Dynamics of Large-Scale Plastic Deformation and the Necking Instability in Amorphous Solids

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We use the shear transformation zone (STZ) theory of dynamic plasticity to study the necking instability in a two-dimensional strip of amorphous solid. Our Eulerian description of large-scale deformation allows us to follow the instability far into the nonlinear regime. We find a strong rate dependence; the higher the applied strain rate, the further the strip extends before the onset of instability. The material hardens outside the necking region, but the description of plastic flow within the neck is distinctly different from that of conventional time-independent theories of plasticity.

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Conventional descriptions of plastic deformation in solids consist of phenomenological rules of behavior, with qualitative distinctions between time-independent and time-dependent properties, and sharply defined yield criteria. Plasticity, however, is an intrinsically dynamic phenomenon. Practical theories of plasticity should consist not of intricate sets of rules, but of equations of motion for material velocities, stress fields, and other variables that might characterize internal states of solids. Roughly speaking, a theory of plasticity, especially for an amorphous solid, should resemble the Navier-Stokes equation for a fluid, with the pressure replaced by a stress tensor, and the viscous forces replaced by a constitutive law relating the rate of plastic deformation to the stresses and internal state variables. That constitutive law should contain phenomenological constants, analogous to the bulk and shear viscosities, that are measurable and, in principle, computable from molecular theories. Yield criteria, work hardening, hysteretic effects, and the like would emerge naturally in such a formulation.

The goal of the STZ (shear transformation zone) theory of plasticity [1–7], from its inception, has been to carry out the above program. In this paper we show how the STZ theory describes a special case of large-scale yielding, specifically, the necking instability of a strip of material subject to tensile loading. There is a large literature on the necking problem. References that we have found particularly valuable include papers by Hutchinson and Neale [8], McMeeking and Rice [9], and Tvergaard and Needleman [10]. Our purpose here is to explore possibilities for using the STZ theory to investigate a range of failure mechanisms in amorphous solids, possibly including fracture. We are able to follow the necking instability far into the nonlinear regime where the neck appears to be approaching plastic failure while the outer regions of the strip become hardened and remain intact. We find that necking in the STZ theory is rate dependent; the instability occurs at smaller strains when the strip is loaded slowly. One especially important element of our analysis is our ability to interpret flow and hardening in terms of the internal STZ variables.

To make this problem as simple as possible, we consider here only strictly two-dimensional, amorphous materials. By "strictly," we mean that elastic and plastic displacement rates are separately planar as in two-dimensional molecular dynamics simulations. The two-dimensional STZ equations presented in this paper are based on earlier work by Falk, Langer, and Pechenik [7,11,12]. We use Eulerian coordinates in which, as in fluid dynamics, the variables x_i denote the current physical positions of material elements. Let the system lie in the $x_1 = x$, $x_2 = y$ plane, and write the stress tensor in the form: $\sigma_{ij} = -p\,\delta_{ij} + s_{ij}$, $p = -\frac{1}{2}\,\sigma_{kk}$, where p is the pressure and s_{ij} is the deviatoric stress—a traceless, symmetric tensor. In analogy to fluid dynamics, let $v_i(x, y, t)$ denote the material velocity at the physical position x, y, and time t. Then the acceleration equation is [13]

$$\rho\,\frac{dv_i}{dt} = \frac{\partial \sigma_{ij}}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial s_{ij}}{\partial x_j}. \tag{1}$$

Here, ρ is the density which, because we shall assume a very small elastic compressibility and volume conserving plasticity, we shall take to be a constant. The symbol d/dt denotes the material time derivative acting on a scalar or a vector field:

$$\frac{d}{dt} \equiv \frac{\partial}{\partial t} + v_k\,\frac{\partial}{\partial x_k}. \tag{2}$$

Our first main assumption is that the rate of deformation tensor can be written as the sum of linear elastic and plastic contributions:

$$D_{ij}^{\rm total} \equiv \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) = \frac{\mathcal{D}}{\mathcal{D}t}\left[\frac{s_{ij}}{2\mu} - \frac{p}{2K}\,\delta_{ij}\right] + D_{ij}^{\rm plast}, \tag{3}$$

where μ is the shear modulus, $K = \mu(1 + \nu^*)/(1 - \nu^*)$ is the two-dimensional inverse compressibility (or bulk modulus), and ν^* is the two-dimensional Poisson ratio. The symbol $\mathcal{D}/\mathcal{D}t$ denotes the material time derivative acting on any tensor, say A_{ij}:

$$\frac{\mathcal{D}A_{ij}}{\mathcal{D}t} \equiv \frac{\partial A_{ij}}{\partial t} + v_k \frac{\partial A_{ij}}{\partial x_k} + A_{ik}\,\omega_{kj} - \omega_{ik}\,A_{kj}; \quad (4)$$

and ω_{ij} is the spin:

$$\omega_{ij} = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i}\right). \quad (5)$$

