Front propagation at the onset of plastic yielding

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The existence of a finite threshold, the yield stress, for the onset of plastic yielding is a universal feature of plasticity. This jamming-unjamming transition is naturally accounted for by the dynamics of a bistable internal state field. We show, within the athermal shear transformation zone theory of amorphous plasticity, that the transition is accompanied by the propagation of plastic fronts. We further show that the mean-field theory cannot select the velocity of these fronts, and go beyond the mean-field description to include fluctuations and correlations effects, resulting in additional nonlocal terms in the equations. Finally, we demonstrate that these terms, with an associated intrinsic length scale, provide a velocity selection mechanism for the plastic fronts.

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I. INTRODUCTION

A complete understanding of the dynamics of plastic deformation in low-temperature, or athermal, amorphous systems remains a major theoretical challenge in statistical and condensed matter physics. The response of these systems to the application of external driving forces exhibits some universal features like a transition from jamming to flow at the yield stress, orientational memory effects of recent deformation, and strain localization [1]. In this work we focus on the spatiotemporal patterns associated with the transition from jamming to flow at the onset of plastic yielding, in the framework of the recently developed athermal shear transformation zone (STZ) theory of amorphous systems [2,3]. This transition is controlled by the applied stress. For stresses below a material-dependent threshold, the yield stress, these systems exhibit elastic deformation as well as transient plastic flow that vanishes at a finite time. The resulting state is "jammed" in the sense that it carries a finite stress without flowing. On the other hand, for stresses that exceed the yield stress, these systems exhibit persistent plastic flow, implying some remarkable "unjamming" (or yielding) transition at the yield stress.

A major difficulty in developing a theory of amorphous plasticity, which among other things should predict plastic yielding at a finite yield stress, is that the identity and characteristics of the microstructural objects that "carry" plastic deformation in amorphous (disordered) systems remain quite elusive. However, a growing body of experimental and simulational evidence seems to point toward a unifying picture in which low-temperature amorphous plasticity involves stressdriven configurational rearrangements of localized regions composed of a small collection of the relevant elementary entities (e.g., particles, molecules, grains, colloids, bubbles) [4]. The existence of such a unifying picture, which is independent of the elementary entities and their microscopic interactions, is fully consistent with the existence of universal features mentioned above.

In line with this accumulating evidence, the athermal shear transformation zone theory of amorphous plasticity views STZs as localized groups of particles that are more susceptible to shearing transformation under stress than their surroundings. Upon surpassing a local threshold a STZ can undergo a finite irreversible shear in a given direction. Once transformed, due to a local redistribution of stresses, a STZ resists further deformation in that direction, but is particularly sensitive to reverse shear deformation if the local applied stress changes sign. Therefore, a STZ is conceived as a two-state system that can transform between its internal states depending on the magnitude and direction of the local stress. In addition, the stress redistribution that accompanies a STZ transition can induce the creation and annihilation of other STZs at a rate proportional to the local energy dissipation (recall that thermal fluctuations are assumed to be absent or negligible). The minimal two-state assumption, along with the deformation-driven creation and annihilation of STZs, provides a mechanism for retaining and losing orientational memory of previous deformation and is sufficient to capture the transition from jamming to flow at a finite yield stress.

We choose to study the spatiotemporal characteristics of the unjamming transition using STZ theory for two major reasons. First, the existence of the transition is described in this theory, as will be explained in detail below, by an exchange of dynamic stability in the equations of motion for an internal state field. More generally, STZ theory aims at identifying proper internal state fields (order parameters) and proposes equations of motion for these based on microscopic insights, symmetries and conservation laws [2,3]. We find such an approach very appealing. Second, recent work has shown that the STZ equations capture a variety of phenomena observed in computer simulations and laboratory experiments [5-13]. Most relevant for our purposes here are the results reported in [12,13]. In [12], the two-state nature of STZs was observed directly in bubble-raft experiments and two-dimensional foam simulations. It was found that groups of bubbles can make transitions, the so-called T1 events that are realizations of STZ transitions in foam, between two states if the direction of the applied force is reversed shortly after an event occurs. However, if the force is not reversed until after other events have occurred nearby, then the orientational memory is lost, implying that a STZ is annihilated. In $\begin{bmatrix} 13 \end{bmatrix}$ the STZ equations were shown to agree quantitatively with transient shear reversal behavior of a granular flow in a We proceed by introducing the relevant mean-field STZ equations in Sec. II, where we also discuss the existence of the transition from jamming to flow at a finite yield stress and the physics behind it. In Sec. III we focus on the spatiotemporal characteristics of the unjamming transition. We show that there exist propagating front solutions if the equations are modified to include effects beyond the mean field as well as an intrinsic length scale. Section IV offers some concluding remarks.

