

Athermal shear-transformation-zone theory of amorphous plastic deformation. I. Basic principlesEran Bouchbinder,¹ J. S. Langer,² and Itamar Procaccia¹¹*Department of Chemical Physics, The Weizmann Institute of Science, Rehovot 76100, Israel*²*Department of Physics, University of California, Santa Barbara, California 93106-9530, USA*

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We develop an athermal version of the shear-transformation-zone (STZ) theory of amorphous plasticity in materials where thermal activation of irreversible molecular rearrangements is negligible or nonexistent. In many respects, this theory has broader applicability and yet is simpler than its thermal predecessors. For example, it needs no special effort to assure consistency with the laws of thermodynamics, and the interpretation of yielding as an exchange of dynamic stability between jammed and flowing states is clearer than before. The athermal theory presented here incorporates an explicit distribution of STZ transition thresholds. Although this theory contains no conventional thermal fluctuations, the concept of an effective temperature is essential for understanding how the STZ density is related to the state of disorder of the system.

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I. INTRODUCTION

The shear-transformation-zone (STZ) theory of amorphous plasticity, to date, has been applied most successfully to “thermal” glassy systems at temperatures high enough that they exhibit linear viscosity and that nonlinear flow at larger driving stresses is controlled by thermally activated processes [1,2]. Our purpose here is to examine the opposite, “athermal” situation, where the ambient temperature is negligible, and all rearrangements of the constituent elements are driven entirely by applied forces. Systems of the kind to be discussed here include noncrystalline solids well below their glass temperatures, dense granular materials, and various kinds of soft materials such as foams, colloids, and the like.

An increasingly useful source of information about these systems is numerical simulation which, while limited in comparison with laboratory experiments on real materials, has certain compensating advantages. For example, athermal materials seem to be intrinsically unstable against nonuniform failure via shear banding or fracture. Such instabilities are much more difficult to observe and control in the laboratory than in large-scale computations. One of our main goals in this project is to develop a predictive description of athermal plasticity—an analog of the Navier-Stokes equation for amorphous solids—that can be used in heterogeneous situations. In the present paper and its sequel [3], however, we confine our attention to spatially homogeneous systems and test our results by comparing with simulations rather than experiments. Another advantage of numerical simulation is that it allows us to observe internal states of the system that are not easily accessible in laboratory experiments. That capability is a central feature of the following paper.

From its inception, the STZ theory has been built on the flow-defect theories of Turnbull, Cohen, Argon, Spaepen, and others. [4–11] It describes plastic deformation in amorphous solids, or solidlike materials, but not in liquids. The assumption is that irreversible molecular (or granular) rearrangements occur only at sparsely distributed sites—the STZ’s—within an otherwise elastic material. The validity of this assumption was demonstrated explicitly in [12], but it

goes back to essentially all of the previously cited earlier work. The STZ model is strictly valid only when the local rearrangements occur infrequently and independently of each other, and when they require either substantial thermal activation or, in the athermal situations of interest here, sufficiently large external driving forces. If the activation energy or work needed to drive a rearrangement is small of order $k_B T$, or if the sites at which rearrangements occur cover most of the system, then the material is effectively a liquid and STZ theory is not applicable.

We visualize an STZ as a localized group of molecules that is more susceptible than its neighbors to a shearing transformation in some direction. That is, these molecules must collectively surmount only a relatively small energy barrier in order to undergo an irreversible shear. Once this happens, it seems reasonable to suppose that they will resist further shear in the original direction, but may be especially susceptible to a reverse shear. One might imagine that the first transition has redistributed the local stresses in such a way as to favor a reverse transition if the applied stress changes sign. We see no strong requirement that the reverse transition must bring the molecules back to exactly their original positions; but it is this approximate picture that suggests a two-state model of STZ’s.

