Dynamics of shear-transformation zones in amorphous plasticity: large-scale deformation in a two-dimensional geometry

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(Dated: September 2005)

A two-dimensional version of the shear-transformation-zone (STZ) theory by Falk and Langer is explored numerically. Two different geometries are used to simulate uniaxial tension experiments where materials are subjected to constant strain rates. In the first setup, a rectangular specimen is given an imperceptible indentation, allowing it to neck at the center. The dynamics are explored systematically by varying both the straining capability of the STZs \( (\varepsilon_0) \) and the external strain rate. Higher values of \( \varepsilon_0 \) increase the plastic flow and result in sharper necks. Decreased values of the external strain rate result in the formation of narrow shear bands, consistent with the absence of thermal relaxation mechanisms in the model. In the second configuration, the equivalent of pre-annealed materials are explored. Here, the sample is initially square and the edges are made rough in order to encourage the formation of shear bands. With respect to \( \varepsilon_0 \) and the external strain rate, the results show trends similar to those in the necking simulations. The pre-annealing was modeled by using a low initial density of STZs. This had most effect when \( \varepsilon_0 \) was large, contributing to the localization of the strain and making the material appear more brittle.

PACS numbers: 62.20.Fe, 46.35.+z, 83.60.Df, 81.40.Lm

Keywords: plasticity, shear banding, necking, numerics, STZ

I. INTRODUCTION

The goal of the continuum shear-transformation-zone (STZ) theory is to describe plastic deformation in amorphous solids on a mesoscopic scale, averaging out some of the microscopic, discrete details. The plastic deformation is described in terms of flow rates, similar in approach to that of the Navier-Stokes model \(^1\) although the scalar pressure has been replaced with a stress tensor.

The STZ theory was constructed by Falk and Langer \(^2\) \(^3\) \(^4\) \(^5\) \(^6\) \(^7\) \(^8\) \(^9\) \(^10\) \(^11\) \(^12\) \(^13\) \(^14\) \(^15\) \(^16\) \(^17\) \(^18\), and originated with the assumption that plastic deformation is limited to, and defined as, the non-affine transformation of particles in localized areas or zones. This was based on similar ideas made by Argon, Spaepen, and others who described creep in metallic glasses in terms of local, molecular transitions or rearrangements \(^10\) \(^11\) \(^12\) \(^13\) \(^14\) \(^15\) \(^16\) \(^17\) \(^18\). This, in turn, grew out of theories by Turnbull, Cohen, and others, who suggested that the observed behavior in the amorphous metals could be described by linking the transition rates to local free-volume fluctuations \(^12\) \(^16\) \(^17\) \(^18\). This paper, continuing the work reported in \(^19\), presents a two-dimensional model that describes elastic and plastic dynamics in an amorphous solid; the STZ theory supplies the model with a plastic-flow description. The main contribution of this paper is the exploration of the STZ theory in a spatially extended system, focusing on features introduced by having an inhomogeneous geometry. Section \(^II\) presents a tensorial version of the STZ theory that was developed in \(^20\) and based on both the scalar model developed earlier by Falk and Langer, as well as some of Falk’s initial ideas of how to write the theory in a two-dimensional setting \(^2\).

The remaining part, which forms the core of the paper, reviews two sets of numerical uniaxial-tension constant-strain-rate simulations of the two-dimensional, tensorial STZ model. First, Section \(^III\) gives a brief discussion of the implementation. Then the first set is presented in Section \(^IV\) exploring how the plastic flow affected the dynamics during necking. The second set is described in Section \(^V\) relating the pre-annealing of amorphous materials to increased strain localization and brittle behavior. The paper is concluded in Section \(^VI\).