II. ELEMENTS OF THE ATHERMAL SHEAR TRANSFORMATION ZONE THEORY

Consider a two-dimensional athermal amorphous system under the application of a pure shear stress s. The two states of a STZ are oriented along the principal axes x (the direction of the force) and y (the perpendicular direction), and denoted by \pm . The number densities of STZs in the \pm states are denoted by n_+ . The configurational disorder of the system is characterized by an effective disorder temperature χ that is assumed to govern the total density of the STZ, with $n_{\infty}e^{-1/\chi}$ being the steady state density of the STZ under persistent deformation. χ was shown very recently to play an important role in the deformation dynamics of amorphous solids [6-10]; however, its dynamics in the present context are not of prime interest and will not be discussed. The internal state fields n_+ and χ , in addition to the applied stress *s*, determine the macroscopic plastic rate of deformation $D^{\rm pl}$ according to [3]

$$\tau_0 D^{\rm pl} = \lambda [R(s)n_- - R(-s)n_+], \tag{1}$$

$$\tau_0 \dot{n}_{\pm} = R(\pm s) n_{\pm} - R(\pm s) n_{\pm} + \Gamma \left(\frac{n_{\infty} e^{-1/\chi}}{2} - n_{\pm} \right).$$
(2)

Here λ is a material-specific parameter with the dimensions of area. τ_0 is the basic time scale and $R(\pm s)/\tau_0$ are the rates for forward and backward transitions, respectively. The athermal condition implies that R(s) vanishes for s < 0, i.e., there are no transitions in the direction opposite to the direction of the applied force [3].

Equation (1) simply states that the macroscopic plastic rate of deformation D^{pl} results from STZ transitions between their two internal states, depending on the driving force through R(s) and on the population of STZs in each of the two states. Equations (2) are master equations for the population densities n_{\pm} themselves. The first two terms on the right-hand side describe the number-conserving process in which STZs change their state from + to - or vice versa. The third term on the right-hand side is a coupling term that accounts for interactions between STZs. As mentioned above, the stress redistribution that accompanies a STZ transition can induce the creation and annihilation of other STZs. This is a crucial aspect of the theory. The rate of STZ creation, Γ , which is a positive definite scalar, is assumed to be proportional to the rate of plastic dissipation $2sD^{\text{pl}}$ [2,3]. For low temperature we obtain [2,3]

$$\Gamma = \frac{2\tau_0 s D^{\rm pl}}{s_v \epsilon_0 e^{-1/\chi}},\tag{3}$$

where s_y is a material-specific parameter of stress dimension, which is shown below to be equal to the yield stress. s_y has an interesting physical meaning: it quantifies how much of the dissipated energy is invested in creating new STZs. When it is large, only a small amount of the dissipated energy is invested in creating new STZs (available for irreversible transitions) and vice versa. This interpretation immediately suggests that s_y is related to the yield stress; see [14] for a discussion of this issue from an entropic point of view.

We proceed by setting the total STZ density to its steady state value, $n_++n_-=n_{\infty}e^{-1/\chi}$, and by defining an orientational order parameter *m* (which is generally a tensor; see [8]) as

$$m \equiv \frac{n_{+} - n_{-}}{n_{+} + n_{-}}.$$
(4)

This internal state field represents the bias of the STZ populations between the \pm states. With these choices we can rewrite Eqs. (1) and (2) as

$$\tau_0 D^{\rm pl} = \epsilon_0 e^{-1/\chi} \mathcal{C}(s) \left[\operatorname{sgn}\left(\frac{s}{s_y}\right) - m \right], \tag{5}$$

$$\tau_0 \dot{m} = 2\mathcal{C}(s) \left[\operatorname{sgn}\left(\frac{s}{s_y}\right) - m \right] \left(1 - \frac{sm}{s_y}\right).$$
(6)

Here $\epsilon_0 \equiv \lambda n_\infty$ and

$$\mathcal{C}(s) \equiv \frac{R(s) + R(-s)}{2}.$$
(7)

The theoretical framework in which the amorphous system is characterized by coarse-grained internal state fields, in addition to stress and strain, is a major point of divergence compared to other approaches [2] and plays a crucial role in the discussion below, where the field m is the central object.