A primary rationale for the two-state model is that it provides a simple mechanism by which the system retains orientational memory of prior deformations. Along with the dynamic transition between jammed and flowing states, orientational memory is one of the universal features of amorphous plasticity that we believe must be captured by any satisfactory theory. A related requirement for an acceptable theory is that it must include a mechanism by which orientational memory is lost during deformation. Here that mechanism is the annihilation and creation of STZ’s at a rate proportional to the rate of energy dissipation. Under athermal conditions, annihilation and creation occur only in response to STZ transitions; thus this mechanism may also be seen as a rough description of the cascades of rearrangements following STZ-like events seen by Maloney and Lemaitre [13,14], and emphasized by Argon and Demkowicz in papers to be discussed in a sequel to this one. [15–18]

The defining feature of an athermal system is the constraint that, because thermal activation of transitions is negligible or nonexistent, molecular rearrangements occur only in response to driving forces. No motion occurs in the absence of such forces, and no rearrangement moves in a direction opposite to that in which the force is applied. In other words, molecular configurations cannot move uphill in energy as they may when thermal fluctuations are present. Stress-induced shear transformations are intrinsically irreversible events. Work is done on the system as the STZ's are driven over energy barriers, and energy is dissipated as the system moves downhill toward new stable states. In contrast to the picture proposed in earlier papers [12,25,26] which assumed only one kind of STZ, the model to be developed here allows STZ's to occur with a range of different sizes and transition thresholds. With this generalization, the STZ model may undergo limited irreversible deformations when the applied stresses are less than the nominal yield stress. The onset of athermal flow at an apparent yield stress then must be a dynamic phenomenon. As in the original STZ theories, it occurs when there is an exchange of stability between the jammed steady states, where nothing is moving, and the flowing steady states, where motion-induced annihilation and creation of STZ's balances the rate at which zones are inactivated by forward transitions. In this way, the STZ picture describes the dynamics of plastic yielding by the same mechanism that it uses to describe the memory effects mentioned above.

Although ordinary thermal fluctuations are absent in the athermal models discussed here, the concept of an effective disorder temperature is essential. Some of the earliest work in this field recognized that the density of flow defects could be related to an intensive quantity such as the free volume v_f (the inverse of the derivative of an entropy with respect to the volume). Intensive quantities of this kind characterize the state of the system as a whole and not just that of a subset of its degrees of freedom. Thus Cohen and Turnbull in 1959 [4] (see also Spaepen [5]) proposed that the density of flow defects in an amorphous solid be proportional to $\exp(-\text{const}/v_f)$, and not just to v_f itself. In Ref. [2], one of us (J.S.L.) argued that the appropriate generalization of free volume is an effective temperature T_{eff} that characterizes the state of configurational disorder in the system. T_{eff} equilibrates to the ambient temperature T at high T , but may fall out of equilibrium at low T where disorder is generated by the atomic-scale, configurational rearrangements that accompany mechanical deformation. If $T_{\text{eff}} = (E_{\text{STZ}}/k_B)\chi$, where E_{STZ} is a characteristic STZ formation energy, then the STZ density is proportional to the Boltzmann factor $\exp(-1/\chi)$. This is a direct analog of the free-volume formula and, in fact, reduces to it in the case of a system under constant pressure with a positive "effective" thermal expansion coefficient. Importantly, the time variation of the STZ density is governed by the dynamics of χ . (For more information about effective-temperature theories, see Refs. [19–24].)

The scheme of this paper is as follows. We review and reformulate basic features of the STZ theory in Sec. II. Then, in Sec. III, we derive the athermal equations of motion for the STZ state variables, propose a specific form for the athermal rate factor, and show a few illustrative examples of how

the theory behaves in various experimental situations and with various choices of the constituent parameters.

II. STZ BASICS

The STZ theory is a phenomenological construction. Our strategy has been to start with what amounts to a caricature of an amorphous material, specifically, a model in which applied stresses and two-state STZ's remain aligned along fixed axes. We deduce from this rudimentary model the internal state variables that are needed to describe its behavior, and then derive equations of motion for those variables. When applying the theory to more realistic situations in three dimensions, at least in simple geometries such as those we encounter here, we assume that we can retain the form of our equations of motion but replace certain state variables by tensors when required by symmetry. In short, we see how far we can go with minimal models and, to the extent possible, test these models by comparing our theoretical predictions with experimental data as in Refs. [1,2].

Accordingly, we start by considering a two-dimensional system, and subject it only to pure shear deformation oriented along a fixed pair of principal axes x and y . It is sufficient for present purposes to assume that the population of STZ's consists simply of zones oriented along the two principal axes of the deviatoric stress tensor, which we take to be $s_{xx} = -s_{yy} = s$ and $s_{xy} = 0$. Choose the "+" zones to be oriented (elongated) along the x axis, and the "-" zones along the y axis. We assume that the STZ's occur in many different varieties, with the symbol α representing, for example, their actual orientations with respect to the stress axes as in Ref. [26] or, explicitly in what follows, their transition thresholds. Thus we denote the population density of zones oriented in the " \pm " directions by the symbol $n_{\pm}(\alpha)$.