II. THE TENSORIAL STZ MODEL

The numerical simulations described in this paper uses the so-called quasi-linear tensorial STZ model in two dimensions, given below. When combined with boundary conditions, it can be used to describe both the elastic and plastic dynamics of an amorphous solid in a spatially extended geometry. The equations are

\[
\left(1 + \nu_2 \right) \frac{1}{2\mu} \frac{Dp}{Dt} = -\frac{1}{2} \nabla \cdot \mathbf{v}, \quad (1a)
\]

\[
\frac{1}{2\mu} \frac{D\delta_{ij}}{Dt} = \dot{D}_{ij}^{\text{tot}} - D_{ij}^{\text{pl}}, \quad (1b)
\]

\[
\frac{Dv_i}{Dt} = \frac{\partial s_{ji}}{\partial x_j} - \frac{\partial p}{\partial x_i}, \quad (1c)
\]

\[
\frac{DA}{Dt} = \Gamma(1 - A), \quad (1d)
\]

\[
\frac{D\Delta_{ij}}{Dt} = \frac{1}{\varepsilon_0} D_{ij}^{\text{pl}} - \Gamma \Delta_{ij}, \quad (1e)
\]

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with
\[
\tilde{D}_{ij}^{\text{tot}} = \frac{1}{2} \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) - \frac{1}{2} \nabla \cdot \mathbf{v}, \quad (1f)
\]
\[
\frac{1}{\epsilon_0} D_{ij}^{\text{pl}} = (\Lambda s_{ij} - \Delta_{ij}), \quad (1g)
\]
and
\[
\Gamma = \frac{2\Lambda \left( \frac{1}{\epsilon_0} \tilde{D}^{\text{pl}} \right)^2}{(1 + \Lambda)(\Lambda^2 - \Delta^2)}. \quad (1h)
\]

The variables here are the pressure \(p\), the deviatoric stress \(s_{ij}\), the velocity \(v_i\), the relative density of STZs \(\Lambda\), and the STZ alignment \(\Delta_{ij}\). \(\tilde{D}_{ij}^{\text{tot}}\) and \(D_{ij}^{\text{pl}}\) are total and plastic rates of deformation, respectively. The tilde on the former indicates that only the deviatoric part of the tensor is being used (that is, the trace has been subtracted from it). \(\Gamma\) is proportional to both the rate at which energy is dissipated through plastic deformations and the strain rate capability of the STZs \(\epsilon_0\). The temporal derivatives \(D/Dt\) and \(D/\partial t\) both include an advective term, and the latter also takes rotation into account. The complete derivation of these exact equations can be found in [20]; see also [21, 22, 23, 24].

Concerning expressions for the stored energy, it was found in an earlier publication [21] that the plastic dissipation is given by
\[
Q = 2\epsilon_0\Lambda \Gamma, \quad (2)
\]
and the plastic energy density
\[
\psi^{\text{pl}} = \epsilon_0 \left( \frac{\Lambda^2 + \Delta^2}{\Lambda} \right). \quad (3)
\]
In addition, the elastic and kinetic energy densities are given by
\[
\psi^{\text{el}} = \frac{\sigma_{ij} \varepsilon_{ij}}{2} = \frac{1}{2\mu} \left[ \left( 1 - \nu_2 \right) \mu \frac{p^2}{1 + \nu_2} \right], \quad (4)
\]
\[
\psi^{\text{kin}} = \frac{1}{2} \rho v^2 \mu = \frac{1}{2} \rho v_x^2 + \frac{1}{2} \rho v_y^2, \quad (5)
\]

One possible interpretation of how plastic deformation might be described by the STZ model, involves the flipping of STZs. A deformation caused by some STZs flipping, will encourage the internal stress distribution to change, which in turn will flip even more STZs as well as create new ones and annihilate existing ones. It takes energy to flip an STZ. The work done on it could even be considered reversible, if one could make the STZ flip back again. Then again, the STZ could make it back to its original position without releasing any energy by being annihilated and recreated, corresponding to permanent deformation. Since, theoretically, one could regain the energy in the flipped STZ if one could make all the STZ flip back again without any of them being annihilated, a reasonable interpretation of stored plastic energy \(\psi^{\text{pl}}\) could be the energy stored in the flipped STZs. In practice, though, plastic deformation is an irreversible process; some of the stored plastic energy would be lost if the STZs were to flip back, since this flipping would cause further deformations and thus more creation and annihilation of STZs. The plastic dissipation \(Q\) can be interpreted as the energy lost when an STZ is annihilated and recreated.

Simplified, zero-dimensional models using a non-tensorial version of the STZ equations have been explored in earlier publications [3, 4, 6, 7, 8]. The current manuscript concentrates on the effects of a two-dimensional geometry.