In [13], Eqs. (5) and (6) were directly applied to predict transient granular flow in experiments of shear reversal in a Taylor-Couette cell. The theory was shown to agree well with the experimental data, encouraging us to study it further in the present context. The first issue to be discussed is the stable steady state solutions of Eq. (6). It has two stationary solutions: (1) a jammed state with $m = \pm 1$ (depending on the sign of *s*), where all the STZs are in either the + or the – state, and $D^{\text{pl}}=0$ in Eq. (5); and (2) a flowing state with $m = s_y/s$ and $D^{\text{pl}} \neq 0$ in Eq. (5).

These two solutions coincide at $s/s_y = \pm 1$. It is straightforward to show that the jammed state is dynamically stable for $|s| \leq s_y$, while the flowing state is dynamically stable for $|s| \geq s_y$. An exchange of stability occurs at $s = s_y$, which indeed shows explicitly that s_y is the yield stress. The fact that s_y was introduced in Eq. (3) as a proportionality constant between the rate of STZ creation, Γ , and the rate of energy dissipation, $2sD^{\text{pl}}$, is yet another point of divergence with respect to standard approaches. In STZ theory the yield stress s_y , as was explained before, is intimately related to the ability of the material to create new STZs as a result of plastic dissipation, i.e., STZ transitions in nearby locations [14]. In this interpretation, a material can yield, i.e., support steady plastic flow, if enough STZs per unit time are created due to other STZ transitions. If this rate is not sufficiently large, then existing STZs are exhausted in transitions at a given direction and not enough new STZs are available for additional transitions that are needed for attaining a steady state. For a given applied stress, whether or not Γ is large enough is determined by s_y . This is an entropic effect [14] and it is the essence of yielding in STZ theory.

As a result, the onset of plastic yielding at a finite threshold is a *dynamic* phenomenon manifested as an exchange of stability of the bistable field m [2]. These results have similar implications for strain-rate- $(\dot{\gamma}$ -) controlled experiments (complementary to the stress-controlled experiments discussed up to now), where the existence of a finite yield stress means that a steady state with a finite stress is obtained in the limit $\dot{\gamma} \rightarrow 0$. The existence of a dynamic threshold is a signature of an underlying bistability (or multistability), which is a natural way to get a finite dissipation at a vanishing strain rate. Note that all these conclusions are entirely independent of the material function C(s). We thus propose that the bistability of the orientational order parameter m is a crucial feature of the theory of amorphous plasticity.

III. THE TRANSITION FROM JAMMING TO FLOW

We now proceed to analyze the spatiotemporal characteristics of this jamming-unjamming transition. We substitute Eq. (5) into Eq. (6) to obtain

$$\tau_0 \dot{m} = 2\mathcal{C}(s)(1-m) \left(1 - \frac{ms}{s_y}\right),\tag{8}$$

where we have assumed s > 0. Consider then an experiment in which the stress is ramped to a constant value smaller than the yield stress (i.e., $s < s_y$). The system is assumed to be initially undeformed and isotropic such that the orientational order parameter satisfies m(t=0)=0. Equations (5) and (8) then predict that subyield plastic deformation occurs as mrelaxes to the jamming fixed point m=1 on a typical time scale $\tau_{iam}(s)$,

$$\tau_{\rm jam}(s) \simeq \frac{\tau_0}{2\mathcal{C}(s)(1-s/s_{\gamma})},\tag{9}$$

during which $D^{\text{pl}} \rightarrow 0$. The jamming time scale $\tau_{\text{jam}}(s)$ diverges as $s \rightarrow s_y^-$, i.e., approaching the yield stress from below, and as $s \rightarrow 0^+$. The latter divergence is a result of the athermal condition, leading to $\mathcal{C}(s \rightarrow 0) \rightarrow 0$ [3]. Therefore, Eq. (9) predicts that jamming is obtained by progressively slower creeplike subyield deformation as *s* approaches either 0 or 1. Moreover, it provides a way to measure the phenomenological function $\mathcal{C}(s)$ in the range where the jamming time is experimentally (or simulationally) accessible.

