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Statistical physics of the yielding transition in amorphous solids

Smarajit Karmakar, Edan Lerner, and Itamar Procaccia
Department of Chemical Physics, The Weizmann Institute of Science, Rehovot 76100, Israel
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The art of making structural, polymeric, and metallic glasses is rapidly developing with many applications. A limitation is that under increasing external strain all amorphous solids (like their crystalline counterparts) have a finite yield stress which cannot be exceeded without effecting a plastic response which typically leads to mechanical failure. Understanding this is crucial for assessing the risk of failure of glassy materials under mechanical loads. Here we show that the statistics of the energy barriers ΔE that need to be surmounted changes from a probability distribution function that goes smoothly to zero as $\Delta E=0$ to a pdf which is finite at $\Delta E=0$. This fundamental change implies a dramatic transition in the mechanical stability properties with respect to external strain. We derive exact results for the scaling exponents that characterize the magnitudes of average energy and stress drops in plastic events as a function of system size.

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In this Rapid Communication we focus on the statistical physics of the yielding transition at very low temperatures and quasistatic external straining conditions (the so-called athermal quasistatic or AQS limit), where very precise simulation results exist for the dependence of energy and stress drops in plastic events as a function of system size [1]. Consider Fig. 1 which demonstrates the nature of the yielding transition. We plot here the conditional mean energy drop in a plastic event as a function of the external strain γ for two-dimensional systems (see below) consisting of N particles, with N ranging between 484 and 20 164. To read this figure properly, one should understand that in some realizations there are no plastic events at all at a given external strain. What is measured here is the size of the mean energy drop if such a (single) drop happened at an external strain value between γ and $\gamma+d\gamma$, averaged over numerous realizations of the random structure of the system (see below for details). We see that in the early stages of the loading, the plastic events are localized and the amount of energy released in events is system-size independent. This is followed by a smooth rise in these curves, showing an increasingly sharper transition to the plastic flow state in which the plastic events become nonlocalized avalanches whose total-energy release increases with the system size. This very interesting system-size dependence will be quantified below. We note in passing that the stress itself cannot be a proper order parameter; states with the same stress level (shown, for example, in Fig. 1 as two magenta circles) have very different conditional mean plastic energy drops. Here we explore the statistical physics that is responsible for the difference between these isostress states, which also have very similar potential energy and pressure. We point out that the precise nature of this *strain-induced* transition from the solidlike jammed state to the steady flow state, where the plastic flow events resemble liquidlike dynamics, is still unclear. Although the increasing availability of computational power has recently led to many important observations and conclusions regarding the statistics of the steady flow state [1–3], a clear-cut identification of the physics that control the *approach* toward steady state has not been presented yet. The aim of this Rapid Communication is to close this gap and to offer some exact results. We stress that this desired analysis is best conducted in the AQS limit since much is known there about the nature of the plastic events themselves, as these are determined by mechanical instabilities which can be seen as a saddle node bifurcation in which the lowest eigenvalue of the Hessian matrix going through zero [4–6]. Denote the potential energy of the system as $U(\boldsymbol{r}_i)$, where $\boldsymbol{r}_i$ are the positions of the particles, and the Hessian matrix as $H_{ij}\equiv\partial^2 U/\partial\boldsymbol{r}_i\partial\boldsymbol{r}_j$. The Hessian is a real symmetric matrix; we denote its lowest eigenvalue (excluding the Goldstone modes) as λ_P. It was established [4,6] that when the external strain γ reaches a critical value γ_P, λ_P vanishes with a square-root singularity, i.e., such that $\lambda_P\propto\sqrt{\gamma_P-\gamma}$. We will show that this simple singularity determines the numerical values of a number of interesting exponents that appear in the statistical analysis [7].