### III. NUMERICAL SETUP

In order to explore the tensorial version of the STZ theory given in Eqs. (1), a couple of two-dimensional geometrical configurations were implemented and simulated numerically. For this purpose, a C++-program using finite-difference algorithms on a regular grid with a second-order explicit time-stepping scheme to integrate the equations was written from scratch. This section will give a brief overview over the numerical implementation of the model, including the mapping of the variables onto a unit square, numerical algorithms and approximations, and boundary conditions.

The two-dimensional STZ theory was implemented numerically in order to simulate uniaxial tension experiments where material specimens were strained at constant rates. The velocity was controlled along the top and bottom edges (the “grips”), while the left and right boundaries were assumed to have no normal stresses and were allowed to deform; see Fig. [1].

Two sets of simulations were performed; in the first set the material was made to neck (Section [V]), while in the second set the samples were given rough boundaries in order to encourage the formation of shear bands (Section [V]). In the necking simulations, a small indentation was applied at the center of the material to break the symmetry and to encourage the neck to form in the middle. In addition, the material was assumed to be symmetric across both the \(x\)- and \(y\)-axis, so only a quarter of the system was modeled numerically. In the simulations with rough boundaries, the left and right edges were made stress-free and independent of each other, and no symmetry assumptions were used. The bottom of the material was held fixed while the top was subjected to a constant strain rate.

One aim when introducing the two-dimensional model
was to find out how it differed from the zero-dimensional description, in particular with respect to geometrical inhomogeneities. After deciding to investigate constant strain rate simulations, it seemed sufficient to only allow the sides to deform, while keeping the grips straight. It was assumed that the free boundaries could be described by functions that were single valued: \(X(y,t), X^0(y,t), X^1(y,t)\) had no normal stresses, that is, \(\sigma_{nn} = 0\). In the necking simulations on the left, the material was assumed to be symmetric across the \(x\) and \(y\) axes; thus only the upper right-hand corner of the material was actually simulated. In the simulations on the right, the lower edge was held fixed.

All the simulations were done at constant strain rate. This was enforced by controlling the \(y\)-component of the velocity, \(v_y\), at the grips (the top and bottom boundaries in Fig. 1). For example, in the necking simulations the grip velocity was given by

\[
v_y[x, y = \pm Y(t), t] = \pm Y(t)D^{tot},
\]

where \(D^{tot}\) was the constant strain rate. Since the velocity was applied to all the nodes along the top and bottom, these edges remained straight. The position of the edge as a function of time, using that \(v_y[x, y = Y(t), t] = \partial_t Y(t)\), was therefore

\[
Y(t) = Y(0) \exp(tD^{tot}).
\]

In addition to controlling \(v_y\), the variables \(\tau\) and \(\Delta\) were kept at zero along the grips, effectively removing any shear there.

At the free boundaries, which comprised \(X(y,t)\) in the necking simulations and \(X^0(y,t)\) and \(X^1(y,t)\) in the others, the normal stress \(\sigma_{nn}\) and shear stress \(\sigma_{nt}\) were set to zero, while the tangential stress \(\sigma_{tt}\) was left untouched.

The simulations were carried out on a uniform rectangular grid using finite-difference approximations for the spatial derivatives. The fields were integrated forward in time using the mid-point method, also known as the second-order Runge-Kutta scheme, as well as an adaptive time-step technique called step-doubling.

When implementing the STZ equations of motion, a numerical viscosity \(\eta \nabla^2 p(\zeta)\) was added to the velocity variables on the mapped grid. This was needed because the first-order derivatives were discretized using a central-difference algorithm; with no higher-order spatial derivatives, the grid-points had a tendency to “decouple”
into two sets of nodes like the black and white squares on a chess board. Note that since the Laplacian was applied to the velocities on the mapped grid (that is, on the unit square) and not to the usual velocities, the diffusion term would only be a “proper” viscosity where the material was undeformed.

Since the added viscosity was only meant as a numerical tool, it was important to monitor any changes it made to the physical results. The influence of the viscosity was minimized by performing successive runs with smaller and smaller values of $\eta$. If the numerical viscosity was chosen too high, the results would look nice and smooth, but when compared to simulations with lower values of $\eta$, it became clear that the added viscosity was smearing out sharp features such as shear bands. On the other hand, when too small values of $\eta$ were used, large gradients caused by the “decoupling” would make the simulations more unstable. This was particularly pronounced at the border (where values were calculated through extrapolation) and in larger grids.