With these conventions, the plastic strain rate—more generally, the plastic part of the rate-of-deformation tensor—is

$$D_{xx}^{\text{pl}} = -D_{yy}^{\text{pl}} \equiv D^{\text{pl}} = \frac{\lambda}{\tau_0} \int d\alpha [R_{\alpha}(\tilde{s})n_{-}(\alpha) - R_{\alpha}(-\tilde{s})n_{+}(\alpha)]. \quad (2.1)$$

Here, λ is a material-specific parameter with the dimensions of volume (or area in strictly two-dimensional models), which must have roughly the same order of magnitude as the volume of an STZ, that is, a few cubic or square atomic spacings. τ_0 sets a time scale for these processes. The integration is over the relevant space of parameters α . The integrand is the net rate per unit volume at which α -type STZ's transform from "-" to "+" orientations. $R_{\alpha}(\tilde{s})/\tau_0$ and $R_{\alpha}(-\tilde{s})/\tau_0$ are the rates for forward ("-" to "+") and backward ("+" to "-") transitions, respectively. For later convenience, we have written these rates as functions of a dimensionless stress $\tilde{s} = s/s_y$, where s_y will turn out to be the dynamic yield stress in the athermal theory. At present, we need to think of s_y only as a characteristic scale for measuring stresses.

The next step is to postulate a master equation for the populations $n_{\pm}(\alpha)$. As before, we do this in a mean-field approximation. Using earlier notation, we write

$$\begin{aligned} \tau_0 \dot{n}_{\pm}(\alpha) = & R_{\alpha}(\pm \bar{s}) n_{\mp}(\alpha) - R_{\alpha}(\mp \bar{s}) n_{\pm}(\alpha) \\ & + \Gamma(\bar{s}) \left(\frac{n_{\infty}(\alpha)}{2} e^{-1/\chi} - n_{\pm}(\alpha) \right). \end{aligned} \quad (2.2)$$

The first pair of terms on the right-hand side describes the same switching back and forth of the STZ's that appears in Eq. (2.1). The last terms describe the creation and annihilation of zones at a rate $\Gamma(\bar{s})/\tau_0$ that, in a mean-field sense, we assume to be the same for both $n_+(\alpha)$ and $n_-(\alpha)$, independent of α and of local properties of the system. Γ is a non-negative, scalar quantity that vanishes when the rate of deformation is zero; in earlier papers [25,26] we have argued that it must be proportional to the rate per STZ at which mechanical work is dissipated via irreversible plastic deformation. $n_{\infty} \exp(-1/\chi)$ is the steady-state density of STZ's achieved by the system during persistent deformation. As discussed in the Introduction, χ is the effective temperature measured in units of the STZ formation energy. In writing this part of Eq. (2.2), we are using the principle of detailed balance to fix the ratio of the annihilation and creation rates. Note that Eq. (2.2) contains no aging or spontaneous relaxation, consistent with the assumption that thermal fluctuations are absent.

Now suppose that $n_{\pm}(\alpha) = n_{\pm} p(\alpha)$ and $n_{\infty}(\alpha) = n_{\infty} p(\alpha)$, where $p(\alpha)$ is a normalized distribution over α . At this point, we make the important simplifying assumption that $p(\alpha)$ is not itself a dynamical quantity that changes during deformation. Performing the integration in Eq. (2.1), we find that

$$D^{\text{pl}} = \frac{\lambda}{\tau_0} [R(\bar{s}) n_- - R(-\bar{s}) n_+], \quad (2.3)$$

where

$$R(\bar{s}) = \int R_{\alpha}(\bar{s}) p(\alpha) d\alpha. \quad (2.4)$$

Similarly, we integrate both sides of Eq. (2.2) over α to obtain

$$\tau_0 \dot{n}_{\pm} = R(\pm \bar{s}) n_{\mp} - R(\mp \bar{s}) n_{\pm} + \Gamma(\bar{s}) \left(\frac{n_{\infty}}{2} e^{-1/\chi} - n_{\pm} \right). \quad (2.5)$$

Thus we recover exactly the earlier equations of motion for the STZ populations, but with a modified interpretation of the rate factors.