The plastic part of the rate-of-deformation D_{ij}^{plast}, like s_{ij}, is a traceless symmetric tensor, thus the plastic deformations are area conserving. For present purposes, we use a simple, quasilinear form of the STZ theory in which

$$D_{ij}^{\text{plast}} = \epsilon_0\, q_{ij}(s, \Delta); \qquad q_{ij}(s, \Delta) = s_{ij} - \Delta_{ij}, \quad (6)$$

and ϵ_0 is a material-specific constant. The traceless, symmetric tensor Δ_{ij} is the internal state variable mentioned earlier. It is proportional to a director matrix that specifies the orientation of the STZs; its magnitude is a measure of the degree of their alignment. The equation of motion for Δ_{ij} is

$$\frac{\mathcal{D}\Delta_{ij}}{\mathcal{D}t} = q_{ij} - \frac{1}{2}\,|q_{km}\,s_{km}|\,\Delta_{ij}. \quad (7)$$

In Eq. (6), Δ plays—very roughly—the role of the "back stress" or "hardening" parameter in conventional theories of plasticity [14–16], a major difference being that Δ emerges directly from a rate equation governing the population of STZs and is, in principle, a directly measurable quantity [1,17]. If the second term on the right-hand side of Eq. (7) were missing, then Δ would be proportional to the integrated plastic strain. This second term, however, which is produced by the creation and annihilation of STZs, is a crucial element of the STZ theory. As we shall show briefly below, this term produces the exchange of dynamic stability between viscoelastic and viscoplastic states that replaces the conventional assumptions of yield surfaces and other purely phenomenological rules of behavior.

With one important exception, Eqs. (6) and (7) constitute a tensorial version of the original STZ theory obtained by linearizing the stress dependence of the rate factors and rescaling. Because of the linearization, these equations do not properly describe memory effects present in the full theory that are important when the system is unloaded or reloaded, but this will not affect our results until the system reaches the necking instability. Only after the neck starts to flow plastically, causing the hardened regions to unload, will we need the full nonlinear theory to determine if the observed behavior is pertinent. We have chosen the rescaling so that all stresses and moduli are expressed in units of the plastic yield stress. We also have assumed that the local density of STZs is always at its equilibrium value so that we do not need to solve an extra equation of motion for that field (denoted by the symbol Λ in earlier papers).

The important exception alluded to above is the presence of the absolute-value bars in Eq. (7). The expression inside the bars is proportional to the rate at which plastic work is being done on the system, a quantity which appears in the original theory as a non-negative factor in the STZ annihilation and creation rates. A negative value of this quantity would be unphysical. In earlier studies of spatially uniform systems, this quantity always remained positive; however, we have observed negative values in the present calculations. The absolute value prevents such unphysical behavior and is consistent with the intent of the original theory. We emphasize, however, that this term contains some of the principal assumptions of the STZ theory. There are other possibilities for it (see, for example, [2]); and it will be interesting to explore the physical significance of these variations of the model.

To understand the transition between viscoelastic and viscoplastic behaviors at the yield stress, and the role played by the state variable Δ, it is easiest to look first at a uniform system under pure shear. Let $s_{xx} = -s_{yy} = s$, $s_{xy} = 0$, $\Delta_{xx} = -\Delta_{yy} = \Delta$, $\Delta_{xy} = 0$; and consider a situation in which s is held constant. Equations (3) and (7) become

$$\dot{\varepsilon} = \epsilon_0\,(s - \Delta), \quad (8)$$

$$\dot{\Delta} = (s - \Delta)(1 - s\Delta), \quad (9)$$

where $\dot{\varepsilon}$ is the total strain rate. At $s = 1$, these equations exhibit an exchange of stability between the nonflowing steady-state solution with $\dot{\varepsilon} = 0$, $\Delta = s$ for $s < 1$, and the flowing solution with $\dot{\varepsilon} \neq 0$, $\Delta = 1/s$ for $s > 1$. As explained in earlier publications, the steady-state system is "jammed" or "hardened" in the direction of the applied stress for $s < 1$; whereas, for $s > 1$, new STZs are being created as fast as existing ones transform, and there is a nonzero plastic strain rate.