The simulations were most sensitive to the value of $\eta$ at low strain rates, basically because there was more time (per strain) to dampen out the velocities. When running as slow as $D_{\text{tot}} = 10^{-5}$ on the larger (more unstable) grids used in Section IV there were no values of $\eta$ that gave satisfactory results; even the smallest stable value of $\eta$ would be too large, resulting in unacceptable amounts of artificial dissipation and influencing the behavior too much. Even for the smaller grids in the necking simulations of Section IV the slowest strain rate $D_{\text{tot}} = 10^{-5}$ was hard to accommodate. In the end, it was found that $\eta = 0.02$ (which in fact turned out to be a good choice for all the simulations) enabled the slowest simulation to reach 5% strain while having only a small impact on the physical results. The influence due to the exact choice of $\eta$ for higher strain rates was usually imperceptible.

IV. NECKING

Irregular geometry in a two-dimensional, externally loaded sample of material can cause stress localizations and shear banding. Compared to a zero-dimensional model, two spatial dimensions add elastic deformation and inertia. As long as the elastic strains are small, the speed of sound high, and the rate of total deformation low, the difference between a zero-dimensional and a uniform two-dimensional system is minimal. Generally speaking, metallic glasses have two modes of deformation: homogeneous and inhomogeneous. A transition from the former to the latter will occur when a material is strained and the stress localizations from the irregular geometry start causing shear bands. The simulations described in this and the next section illustrates this transition. Some earlier work can be found in 14.

A. Simulations

One way of exploring the effect of a non-trivial geometry is to look at the dynamics of a material while it is necking. A series of simulations were run where a rectangular $2 \times 8$ piece of material was elongated in the $y$-direction at a constant strain rate. The material was slightly indented in the middle, where the width was reduced by 1%. Specifically, the right-hand boundary was given by $X(y,t = 0) = 1 - \delta(y)$, where $\delta(y) = 0.01\exp[-\ln 2(y/0.1)^2]$. This perturbation to the geometry was added to break the symmetry and to help trigger any potential instabilities. The material (or rather, a quarter of it) was mapped onto an $11 \times 41$ regular grid, using the transformation of variables described in Section III. The size of the grid was verified to be large enough to support the desired accuracy, as a comparison with some test runs on a larger $21 \times 81$ grid gave almost identical results. The shear modulus was set to $\mu = 100$ and the density $\rho = 1$; since the speed of sound is proportional to $\sqrt{\mu/\rho}$, a lower value of $\mu$ would have jeopardized the assumption that the elastic deformations were instantaneous. Conversely, an increased value of $\mu$ would demand notably more resources computationally. All the necking simulations had $\Lambda_0 = 1$, and the numerical viscosity was chosen to be $\eta = 0.02$, based on the discussion in Section III.

Fig. 4 shows the outlines of material samples in two separate simulations. The solid outlines were the initial configurations; notice that the indentations are hardly visible. The dashed outlines represent the configurations after the systems had been strained. The simulation on the left was strained an order of magnitude faster than the one on the right. While the former had a smooth neck, the latter had a more irregular boundary due to shear bands.

In general, shear bands would appear more readily when the material was strained at a lower rate. The left part of Fig. 4 shows the plastic dissipation $Q$ as given by Eq. 21 in a simulation with $D_{\text{tot}} = 10^{-4}$, $\epsilon_0 = 0.03$, and $\Lambda_0 = 1$ after it had strained roughly 6%. The right-hand side displays, for the same simulation, the velocity field with the uniform part $v_{\text{uniform}} = (0,yD_{\text{tot}})$ subtracted away. These figures show that the material no longer was deforming uniformly. Stress concentrations radiating out from each notch at roughly $45^\circ$ increased the plastic dissipation, and thus the plastic deformation, along these shear bands. As can be seen in the velocity plot, the whole central piece of the neck became narrower, and this is what caused the irregular boundaries seen on the right-hand side of Fig. 4.