Below we employ a model glass-forming system with point particles of two "sizes" but of equal mass m in two and three dimensions (2D and 3D, respectively), interacting via a pairwise potential which has been fully described in [8]. The experiments performed are as follows: for undeformed isotropic systems we measured the strain at which the first plastic event takes place and denoted it as $\Delta\gamma_{\rm iso}$. Each such mea-

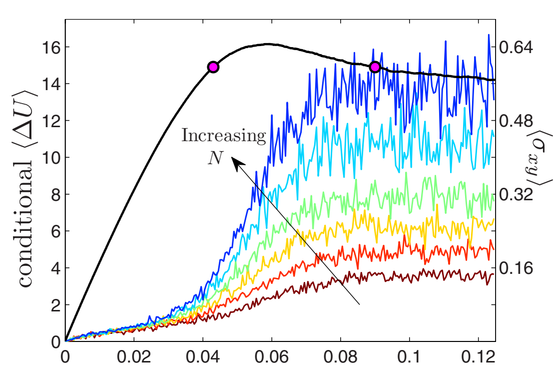

FIG. 1. (Color online) Evolution of the conditional mean energy drops with the loading, for all system sizes simulated, increasing from bottom to top. Superimposed (scale on the right ordinate) is the mean stress vs strain curve for the largest system of $N=20\,164$. The magenta dots represent equistress states but of highly different stability properties.

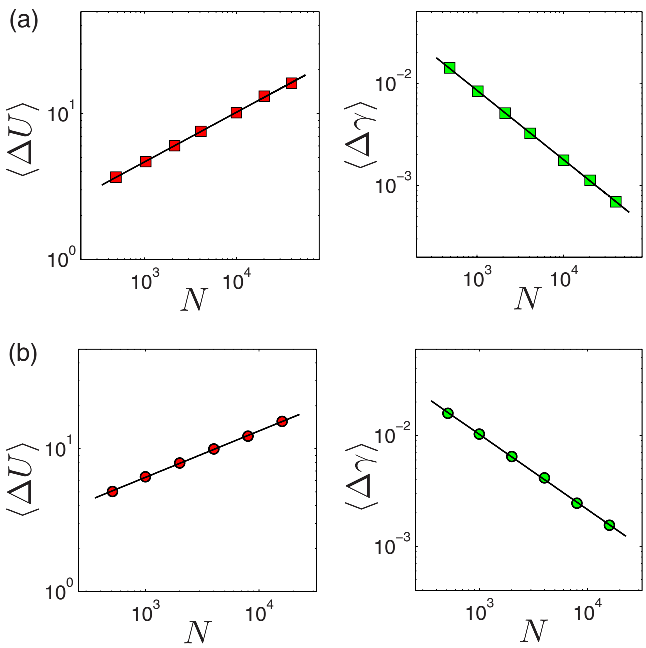

FIG. 2. (Color online) Panel (a). Mean energy drop $\langle \Delta U \rangle$ and mean strain interval $\langle \Delta \gamma \rangle$ in two dimensions as functions of system size, measured in AQS simulations of steady plastic flow of a model glass former, see text. Panel(b). The same for three dimensions. The continuous lines represent the scaling laws (1). The scaling exponents are the same in 2D and 3D.

surement was performed on a freshly produced amorphous solid, quenched from the high-temperature liquid at the rate of $5\times 10^{-5}\frac{\varepsilon}{k_B\tau}$. Then the AQS scheme (see [8] for details) was utilized to strain the system up to the first mechanical instability occurring at some strain value $\Delta\gamma_{\rm iso}$. Statistics of $\Delta\gamma_{\rm iso}$ were collected for a variety of system sizes, see below. In the elastoplastic steady state we first strained statistically independent systems for 100% strain to reach stationarity and then collected statistics as shown below.

In the steady flow state, the statistics of the energy drops ΔU, the stress drops $\Delta\sigma$, and the strain intervals between successive flow events $\Delta\gamma$ become stationary. Quite surprisingly, one finds that the averages of these quantities obey scaling relations with the same exponents in two and three dimensions:

$$\langle \Delta U \rangle \sim \bar{\epsilon} N^{\alpha}, \quad \langle \Delta\sigma \rangle \sim \bar{s} N^{\beta}, \quad \langle \Delta\gamma \rangle \sim N^{\beta}. \tag{1}$$

In Fig. 2 the mean energy drop $\langle \Delta U \rangle$ and mean strain interval $\langle \Delta\gamma \rangle$ for our model system are displayed, together with the scaling laws [Eq. (1)]. We show results in the upper panels in two dimensions, in the lower panels in three dimensions, and in both $\alpha \approx 1/3$ and $\beta \approx -2/3$. A scaling relation $\alpha - \beta = 1$ was already established before [2]. In this Rapid Communication we propose that the respective values 1/3 and $-2/3$ are exact.