Before writing an equation of motion for χ , and then moving on to the specifics of the athermal theory, we reintroduce some convenient notation and rewrite the equations of motion in the form in which we shall use them. We define the following dimensionless quantities:

$$\epsilon_0 \equiv \lambda n_{\infty}, \quad (2.6)$$

$$\Lambda \equiv \frac{n_+ + n_-}{n_{\infty}}, \quad (2.7)$$

$$m \equiv \frac{n_+ - n_-}{n_+ + n_-}, \quad (2.8)$$

$$\mathcal{C}(\bar{s}) \equiv \frac{1}{2} [R(\bar{s}) + R(-\bar{s})], \quad (2.9)$$

$$\mathcal{T}(\bar{s}) \equiv \frac{R(\bar{s}) - R(-\bar{s})}{R(\bar{s}) + R(-\bar{s})}. \quad (2.10)$$

Then Eq. (2.3) is

$$\tau_0 D^{\text{pl}} = \epsilon_0 \Lambda \mathcal{C}(\bar{s}) [T(\bar{s}) - m] \quad (2.11)$$

and Eq. (2.5) becomes a pair of equations for m and Λ :

$$\tau_0 \dot{m} = 2\mathcal{C}(\bar{s})(\mathcal{T}(\bar{s}) - m) - \frac{m\Gamma(\bar{s})}{\Lambda} e^{-1/\chi} \quad (2.12)$$

and

$$\tau_0 \dot{\Lambda} = \Gamma(\bar{s})(e^{-1/\chi} - \Lambda). \quad (2.13)$$

Using the preceding notation, we choose the equation of motion for the effective temperature χ to be the athermal version of Eq. (3.5) in Ref. [2]. So far, none of the ingredients of our equations of motion have been written specifically in their athermal forms; but here we deviate by dropping terms that refer explicitly to mechanisms by which χ relaxes to the ambient temperature. Thus

$$\tau_0 c_0 \dot{\chi} = \epsilon_0 \Lambda \Gamma(\bar{s}) (\chi_{\infty} - \chi). \quad (2.14)$$

This is basically an expression of the first law of thermodynamics. The left-hand side is the time rate of change of the configurational internal energy roughly approximated as the product of the effective temperature χ multiplied by a specific heat c_0 . The latter quantity is expressed in units of k_B per atom and thus is of order unity. The right-hand side of Eq. (2.14) is proportional to the rate of energy dissipation per unit volume, that is, the dissipation rate per STZ Γ multiplied by the STZ density Λ .

The last factor on the right-hand side of Eq. (2.14) appears because there must be an upper bound on χ ; the disorder temperature cannot simply increase indefinitely under continued athermal deformation but, rather, must settle to some steady-state value χ_{∞} . That limiting behavior has been demonstrated explicitly by Ono *et al.* in simulations of a sheared foam [19], in which the authors showed that a variety of different definitions of an effective temperature for an athermal system are consistent with each other. They also found that χ_{∞} has a nonzero value at sufficiently small strain rates and increases, as argued in Ref. [2], only when the strain rate becomes comparable to other relevant, internal, inverse time scales. In Ref. [2], the small-strain-rate value of χ_{∞} was estimated to be roughly the ratio of the yield stress to the shear modulus or, more or less equivalently, the ratio of the glass temperature to the STZ formation energy. If the former estimate can be taken literally, then Johnson's analysis of yield strengths in a wide range of glasses in Ref. [27] implies that χ_{∞} is a universal number of order 0.02–0.04. That value is consistent with the one found in Ref. [2], where a direct estimate of the STZ energy in a metallic glass was available from viscosity measurements.

The preceding estimates of χ_{∞} give us useful insight regarding the general structure of the STZ theory summarized

by Eqs. (2.11)–(2.14). In our atomic units, the density n_∞ should be of order unity, and ϵ_0 as defined in Eq. (2.6) also must be of order unity. Thus, if χ_∞ is small of order 0.1 or less, the density of STZ's, $\Lambda \equiv \exp(-1/\chi_\infty)$, is of order 10^{-3} or appreciably smaller, consistent with our basic assumption that the STZ's are rare defects that interact only weakly with each other. In retrospect, we recognize that earlier STZ theories that did not include the effective temperature, e.g., Ref. [1], required improbably large values of the STZ density in order to agree with experiment.