In a uniform STZ material, the rate of deformation $D^p$ increases drastically when the deviatoric stress $|s|$ becomes larger than unity 19 20 21. In steady state, any area with $|s| > 1$ can be considered to be flowing plastically, while regions with $|s| < 1$ are jammed. This applies to the tensorial version of the theory, too, when measuring the deviatoric stress by the invariant $\tilde{s} = \sqrt{s^2 + \tau^2}$.
FIG. 3: Examples of the geometry in two numerical experiments. The solid outlines are the initial configurations — the initial indentations are hardly visible. The dashed outlines represent the geometry after the left and right samples were strained 24% and 10%, respectively. The strain rate in the left simulation was $D_{\text{tot}} = 10^{-3}$, ten times higher than on the right. In both simulations $\mu = 100$, $\nu = 0.5$, $\epsilon_0 = 0.03$, $\Lambda_0 = 1$, and the initial size of the samples were $2 \times 8$.

also known as the maximum shear stress. Fig. 4 shows a series of snapshots from a necking simulation where the interior has been shaded according to the values of $\bar{s}$; the darker the shade, the higher the value (notice that the strain is plotted against the total stress $\sigma_{yy}$ at the grip, and since $\sigma_{xx} = \sigma_{xy} = 0$ there, one has that $\sigma_{yy} = 2\bar{s}$). At low strains the stress was uniform, but as the material necked the stress concentrated in the center. The black lines that appear in the last four snapshots mark the boundary between $\bar{s} < 1$ and $\bar{s} > 1$. The steady-state solutions suggest that the area between the lines were flowing plastically, while the regions on either end, outside the lines, were more or less jammed. As the neck grew more pronounced, the plastically flowing area would shrink, making a smaller and smaller area responsible for accommodating the ever increasing global strain. In addition, the jammed areas would relax (notice how the ends grew lighter in the final snapshots) and contract along the strained $y$-axis while releasing stored energy. This decrease in strain at the ends had to be compensated by increasing the strain even further in the middle.

The graph below the snapshots plots the true stress $\sigma_{yy}$ at the grips as a function of the total true strain $\varepsilon_{yy}$. The true stress (at the grip) is defined as the force divided by the current width of the material, both measured at the grip. The true, or logarithmic, total strain is defined as $\varepsilon_{yy}^\text{tot} = \ln[L_y(t)/L_y(0)]$, where $L_y(t)$ is the length of the material at time $t$. The snapshots were marked on the graph as circles. The first snapshot was taken while the material was in the “elastic phase”, while the second was taken just as the material was about to yield. This explains why the two first snapshots seem so uniform. Note that since the plotted stress was measured at the grips, it corresponds to the shading at the ends of the material.

To illustrate how the parameters affect the material behavior, Figs. 6 and 7 show further plots where the true stress $\sigma_{yy}$ at the grip was plotted against the true total strain $\varepsilon_{yy}^\text{tot}$, comparing curves for various values of $\epsilon_0$ and $D_{\text{tot}}$. In Fig. 6 all the simulations were strained at a rate of $D_{\text{tot}} = 10^{-3}$ while $\epsilon_0$, the amount of strain caused by flipping STZs, was varied. In simulations with a higher $\epsilon_0$, the material needed to be strained further before reaching the yield stress. This is because more of the work done on the system was stored as plastic energy; it was only the elastic deformations that contributed to the rising stress. In fact, the slope of the stress-strain curves in the “elastic” regime, which corresponds to the
FIG. 5: The graph shows the true stress $\sigma_{yy}$ at the grips as a function of the total strain $\varepsilon_{yy}^{\text{tot}}$. Snapshots of the system were taken at six different strains, and the interior was shaded according to the value of the maximum shear stress $\bar{s} = \sqrt{s^2 + \tau^2}$. The black lines in the four last snapshots show where $\bar{s} = 1$, suggesting that the area between the lines ($\bar{s} > 1$) was flowing plastically while the areas at the ends ($\bar{s} < 1$) were jammed. ($D_{\text{tot}} = 10^{-3}, \epsilon_0 = 0.03, \Lambda = 1$)

**FIG. 6:** The true stress $\sigma_{yy}$ at the grip plotted against the true total strain $\varepsilon_{yy}^{\text{tot}}$ for selected values of $\epsilon_0$. As $\epsilon_0$ was increased, it took longer (in terms of strain) for the material to reach the yield stress, since less of the deformation was stored as elastic energy (and more as plastic). Once the yield stress was reached, a higher value of $\epsilon_0$ allowed for more plastic deformation and thus a quicker relaxation of the stress. ($D_{\text{tot}} = 10^{-3}, \mu = 100, v_2 = 0.5, \Lambda = 1$)

After the system reached yield stress, the simulations with high strain rates took a lot longer (in terms of strain) before they would neck. The higher strain rate meant a steady-state stress even further above unity (the “yield stress”), which in turn meant that small geometric inhomogeneities would not be able to separate the stress into regions of $\bar{s} > 1$ and $\bar{s} < 1$. For the low strain rate simulations, the stress localization was more pronounced, and for the lowest rate, the shear bands were so sharp that the numerics was not able to strain the material beyond 5%.