The yielding transition is underlined by the fact that for the first plastic event when strained from a freshly quenched isotropic state the statistics is entirely different, with $\Delta U \sim N^0$ representing a localized event without any system-size dependence. On the other hand the first plastic event

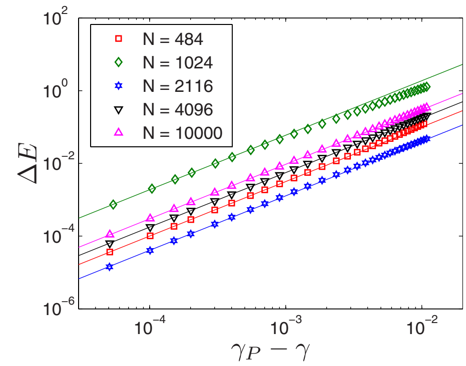

FIG. 3. (Color online) Scaling of energy barriers for various system sizes, see [8] for details. The slope of the continuous lines is 3/2.

does not occur for any infinitesimal value of γ and careful measurement of the mean strain interval $\langle \Delta\gamma_{\rm iso} \rangle$ that separates the undeformed state from the first plastic event results in a scaling law

$$\Delta\gamma_{\rm iso} \sim N^{\beta_{\rm iso}}, \quad \beta_{\rm iso} \approx -0.62. \tag{2}$$

How can we understand the difference between β and $\beta_{\rm iso}$ and what determines their numerical values?

Starting from any given mechanically stable state, at the undeformed state or at the steady state, the system has a set of $O(N)$ energy barriers ΔE which are coupled to the external strain. One of those needs to be surmounted in order to have a plastic event. In AQS conditions the one chosen will be the one which has the smallest $\Delta\gamma_{\rm iso}$ (in the isotropic state) or the smallest $\gamma_P - \gamma$ (in the steady state). As a function of the external strain this barrier reduces until it vanishes at the saddle node bifurcation where λ_P vanishes [4–6]. In Refs. [8,9] it was shown that the manner in which the energy barrier vanishes is determined by the saddle node singularity. In other words, it was established that close to γ_P

$$\Delta E \propto \lambda_p^3 \sim (\gamma_P - \gamma)^{3/2}. \tag{3}$$

We stress that this result is valid, sufficiently close to γ_P, equally well when starting from equilibrium, where γ_P represents the value of the strain for the *first* plastic event, or in the steady state, where γ_P is any value of the strain where a plastic event occurs. It turns out that the scaling law [Eq. (3)] is obeyed, at least in the class of models in which the potential is purely repulsive, for a very long range of $\gamma_P - \gamma$, see Fig. 3. We will use this in this Rapid Communication, coming back to the question of universality at the end.

In terms of distributions, the possible plastic events can occur anywhere in the system, and the number of possible sites increases linearly with N. However, we realize that every time that we observe a plastic event in AQS conditions, it is one of the *lowest barriers* out of $O(N)$ barriers that is overcome [10]. We cannot directly measure the distribution of energy barriers but need to concentrate on the extreme statistics regarding the minimal value. In the isotropic solid state we expect a zero probability of finding a zero barrier. Since we have no typical scale at small strain values, the