Our goal now is to see how this exchange of stability occurs in a dynamic, spatially nonuniform situation. Consider a rectangle with straight grips at $x = \pm L(t)$. The upper and lower surfaces, at $y = \pm Y(x, t)$, are free boundaries. We assume symmetry about both the x and y axes so that we need to consider only the first quadrant of the system. On the free upper boundary, the relation between the material velocities and the motion of the surface is

$$\left(\frac{\partial Y}{\partial t}\right)_x = v_y(x, Y, t) - v_x(x, Y, t)\left(\frac{\partial Y}{\partial x}\right)_t. \quad (10)$$

We also must specify stress conditions on this surface:

$$\sigma_{nn} = \gamma\,\kappa = \frac{\gamma\,Y''}{(1 + Y'^2)^{3/2}}; \qquad \sigma_{nt} = 0. \quad (11)$$

Here, γ is the surface tension, κ is the curvature, and the subscripts n and t denote normal and tangential components, respectively. The grips at $x = \pm L(t)$ move outward at a predetermined strain rate, $\dot{L}/L = \Omega$; thus $v_x(L, y, t) = L\,\Omega$ for $0 < y < Y(L, t)$. Note that we do not constrain v_y along this edge; we allow the grip to slide in the y direction.

We wish to study how the shape of the upper surface, $Y(x, t)$, changes as the grips on the sides are moved outward at various strain rates Ω. Rather than trying to track this surface through the most general possible deformations, we assume that $Y(x, t)$ remains single valued and simply make a change of variables:

$$\xi = \frac{x}{L(t)}, \qquad \zeta = \frac{y}{Y(x, t)}. \tag{12}$$

We then transform Eqs. (1), (3), and (7), and the boundary conditions (10) and (11) into equations of motion for the velocity, the stress, the state variable Δ, and the moving boundary Y, all expressed as functions of ξ, ζ, and t. We solve these equations in the fixed square $0 < \xi < 1$, $0 < \zeta < 1$.

In all of the calculations described here, we have used $\rho = 1$, $\mu = 100$, $K = 300$, and $\gamma = 0.1$. Our initial conditions are $L(0) = 4$ and $Y(x, 0) = 1 - \delta(x)$, where $\delta(x) = 0.01\exp(-8x^2)$ is a small deformation that breaks translational symmetry. We chose two values for ϵ_0: 0.1 (hard) and 0.3 (soft), and two values for the strain rate Ω: 0.01 (fast) and 0.001 (slow). The time taken by sound waves to cross the system is approximately $L\sqrt{\rho/\mu} \approx 0.4$. This is smaller than the characteristic time scale for plastic deformation, which we have scaled to unity, and is much smaller than the actual time scales that we observe for our relatively small pulling rates Ω. Thus, our system is elastically quasistationary, and the precise value of ρ is not important.

We have solved these equations on a fixed, nonuniform 80×20 grid in ξ, ζ space, using the implicit differential-algebraic solver DASPK [18]. In order to suppress numerical instabilities, we have added a small viscosity $\rho\eta\nabla^2 v_i$ to the right-hand side of the acceleration Eq. (1), and have set $\eta = 0.1$.

Figure 1 shows initial and final shapes of samples undergoing tensile tests for four different combinations of the two parameters Ω and ϵ_0 as indicated. For clarity, we show the complete strip although only the behavior of the upper right quarter was computed. The final shapes were arbitrarily chosen at the time when the engineering stresses at the grips were roughly half of their peak values (see Fig. 2). There is a necking instability in all four cases, but it occurs at greater strain for the faster pulls. This rate dependence is also apparent in Fig. 2, which shows the engineering stress at the center of the grip, $\tilde{\sigma}_{xx}(L, 0, t) = \sigma_{xx}(L, 0, t)Y(L, t)/Y(L, 0)$ as a function of the engineering strain $\tilde{\varepsilon}_{xx} = [L(t) - L(0)]/L(0)$ for all four cases (remember that $\sigma_{xx} = s - p$, and $s \equiv s_{xx}$).

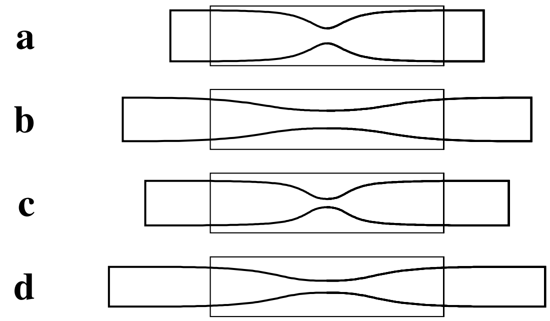

FIG. 1. Initial and final shapes of the material in four numerical tensile tests: (a) $\epsilon_0 = 0.1$, $\Omega = 0.001$; (b) $\epsilon_0 = 0.1$, $\Omega = 0.01$; (c) $\epsilon_0 = 0.3$, $\Omega = 0.001$; (d) $\epsilon_0 = 0.3$, $\Omega = 0.01$.

Thus, although the "softness" parameter ϵ_0 controls the overall plastic response of the material, the onset of the necking instability is controlled by the applied strain rate.