**Fig. 8** compares stress-strain curves of simulations where both $\epsilon_0$ and $D_{\text{tot}}$ were varied. These curves show clearly that the strain rate primarily changed the time between yield and necking, while $\epsilon_0$ controlled the dynamics of both the stress increase before yield and the relaxation after.

On a side note, all the simulations were started at the given (or final) strain rate rather than being ramped up from zero. This was especially important for the high strain rate simulations. If the material had been started from rest, the details of how the strain rate was ramped up would greatly affect the outcome of the simulation. If ramped up too slowly, the material would yield before the final strain rate could be achieved. If the strain rate was turned up too quickly, the speed of sound would no longer be negligible and inhomogeneities would form at the grips due to large stress buildups. To minimize transient effects from the non-zero initial strain rate (such as standing elastic waves in the material), initial values for the other variables in the simulation were calculated in order to...

**effective** shear modulus, has been calculated in [22]. After reaching the yield stress, the systems with a higher $\epsilon_0$ would see a faster relaxation of the stress. This is probably because a high $\epsilon_0$ allowed for a higher plastic rate of deformation at the neck, where the elastic stored energy was released through plastic dissipation. Interestingly enough, a high $\epsilon_0$ meant that most of the stored energy was plastic; that is, the energy was stored in flipped STZs rather than elastic strain (the amount of stored plastic energy cannot easily be deduced from the stress-strain curves).

The effect of varying the total strain rate is shown in **Fig. 7**. The strain rate had little effect on the strain at which the yield stress was reached (although it did influence the initial stress in these simulations; see below).
start the system as close as possible to a steady state. This is why the curve with a strain rate of $D_{\text{tot}}^\text{init} = 10^{-2}$ in Fig. 7 starts with a somewhat higher stress. This is not a numerical effect; it would be true for real experiments as well. See Fig. 2 and the accompanying text for some further information on the effects of a non-zero initial strain rate.

**B. Discussion**

In the previous section, a series of necking simulations with different values of the parameters $\kappa_0$ and $D_{\text{tot}}^\text{init}$ was described. Trends seen in these simulations are discussed in more depth in the text below.

Fig. 4 is a “phase diagram” of the dynamics of the necking simulations, mapping out the behavior as a function of $D_{\text{tot}}^\text{init}$, the total strain rate, and $\kappa_0$, the strain due to flipped STZs (Spaepen uses a similar diagram, which he calls a “deformation map”, when he outlines the behavior of amorphous metals in a graph of the temperature versus the stress [11, 26]). It tries to capture the essence of the behavior described in the simulations above.

Fig. 11 shows how the simulations discussed in the previous section fit into the “phase diagram” of Fig. 4. Since there was more room in this graph, an additional curve and shading was added to show what parameter values would cause the initial stress to lie between $s_0 = 0.1$ and $s_0 = 1$, the latter being the yield stress.

Returning to Fig. 3 the following is an attempt to
yield stress at the same total (that is, elastic and plastic) deformations. Thus the material would always reach the stress. As long as $\bar{\Delta}$ was low, $\Gamma$ was negligible, and few STZs were created or annihilated. This implies that the material needed to dissipate this energy if it were to stay in steady state. In the slow strain rate simulations, it seems that the rate was slow enough that all the dissipated energy could exit through the shear bands; in other words, only the shear bands had stresses above the yield stress. In the simulations with higher strain rates the input of energy per unit time was higher, resulting in energy dissipation throughout the material. This forced the stress to exceed the yield stress everywhere. Remember that if $s > 1$ then $\Delta \to 1/s$, while if $s < 1$ then $\Delta \to s$. Since the plastic flow was proportional to $\epsilon_0(s - \Delta)$ ($A_0 = 1$ in these simulations), the slowly strained materials saw a large difference between the amount of plastic flow in the shear bands and the rest of the material. The stresses would be above the yield stress in the shear bands and below it elsewhere. Notice how the inhomogeneous geometry played a vital role by breaking the symmetry, concentrating the stresses in certain areas, and thus allowing the shear bands to form.