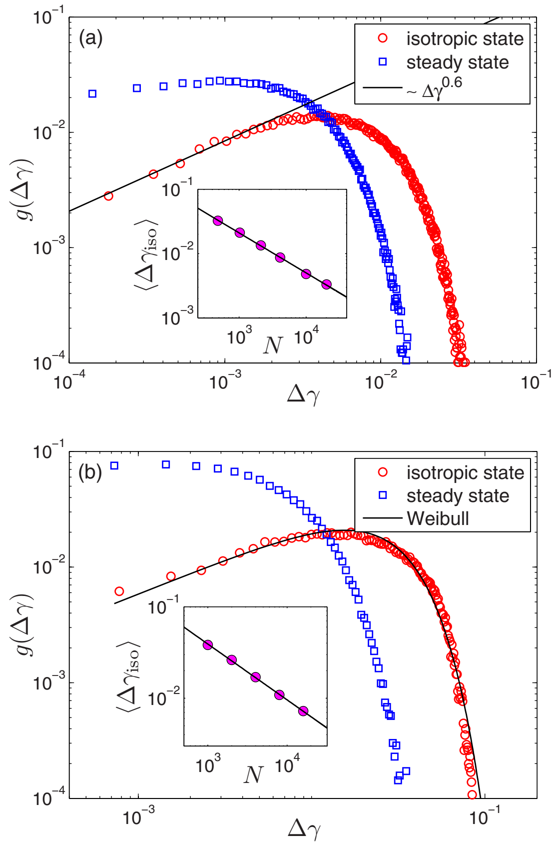

FIG. 4. (Color online) The measured pdf in two dimension for $N=4096$ in panel (a) and in three dimensions for $N=2000$ in panel (b) for the observed value of $x \equiv \Delta\gamma_{\rm iso}$ for isotropic systems (in red) and of $x \equiv \Delta\gamma$ for the steady state (in blue). The scaling law for the mean shown in the inset indicates a value of $\eta \approx 0.6$ for both two and three dimensions. Note the dramatic change in the power-law tail of the distributions at small values of $\Delta\gamma$: in equilibrium the tail guarantees that the probability to see a zero value of ΔE is zero. This is not the case in the steady state, and this is the physical hallmark of the yielding transition. The black line through the red dots in panel (b) is the Weibull distribution Eq. (5).

distribution starts as a power law, leading to a distribution of the form

$$p(x) = x^{\eta} h(x)/Z, \quad Z \equiv \int_0^\infty x^{\eta} h(x) \quad \eta \geq 0, \tag{4}$$

where $h(x)$ decays rapidly for $x \gg 1$. It is well known then that if we now take a set of $N \gg 1$ independent samples from such a distribution, then the probability distribution $g(y,N)$ of the minimal element of the set (denoted $y \equiv \Delta\gamma_{\rm iso}$) is the Weibull distribution [11]

$$g(y,N) = \frac{1+\eta}{y_0}\left(\frac{y}{y_0}\right)^{\eta} \exp\left[-\left(\frac{y}{y_0}\right)^{1+\eta}\right]. \tag{5}$$

In this equation $y_0 \sim N^{-1/(1+\eta)}$ is the mean value of y with respect to the Weibull distribution [12]. A test of this logic is presented in Fig. 4 for systems in three dimensions where we show the distribution of $\Delta\gamma_{\rm iso}$ of isotropic states, in excellent agreement with Eq. (5) with $\eta \approx 0.6$. In two dimensions the scaling with $\eta \approx 0.6$ is also recovered. We expect the distribution of the coefficients of the scaling law [Eq. (3)] to be regular, implying that the probability distribution of the energy barriers has, for low values of ΔE, the form

$$p(\Delta E) \sim (\Delta E)^{\tilde\eta}, \quad \tilde\eta = (2\eta - 1)/3. \tag{6}$$

For $\eta \approx 0.6$ we find $\tilde\eta \approx 1/15 > 0$. This is consistent with the notion of solidity; one expects that for a solid the probability of finding a zero barrier is strictly zero. Finally, the mean value of the minimal values of ΔE scales as predicted by the Weibull distribution, i.e., $\langle \Delta E \rangle \sim N^{-1/(1+\tilde\eta)}$. Substituting this in the mean of Eq. (3) we recover Eq. (2) with the observed exponent $\beta_{\rm iso} \approx -0.62$. We thus conclude that the first plastic event is dominated by extreme statistics of the minimal barriers for plasticity with a probability distribution function (pdf) of the energy barriers that goes to zero for $\Delta E \to 0$ as is expected from a solid.

The picture changes dramatically in the elastoplastic steady state. There the distribution of strain intervals between successive events $\Delta\gamma$ changes qualitatively as seen in Fig. 4: the power-law initial part of the distribution is very shallow, maybe even a constant. Below we model the processes that are responsible for this; skipping the details for a while, here we propose that the hallmark of the yielding transition is that in the elastoplastic steady state the probability to find a zero value of the energy barrier is nonzero, cf. [13]. In other words, the criterion of solidity is no longer applicable. We also cannot expect that the statistics of $\Delta\gamma$ follows the Weibull distribution since the values of γ_P in subsequent plastic events become highly correlated and history dependent. Indeed the steady-state distribution shown in Fig. 4 cannot be fitted to a Weibull distribution. On the other hand we can still expect that the numerical values of the minimal energy barriers that need to be surmounted remain statistically independent due to the avalanches, see next paragraph. The consequence of this is that with N independent random samples of ΔE with a finite probability to find $\Delta E=0$, the scaling of the minimal value must scale like $1/N$ [12]. Using this in Eq. (3) leads to the proposed exact values of $\alpha=1/3$ and $\beta=-2/3$.

