Elastic Constants of Amorphous Solids”, Phys. Rev. E, submitted. Also: arXiv:1004.2198.
[16] S. Karmakar, E. Lerner, and I. Procaccia, “Local Nonlinear Elastic Constants: The Mechanism of Spatial Correlations in Elasto-Plasticity of Amorphous Solids”, in preparation.