In contrast, the value of the strain rate had little effect on the simulations before the stress reached the yield stress. As long as $\Delta$ was low, $\Gamma$ was negligible, and few STZs were created or annihilated. This implies that the deformation before yield was almost reversible, and that the plastic strain was proportional to $\Delta$, the fraction of flipped STZs. Thus the material would always reach the yield stress at the same total (that is, elastic and plastic) strain.

Second, when the parameter $\epsilon_0$ was given high values, the material would have to be strained further before reaching yield stress. This parameter controlled the amount of strain due to flipping STZs, or alternatively, how much of the energy was absorbed in plastic deformations. By combining Eqs. (5) and (4), one can see that a uniform system in steady state with $s \approx 1$ has $\psi^\text{pl}/\psi^\text{el} \approx \epsilon_0 \mu(1 + \nu_2)$ [20]; when this expression was less than unity, most of the strain energy was stored as elastic strain. This would correspond to $\epsilon_0 < 0.007$ in the above simulations, since $\mu = 100$ and $\nu_2 = 0.5$. As $\epsilon_0$ was increased, the STZs were responsible for more of the deformation, and since the stress is only proportional to the elastic strain, the stress would grow more slowly for large $\epsilon_0$. That explains why the materials with the smaller $\epsilon_0$ yielded earlier.

Observing the post-yield dynamics, a large value of $\epsilon_0$ ultimately resulted in sharper necks. After the stress had reached yield, the energy supplied by the work at the grips would no longer be stored in the elastic or plastic deformations (which corresponds to stress and flipped STZs, respectively). Rather, the energy was dissipated through flipping newly created STZs while annihilating the same amount of already-flipped ones. In a homogeneous system the material would just remain in this steady state. In the necking simulations, though, the localized stresses emanating from the indentations perturbed the system enough to change the flow from homogeneous to inhomogeneous. Especially for higher values of $\epsilon_0$, the neck would narrow rapidly, increasing the stress and plastic flow there until the material would snap in two (in practice, the restricted geometry of the numerical grid would not actually allow the material to split, but the neck would become extremely narrow and the time-step would decrease to a value which was, for all practical purposes, zero). This uncontrolled necking was mainly driven by stored energy being released through plastic dissipation at the neck. Interestingly enough, it was the stored plastic energy that supplied almost all of the energy; the stored elastic energy was almost negligible when $\epsilon_0 \gg 1/\mu(1 + \nu_2)$. An interesting question is: How much does the quasi-linear approximation affect the dynamics? In a fully non-linear version of the theory, the STZ transition rates would grow small for low stresses, thus preventing the STZs from flipping back [21]. Potentially, this could prevent some of the release of the stored plastic energy from the areas further from the neck.

A large value of $\epsilon_0$ meant that the material needed to be strained further before the stress reached the yield stress since the plastic flow relaxed some of the stresses. Although it took longer for the material to reach the yield stress, once it did the neck developed more rapidly. This was because the increased plastic flow in the neck allowed the ends to relax and release its stored plastic and elastic energy faster. The relaxation of the stress at the ends added even more strain to the center, contributing to the plastic flow at the neck. Finally, as the neck became thinner, the stress would rise there and increase the already high plastic flow even further. Thus the material would

![Graph](image-url)
neat faster when \( \epsilon_0 \) was high, since that would reinforce this feedback loop.

When \( \epsilon_0 \ll 1/\mu(1 + \nu_2) \), most of the initial work done on the system was stored as elastic energy. After reaching yield stress, the steady-state stress became large (and \( \Delta = 1/\delta \) small) in order to create enough plastic dissipation \( \tilde{D}_{pl} \) to counter the steady input of energy supplied by the work done at the ends of the material. There were some faint shear bands where the stresses showed slightly elevated values, but the plastic dissipation was almost uniform throughout the material when \( \epsilon_0 \) was small.