Suppose now that s/s_y is O(1), but not very close to unity, such that the system becomes jammed on a realistic time scale; then suppose that after jamming the applied stress is ramped again to a value above the yield stress, i.e., $s > s_y$. The system is now in the jammed state, m=1, that is, unstable for $s > s_y$. In these situations we generally expect fluc-

tuations to propagate as fronts, converting an unstable state into a stable one. Therefore, we are looking for translationally invariant solutions of the form m(x,t)=m(x-ut); here we assume that the x dimension is much larger than the y dimension and that the front propagates from left to right. Our task now is to solve Eq. (8) for this ansatz, with the boundary conditions

$$m(x \to -\infty) \to \frac{s_y}{s}, \quad m(x \to +\infty) \to 1.$$
 (10)

The first boundary condition corresponds to the flowing state left behind the front, while the second one corresponds to the jammed state ahead of it. A solution can be readily obtained, yielding

$$m(x,t) = \frac{1 - \left(\frac{s_y^2}{s^2} - \frac{s_y}{s}\right) \exp\left(\frac{-2\mathcal{C}(s)(s/s_y - 1)(x - ut)}{\tau_0 u}\right)}{1 - \left(\frac{s_y}{s} - 1\right) \exp\left(\frac{-2\mathcal{C}(s)(s/s_y - 1)(x - ut)}{\tau_0 u}\right)}.$$
(11)

This seems to be a propagating front solution in which a plastically deforming region, $D^{pl} \neq 0$, invades a jammed region, $D^{pl}=0$.

However, Eq. (11) is not a unique solution of the problem since it is valid for any velocity u. More importantly, a velocity u cannot be selected by Eq. (8) in principle since in the absence of an intrinsic length scale a velocity cannot be dimensionally constructed. Therefore, if we aim at describing the spatiotemporal patterns that accompany the onset of plastic flow, we cannot avoid addressing the fundamental problem of a missing length scale in our theory. In fact, two length scales are already implied within our theoretical framework; a finite STZ density implies a typical distance between STZs, which can be thought of as a microstructural correlation length. This length scale might be relevant as different STZs can interact via the stress and displacement fluctuations generated when a STZ transforms between its internal states. Evidence for the existence of such a length scale was given, for example, in [15,16]; it can be identified with the typical size of areas of quasicrystal-like short-range order of [15] or with the typical size of regions free of liquidlike defects of [16].

The range in which these interactions can affect STZ transitions also implies a length scale, possibly larger than the previous one, that is determined by the combined effect of the magnitude of the stress fluctuation, its range, and the distribution of STZ transition thresholds. This length scale characterizes the scale in which the probability of finding a sufficiently large stress perturbation (that can overcome the local transition threshold) is not exponentially small. Therefore, we should consider *nonlocal* stress fluctuations that can induce STZ transitions at different locations where STZs already exist and are close to their transition threshold. This effect was stressed by several authors [17–19] and was assumed to be the origin of the cascades of rearrangements observed in athermal quasistatic simulations [20]. With this physical intuition in mind, we should extend the homogeneous and local mean-field theory to include some inhomogeneous and nonlocal effects.

In summary, our theory should incorporate nonlocal terms that account for the following physical effects: (i) The stress and displacement fluctuations that are generated by STZ transitions; (ii) the joint spatial probability distribution function of STZ that includes a correlation length; and (iii) the STZ transition threshold distribution. Therefore, we add to the left-hand side of Eqs. (1) and (2) terms that are weighted integrals over existing terms that include the transition rates $R(\pm s)$; these terms represent the idea that STZ transitions from + states to - states (or vice versa) at a given location result in a properly weighted change in the rate of transitions at different locations. Rearranging the modified equations, we arrive at the following equation for m(x,t):

$$\tau_0 \dot{m}(x,t) = 2\mathcal{C}(s) \left[1 - m(x,t)\right] \left(1 - \frac{sm(x,t)}{s_y}\right) + 2\mathcal{C}(s) \left(1 - \frac{sm(x,t)}{s_y}\right) \int_{-\infty}^{\infty} K(x-x') \left[1 - m(x',t)\right] dx'.$$
(12)

The phenomenological kernel K(x) in Eq. (12), whose dimension is (length)⁻¹, represents the physics of STZ correlations and interactions discussed above. The fact that it is a one-dimensional function of x alone already incorporates several approximations. First, there is some evidence that STZ transitions generate quadrupolar elastic fields [17]. Here this anisotropic structure is neglected due to the assumption that the y dimension is much smaller than the x dimension. Second, the kernel K might include some time dependence that accounts, for example, for the wave nature of the stress and displacement fluctuations. We assume that this time dependence can be integrated out without affecting the basic physics we are trying to describe. In choosing a specific functional form for the kernel K(x), we do not want to make any definite claim as to whether the incorporated length scale is a short-distance correlation length or a longer-distance cutoff scale discussed above, but to stress that our theoretical considerations entail the existence of a length scale. Both physical possibilities share the feature that the immobile STZs interact via nonlocal stress fluctuations, which can be schematically described by

$$K(x) = \frac{\alpha}{\ell} \exp\left(-\frac{x^2}{2\ell^2}\right),\tag{13}$$

where ℓ is the characteristic length scale and α is the amplitude. Note that we do not consider here very long-range kernels, i.e., those with power-law tails, as we believe that the STZ transition threshold distribution limits the range in which stress fluctuations can induce STZ transitions, as explained above.