Λ appears as a rate-determining prefactor on the right-hand sides of Eqs. (2.11) and (2.14), which govern the bulk system-wide variables D^{pl} and χ ; but Λ does not appear in a similar way in Eqs. (2.12) or (2.13), which pertain to the dynamics of individual STZ's. It follows that the plastic strain rate and the effective temperature respond much more slowly to changes in stress than they do the internal STZ variables m and Λ , and that the slow dynamics of the effective temperature controls the observable mechanical behavior of the system in most circumstances.

III. ATHERMAL THEORY

The crux of the athermal STZ theory is the choice of the rate factor $R(\tilde{\sigma})$ and the resulting expression for the creation and annihilation factor Γ . An immediate and important simplification follows from the athermal constraint that no motion occurs in a direction opposite to that of the applied force. Thus $R(\tilde{\sigma})$ must vanish if $\tilde{\sigma} < 0$. We then find from Eq. (2.10) that

$$\mathcal{T}(\tilde{\sigma}) = \text{sgn}(\tilde{\sigma}) = \frac{\tilde{\sigma}}{|\tilde{\sigma}|}. \quad (3.1)$$

This result is trivially correct no matter how complicated the transition rate might be. It immediately tells us that jamming—i.e., $D^{\text{pl}}=0$ —occurs only for $m=\pm 1$, depending on the sign of the stress, and that no transitions in either the forward or backward direction are occurring in the jammed state. For example, when $\tilde{\sigma} > 0$ in Eq. (2.3), jamming occurs because both $n_- = 0$ and $R(-\tilde{\sigma}) = 0$.

A second immediate simplification comes from the observation that, with no uphill transitions in energy, all the work done on the system must be dissipated and none can be stored internally. Thus the dissipation rate per STZ, in the dimensionless form required by Eq. (2.5), must be

$$\Gamma(\tilde{\sigma}, m) = \frac{2\tau_0 \tilde{\sigma} D^{\text{pl}}}{\epsilon_0 \Lambda} = 2\tilde{\sigma} \mathcal{C}(\tilde{\sigma}) \left(\frac{\tilde{\sigma}}{|\tilde{\sigma}|} - m \right). \quad (3.2)$$

We thus recover the expression for Γ originally guessed in Ref. [12] but now without the sign problem pointed out there. The work done by the external driving force cannot be negative in the athermal limit because the plastic flow must have the same sign as the stress. [Equation (3.2) can be derived systematically using Pechenik's method [25,26]. That analysis reveals that, in the athermal limit, the recoverable internal energy vanishes for $m^2 < 1$.]

To complete the definition of our model, we must specify a form for $R(\tilde{\sigma})$. Consider just a single species of STZ, and

suppose that the parameter α determines the activation threshold, say, $\tilde{\sigma}_\alpha$. That is, let $R_\alpha(\tilde{\sigma})$ vanish for $\tilde{\sigma} < \tilde{\sigma}_\alpha$, with the understanding that the absence of thermal fluctuations means that the only allowed transitions are those that are driven mechanically by sufficiently large stresses. A convenient, minimal form for $R_\alpha(\tilde{\sigma})$ is

$$R_\alpha(\tilde{\sigma}) = \begin{cases} 2(\tilde{\sigma} - \tilde{\sigma}_\alpha) & \text{for } \tilde{\sigma} > \tilde{\sigma}_\alpha, \\ 0 & \text{for } -\infty < \tilde{\sigma} < \tilde{\sigma}_\alpha. \end{cases} \quad (3.3)$$

This expression is a rough description of an athermal system moving in a double-well potential. The system remains trapped until the applied force $\tilde{\sigma}$ reaches its threshold $\tilde{\sigma}_\alpha$, at which point the unbalanced force rises linearly in $\tilde{\sigma} - \tilde{\sigma}_\alpha$. If the response is dissipative, i.e., frictional or viscous, then the speed at which the system moves away from its original position will also be proportional initially to $\tilde{\sigma} - \tilde{\sigma}_\alpha$. In our case, the proportionality coefficient is incorporated into the factor τ_0^{-1} .