To understand the pdf of strain intervals as measured in the steady state (cf. Fig. 4), we need to explain how the avalanches that occur after every plastic event refresh the statistics and renormalize the pdf to the form seen in Fig. 4. The cumulative energy associated with an avalanche grows subextensively with the system size (like $N^{1/3}$), and therefore the impact of these avalanches remains pertinent in the thermodynamic limit. To model the effect of the avalanches imagine that we consider a population of N energy barriers ΔE_i sampled from a distribution $p(\Delta E)$ which satisfies the two conditions: (i) $p(\Delta E) \sim \Delta E^0$ for $\Delta E \to 0$ and (ii) $p(\Delta E) \to 0$ at least exponentially fast for $\Delta E \gg 1$. The series of plastic drops is then modeled by the following iterative steps; at each step we repeat the following operations: (1) find $\Delta E_{\rm min}$ and record it. (2) For every $\Delta E_i \neq \Delta E_{\rm min}$ transform,

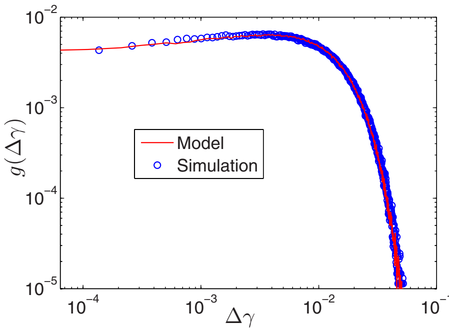

FIG. 5. (Color online) Pdf of the observed strain intervals between avalanches compared to the converged pdf of the iterative model, see text for details. Here $q=2/3$. The agreement indicates the robustness of the model and the crucial role of the avalanches in renormalizing the pdf. Here we opted to show the pdf of strain intervals because it is the directly measurable quantity related to the energy drop by Eq. (3).

$$\Delta E_i \leftarrow (\Delta E_i^{2/3} - \Delta E_{\min}^{2/3})^{3/2}. \quad (7)$$

This step takes into account the fact that what is changed in the simulations is the external strain rather than the energy barriers, and we have used Eq. (3). (3) Remove $\Delta E_{\min}$ and reassign a new number from $p(\Delta E)$ instead of it. (4) To model the decorrelating effect of avalanches, randomly remove qN numbers from the set [$q \in (0,1)$ is some fraction] and reassign new numbers instead of them from $p(\Delta E)$. This iteration scheme is readily performed numerically, leading to a converged pdf that is shown in Fig. 5 in comparison to the simulational pdf. We find an excellent agreement which underlines the crucial effect of avalanches in partially destroying the correlation between subsequent values of $\Delta E_{\min}$. Importantly, the scaling of the mean value is independent to the choice of q in the large N limit. It should be noted that when the same iteration procedure is performed with a pdf that goes to zero at zero like ΔE^{η} (even for very small η), the resulting converged pdf is qualitatively different, preserving the scaling of the mean value $\langle \Delta E_{\min} \rangle \sim N^{-1/(1+\eta)}$. This stresses the importance of the physics of the yielding transition which takes the system from a solidlike to liquidlike state with a qualitative change in $\lim_{\Delta E \to 0} p(\Delta E)$.

The main point of this Rapid Communication is that the yielding transition is characterized by a qualitative change in the nature of the pdfs of the energy barriers for a plastic event in the AQS limit. For the solid the probability to see a vanishing energy barrier is zero. For the elastoplastic steady state this probability is finite. Physically, this transition is the reason for the avalanches that are observed in the steady state—there are many localized configurations with close to zero energy barrier to surmount and any plastic drop anywhere in the system will find it easy to cause all these configurations to cross the instability threshold. The implication of this qualitative change is the change in scaling exponents which are shown in Eqs. (1) and (2). One main result of the Rapid Communication is the derivation of the exact values of the exponents α and β in Eq. (1). We stress that this exact result rests entirely on the availability of the scaling law [Eq. (3)]. Clearly this law is asymptotically true for $\gamma \to \gamma_P$, equally well in 2D and 3D, implying that α and β are dimension independent. However the range of strain values over which this law pertains in the present Rapid Communication is quite amazing, and there is no guarantee that this will remain true in other models which have attractive terms in the potential of molecular degrees of freedom. It is therefore worthwhile to continue to explore the scaling properties of different models in the AQS conditions to delineate the existence of universality classes.

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