To see what is happening internally, we show in Fig. 3 graphs of s and Δ ($\equiv \Delta_{xx}$) along the centerline of the strip (the x axis) for case (a) in Fig. 2 shortly after the sample is starting to neck. According to Eq. (6), the plastic flow rate is proportional to $s - \Delta$. Outside the necking region, $s \cong \Delta \leq 1$; thus the system in this region has hardened and deforms only elastically. Inside the necking region, however, s rises well above unity and Δ becomes small. Here the system has come close to steady-state flow on the $\Delta = 1/s$ branch of stationary solutions of Eq. (9).

This internal structure of the STZ picture of necking dynamics makes it clear that the strain-rate dependence shown in Figs. 1 and 2 is caused by the competition between the rate of elastic loading and the rate at which hardening occurs, the latter being governed by the equation of motion for Δ, Eq. (7). When the loading is slow, Δ grows along with the stress s, and there is little plastic

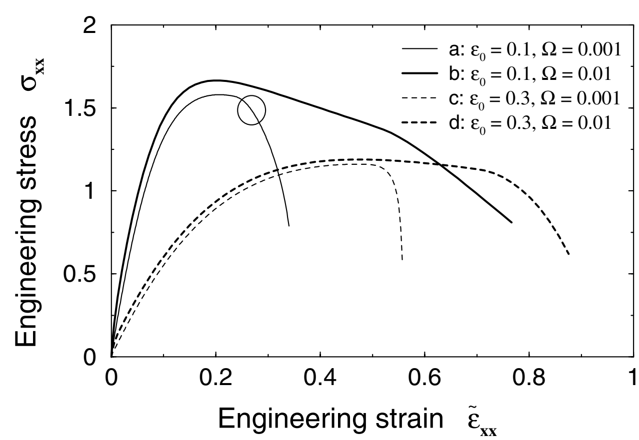

FIG. 2. The engineering stress $\tilde{\sigma}_{xx}$ at the grip plotted against the engineering strain $\tilde{\varepsilon}_{xx}$ for the four cases shown in Fig. 1. The big circle marks the state whose internal properties are shown in Fig. 3.

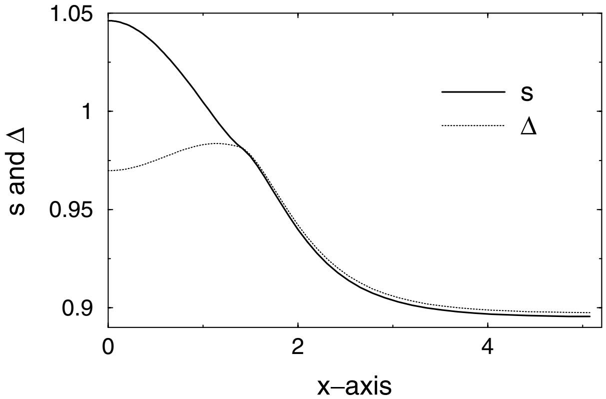

FIG. 3. The deviatoric stress s, and Δ, along the x axis. This picture corresponds to case (a) indicated by the big circle in Fig. 2 shortly after the sample is starting to neck.

flow anywhere until the stress exceeds the yield stress in the necking region. In the opposite limit, when the loading is fast, Δ remains appreciably smaller than s for a longer time during which the material undergoes plastic deformation everywhere. It would be useful to test this prediction of the STZ theory by measuring necking, say, in amorphous metals. We presume that various ingredients of the full STZ theory, such as stress-dependent rate factors and other features that have been ignored here, would be needed to fit experimental data quantitatively, and that we would learn much about the theory from such an effort.

Note that the behavior shown in Fig. 3 is quite different from that predicted by conventional, time-independent plasticity theory, in which there would be a plastic zone with $s \cong 1$ inside the neck, that is, s would remain at the yield stress. We have found no evidence that this conventional behavior occurs in the simulations presented here, even for the smallest pulling speeds. (For cavitation, the STZ theory predicts a conventional plastic zone around a growing hole when the growth rate is very slow [4].) Once the instability sets in, the development of the neck is governed by the elastic energy already stored in the strip. We have confirmed this feature of late-stage necking dynamics by performing numerical experiments in which we stop the motion of the grips, that is, hold them fixed, at various times after the neck has started to form but well before it has grown appreciably. We find that so long as the stored elastic energy is large enough, stopping the remote loading in this way has almost no effect on the neck; it continues to grow just as before, driven by the elastic unloading.

The behavior described in the last sentence — necking driven by stored elastic energy — looks in many ways like fracture, although necking differs from ordinary fracture in that the stress concentration that triggers the instability is due to narrowing of the strip as a whole rather than to a localized defect on just one surface. Nevertheless, the behaviors shown in Fig. 3 (and other, later-stage results not shown here) suggest the onset of a localized, propagating failure mechanism. In order to study the connection between necking and fracture in adequate detail we believe that we shall need to use the full STZ theory and to improve our numerical resolution.

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