For purely athermal systems such as granular materials or foams where there are no other relevant time scales, this interpretation of the rate factor makes sense only if τ_0 is comparable to, or longer than the inverse of the total strain rate. In the opposite limit, where the duration of an STZ transition is very short compared to the interval between transitions, the only relevant time is the inverse strain rate itself. Therefore, the rate of STZ transitions τ_0^{-1} must be proportional to the total strain rate. This is the common limiting situation in which the number of irreversible atomic rearrangements, i.e., STZ transitions, does not depend on the length of time during which the material has been loaded but only on the extent of the deformation. The situation is quite different in molecular solids, even at athermally low temperatures, because then the molecular vibration frequency governs the rate of the forward, stress-enabled transitions across the STZ energy barrier.

According to Eq. (2.4), $R(\tilde{\sigma})$ is the average over rate factors $R_\alpha(\tilde{\sigma})$ with a normalized weight factor that we can denote by $p(\tilde{\sigma}_\alpha)$. In choosing $p(\tilde{\sigma}_\alpha)$, we are led by the following considerations.

(1) If characteristic stresses for a system of interest are of order our scale factor s_y , and if s_y is the only stress scale in the problem, then $p(\tilde{\sigma}_\alpha)$ should have a peak at $\tilde{\sigma}_\alpha \equiv 1$.

(2) The probability of very low thresholds, $\tilde{\sigma}_\alpha \ll 1$, must be vanishingly small. The athermal constraint means that there are no negative thresholds, i.e., no transitions in the direction opposite to the stress. Therefore $p(\tilde{\sigma}_\alpha)$ must be such that $R(\tilde{\sigma})$ vanishes smoothly at $\tilde{\sigma}=0$ and remains zero for all $\tilde{\sigma} < 0$.

(3) We expect that different materials, under different circumstances, will have different threshold distributions, and we therefore need at least one extra parameter that controls the width and/or shape of $p(\tilde{\sigma}_\alpha)$. Our minimal, phenomenological rule for model building implies that we should start by introducing only one such parameter, denoted below by ζ .

A distribution that satisfies all these criteria and is convenient for numerical purposes, is

$$p_{\zeta}(\tilde{s}_{\alpha}) = \frac{\zeta^{\zeta+1}}{\zeta!} \tilde{s}_{\alpha}^{\zeta} \exp(-\zeta \tilde{s}_{\alpha}). \quad (3.4)$$

This distribution has a width of order $\zeta^{-1/2}$ near its peak at $\tilde{s}_{\alpha}=1$. $R(\tilde{s})$ is now obtained from Eq. (2.4):

$$R(\tilde{s}) = 2 \frac{\zeta^{\zeta+1}}{\zeta!} \int_0^{\tilde{s}} (\tilde{s} - \tilde{s}_{\alpha}) \tilde{s}_{\alpha}^{\zeta} \exp(-\zeta \tilde{s}_{\alpha}) d\tilde{s}_{\alpha} \quad (3.5)$$

from which we see that

$$R(\tilde{s}) \approx \begin{cases} \tilde{s}^{\zeta+2} & \text{for } \tilde{s} \rightarrow +0, \\ 2(\tilde{s}-1) & \text{for } \tilde{s} \gg 1. \end{cases} \quad (3.6)$$

Our equations of motion are now conveniently written in the form

$$D^{\text{pl}}(\tilde{s}, m, \Lambda) = \frac{\epsilon_0}{\tau_0}(\tilde{s}, m), \quad (3.7)$$

where

$$q(\tilde{s}, m) \equiv C(\tilde{s}) \left(\frac{\tilde{s}}{|\tilde{s}|} - m \right), \quad (3.8)$$

$$\dot{m} = \frac{2}{\tau_0} q(\tilde{s}, m) \left(1 - \frac{m\tilde{s}}{\Lambda} e^{-1/\chi} \right), \quad (3.9)$$

$$\dot{\Lambda} = \frac{2}{\tau_0} \tilde{s} q(\tilde{s}, m) (e^{-1/\chi} - \Lambda) \quad (3.10)$$

and

$$\dot{\chi} = \frac{2\epsilon_0}{c_0\tau_0} \Lambda \tilde{s} q(\tilde{s}, m) (\chi_{\infty} - \chi). \quad (3.11)$$