Equation (12), with the kernel of Eq. (13), poses a nontrivial front selection problem. As in many other front selection problems [21], there might exist a family of propagating front solutions from which a unique solution is selected dynamically. A complete analysis of Eq. (12) is well beyond the scope of the present work. However, we aim here at demonstrating that the proposed additional terms indeed lead to front selection. With that aim, we first consider the possibility that the nonlocal contribution is a small correction to the mean-field equation and treat Eq. (12) perturbatively, with α being the small parameter in the expansion. We thus write $m=m^{(0)}+\alpha m^{(1)}+O(\alpha^2)$, where $m^{(0)}$ is given in Eq. (11). The first-order equation in α selects the velocity, from which we estimate

$$u \simeq \frac{2\ell \mathcal{C}(s)}{\tau_0} \left(\frac{s}{s_y} - 1\right). \tag{14}$$

It is important to note that the nonlocal term is a singular perturbation in the sense that there is no solution at all in the limit $\alpha \rightarrow 0$.

As we cannot offer a similar analysis for the general case where α is not necessarily small, we studied Eq. (12) numerically by choosing $s > s_v$ and introducing the homogeneous jammed state, m=1, with various localized perturbations. In the numerical calculations we choose, for simplicity, $C(s) = H(s - s_v)(s - s_v)$ for s > 0. Here $H(\cdot)$ is the Heaviside unit step function. We have found that all perturbations converge, for sufficiently large times, to a unique front profile with a unique velocity u. This result shows that indeed the new nonlocal term in Eq. (12) provides a front velocity and profile selection mechanism for the problem at hand. In Fig. 1 we show the numerical front profile for a small amplitude α and the analytic prediction of Eq. (11) (shifted by a few time units for clarity). In the inset we compare the numerical results for the velocity u as a function of s to the prediction of Eq. (14). We observe that in this regime, i.e., for small α , the profile is, to a very good approximation, given by Eq. (11) with the selected velocity satisfying Eq. (14). Upon increasing the amplitude α , the nonlocal term becomes more dominant and the solution of Eq. (11) is no longer accurate. We thus conclude that, in the presence of the nonlocal interaction term, with the associated length scale ℓ , the proposed theory predicts the existence of propagating front solutions that remain to be observed in computer simulations and experiments.

IV. CONCLUDING REMARKS

The main question asked in this paper is: "What are the spatiotemporal characteristics of the transition between a



FIG. 1. (Color online) Propagating *m* front solution of Eq. (12) with α =0.01 and *s*=1.1 (solid line) compared to the analytic prediction given by Eq. (11) (dashed line), shifted by a few time units for clarity. (Inset) The velocity *u* (in units of $2\ell/\tau_0$) as a function of *s*, for both the numerics (open circles) and the prediction of Eq. (14) (solid line).

jammed state found at applied stresses below the yield stress s_y and a homogeneously flowing state found at applied stresses above the yield stress s_y ?" In our opinion, this is a fundamental question in the field of plasticity of amorphous

systems. We addressed this problem in the framework of the recently developed athermal shear transformation zone theory, which in our opinion offers a promising route for developing a predictive theory of amorphous plasticity. This theory describes the phenomenon of plastic yielding at a finite threshold in terms of an exchange of dynamic stability in the equation of motion for an orientational order parameter *m*. Our main result is that this theory predicts the existence of propagating front solutions that accompany the yielding transition provided that nonlocal effects are introduced. The nonlocal terms that account for nonlocal STZ interactions incorporate a length scale that is missing in the original theory. Our predictions for the existence of plastic fronts at the yielding transition should be tested in computer simulations and experiments. This may provide further support for the analytic structure of the developing STZ theory, substantiate the existence of the bistable orientational order parameter m, and shed some light on the missing intrinsic length scale. As the existence of a yield stress is a fundamental property of materials, elucidating the spatiotemporal nature of the yielding transition is of major importance.

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