Equations (3.10) and (3.11) tell us that the only stable, steady-state solutions of the preceding equations must have $\chi = \chi_{\infty}$ and $\Lambda = \exp(-1/\chi_{\infty})$, consistent with our expectation that the system must flow to a fixed point with an STZ density $n_{\infty} \exp(-1/\chi_{\infty})$. Then Eq. (3.9) has two stationary solutions: the jammed state with $m = \pm 1$ (depending on the sign of \tilde{s}) and $D^{\text{pl}} = 0$ and the flowing state with $m = 1/\tilde{s}$ and $D^{\text{pl}} \neq 0$. These two solutions coincide at $m = \tilde{s} = \pm 1$. It is easy to check, as in many earlier STZ papers, that the jammed state is dynamically stable for $|\tilde{s}| < 1$ and the flowing state for $|\tilde{s}| > 1$. An exchange of stability occurs at $\tilde{s}_y = 1$, which justifies our earlier choice of units for the stress. Note that these conclusions are entirely independent of the rate factor, whose stress dependence enters only via the function $C(\tilde{s})$ in the equations of motion.

To look at the time-dependent behavior of these equations, we must include elastic as well as plastic responses. Assume that the total rate of deformation D^{tot} is a linear superposition of elastic and plastic parts, that is,

$$D^{\text{tot}} = \frac{\dot{\tilde{s}}}{2\tilde{\mu}} + D^{\text{pl}}(\tilde{s}, m, \Lambda), \quad (3.12)$$

where $\tilde{\mu}$ is the shear modulus measured in units s_y . In one common class of experiments, the material is sheared at a

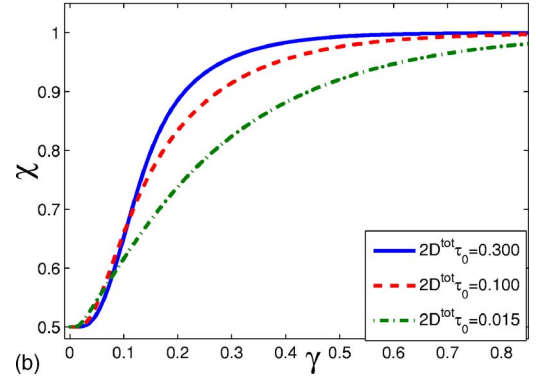
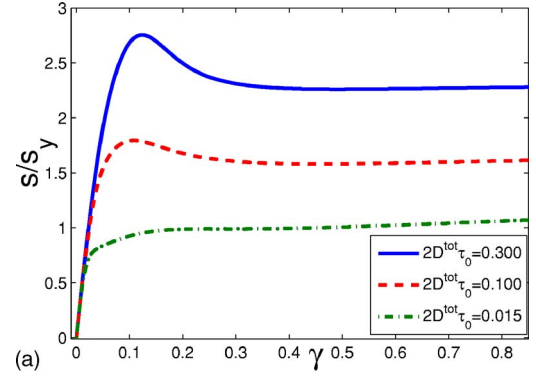


FIG. 1. (Color online) Upper panel: The normalized stress s/s_y as a function of strain γ for different values of the normalized strain rate $2D^{\text{tot}}\tau_0 = \dot{\gamma}\tau_0$. The parameters used in integrating Eqs. (3.13)–(3.16) are $\zeta=1$, $\chi_{\infty}=1$, $\chi_0=0.5$, $\tilde{\mu}=45$, $\epsilon_0=1$, and $c_0=0.25$. The different values of the normalized strain rate (from top to bottom) are $2D^{\text{tot}}\tau_0 = \dot{\gamma}\tau_0 = 0.3, 0.1, 0.015$. The initial values used are $m(\gamma=0)=0$ (i.e., no previous deformation) and $\Lambda(\gamma=0) = \exp(-1/\chi_0)$. Lower panel: The corresponding curves of χ as a function of γ for the three cases. See text for discussion.

fixed rate $D^{\text{tot}} = \dot{\gamma}/2$, and the stress is measured as a function of the strain γ . To model such experiments, we write Eq. (3.12) in the form

$$\frac{d\tilde{s}}{d\gamma} = \tilde{\mu} \left(1 - \frac{2\epsilon_0\Lambda}{\dot{\gamma}\tau_0} q(\tilde{s}, m) \right) \quad (3.13)$$

and similarly transform Eqs. (3.9), (3.10), and (3.11):

$$\frac{dm}{d\gamma} = \frac{2}{\dot{\gamma}\tau_0} q(\tilde{s}, m) \left(1 - \frac{m\tilde{s}}{\Lambda} e^{-1/\chi} \right), \quad (3.14)$$

$$\frac{d\Lambda}{d\gamma} = \frac{2}{\dot{\gamma}\tau_0} \tilde{s} q(\tilde{s}, m) (e^{-1/\chi} - \Lambda), \quad (3.15)$$

and

$$\frac{d\chi}{d\gamma} = \frac{2\epsilon_0}{c_0\dot{\gamma}\tau_0} \Lambda \tilde{s} q(\tilde{s}, m) (\chi_{\infty} - \chi). \quad (3.16)$$

To illustrate the predictions of this theory, we show in Fig. 1 a sequence of stress-strain curves $\tilde{s}(\gamma)$ for different values of $\dot{\gamma}\tau_0$. A corresponding set of graphs of $\chi(\gamma)$ is shown in the lower panel of that figure. For each of these

curves we have used $\zeta=1$ (implying a broad distribution of low-lying thresholds), $\chi_\infty=1$ (a large value, chosen here for illustrative purposes), and an initial value of $\chi=\chi_0=0.5$. We also choose $\bar{\mu}=45$, $\epsilon_0=1$, and $c_0=0.25$. Note that, for small $\dot{\gamma}\tau_0=0.015$ (lower curve, upper panel), the flow stress \tilde{s}_f at large γ is approximately equal to the yield stress, $\tilde{s}_f\cong 1$, and that there is substantial yielding at smaller stresses because ζ is small. For larger values of $\dot{\gamma}\tau_0$, the stress rises nearly elastically to a peak as χ and the number of STZ's increases, and then drops as the plastic flow induces strain softening. The flow stresses are higher in these situations. In all cases, the effective temperature χ ultimately reaches its steady-state value χ_∞ .

A second common class of experiments is that in which the stress rather than the strain is controlled. In this situation, we must solve Eq. (3.12) as written, with $D^{\text{tot}}=\dot{\gamma}/2$ on the left-hand side and \tilde{s} a predetermined function of time t on the right. Figure 2 illustrates a stress-strain curve for a case in which the stress is cycled as shown in the inset. We have chosen the stress to remain always less than the yield stress in order to illustrate the effects of small $\zeta=1$. The material parameters are the same as in Fig. 1. Note the appearance of subyield deformation as before, and also the hysteresis associated with energy dissipation during that deformation.

IV. CONCLUDING REMARKS

The athermal STZ theory appears to be cleaner and more broadly applicable than its predecessors. It does not, of course, replace the thermal STZ theory that is needed to describe plastic deformation of amorphous materials near their glass temperatures; but, even there, the athermal analysis suggests some simplifications that may be useful, for example, in the choice of the transition rates $R(\tilde{s})$. It seems to us that the most important open question in the athermal STZ theory is whether the effective temperature χ is adequate for describing all the relevant internal states of a deforming ma-

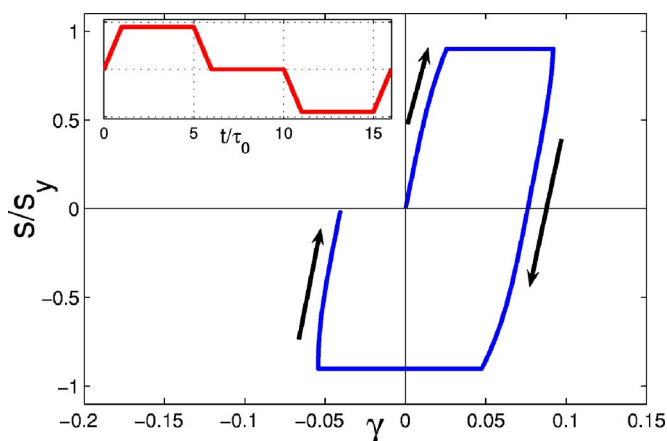


FIG. 2. (Color online) The normalized stress s/s_y as a function of the strain γ for the stress controlled loading shown in the inset. The parameters used are the same as those in Fig. 1. Note that, although the maximum absolute normalized stress is $|s/s_y|=0.9$, significant subyield plastic deformation is visible, in addition to memory effects.

terial, or whether other internal variables may be needed. Our analysis of the simulations by Demkowicz and Argon [15–18], to be described in the sequel to this paper, is aimed at answering this question.

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