V. PRE-ANNEALED MATERIALS

The behavior of a pre-annealed metallic glass is more brittle than both a virgin as-quenched sample and a material that has experienced plastic work. Experiments have shown that metallic glasses that have been annealed below the glass transition temperature seem more brittle, show more pronounced strain softening, and have decreased plastic flow \([26, 31, 32, 33, 34, 35]\). Microscopically, observations showed structural relaxation in the form of more closely packed molecules, corresponding to a macroscopic increase in density. Upon plastic deformation the materials were seen to return to their as-quenched states, including a decrease in the density and a lower packing fraction. Annealing for a longer time or with a higher temperature gave more pronounced changes in the mechanical properties. It is also worth noting that aging the materials over longer periods of time at lower temperatures also made the metallic glasses more brittle \([27]\).

The STZ theory captures the change in behavior due to annealing through \( \Lambda \), the relative density of STZs. When a virgin material is initially quenched from a molten state, the atoms have little time to organize into a closely packed configuration, leaving a “fluffy” structure and a high density of STZs. Annealing the material packs the atoms into a tighter configuration, making \( \Lambda_0 < 1 \). Likewise, if an annealed material is subjected to plastic work, the value of \( \Lambda \) would rise as the tightly packed atoms are “re-fluffed”, leaving more room for local rearrangements.

The version of the STZ theory that is explored numerically in this paper has no mechanism for thermal creep or relaxation, which is reflected in the fact that \( \Lambda \geq 0 \). Thus the model can only simulate pre-annealed materials, by setting the initial value of \( \Lambda \) low \([33]\). Consequently, a material with \( \Lambda_0 < 1 \) and \( \Lambda_0 = 1 \) will from now on be referred to as “pre-annealed” and “worked”, respectively, although the latter could also represent a material in its virgin as-quenched state.

Initially during a constant strain-rate experiment, a small \( \Lambda \) would suppress plastic deformation since there would be very few STZs to flip. As the stress \( \bar{s} \rightarrow 1 \), most of the existing STZs would be flipped, and new ones would have to be created causing \( \Lambda \) to grow. The lower \( \epsilon_0 \) was set, the higher the peak stress and steady-state stress would be, and the faster \( \Lambda \) would grow toward one.

The previous section assumed that \( \Lambda \equiv 1 \) throughout. The current section describes simulations where pre-annealed materials were used during loading, implemented by setting \( \Lambda_0 = 0.01 \). A spatially extended two-dimensional simulation allowed \( \Lambda \) to grow locally, thus making it possible for the material to boost the plastic flow in areas where the stresses were high. As will be seen, this contribution to the inhomogeneous deformation was particularly pronounced for high values of \( \epsilon_0 \).

As in Section IV, the simulations had a shear modulus of \( \mu = 100 \), a density of \( \rho = 1 \), a Poisson ratio of \( \nu_2 = 0.5 \), and a numerical viscosity of \( \eta = 0.02 \). The size of the material was \( 4 \times 4 \), although this time the whole material was simulated (that is, there were no symmetric boundaries). The material was mapped onto a grid measuring 33 \( \times \) 33 nodes. The left and right boundaries \( X^0(y, t) \) and \( X^1(y, t) \) (initially parallel to the \( y \)-axis) were both allowed to deform. The lower boundary was held fixed at \( y = 0 \), while the upper boundary \( Y(t) \) was moved at a constant strain rate (see Section III for further details). The initial density of STZs was set below unity, to \( \Lambda_0 = 0.01 \). In order to encourage inhomogeneous flow, the free boundaries were made jagged by randomly perturbing the width with values up to 1% of the total width (in other words, after the perturbation \( X^1(y, 0) - X^0(y, 0) \in [3.96, 4.04] \)). By setting the seed for the random number generator to the same value for all the simulations, the initial geometry would always be the same.

The simulations in this section illustrate the dynamics of pre-annealed materials in three different ways. First, the distribution and average density of STZs are compared to the dissipated energy and the work done on the systems for different values of \( \epsilon_0 \). Second, the dynamics of pre-annealed and worked materials are compared. And third, the following question is addressed: Would the simulations with higher strain rates experience more pronounced shear bands if they were stopped and held at a fixed strain for the same amount of time it would take a slower simulation to reach that same strain?

A. Variation in \( \epsilon_0 \)

Fig. II compares the average density of STZs

\[
\Lambda_{\text{avg}} = \frac{1}{A} \int_A \Lambda \, dA
\]

(10)

(where \( A \) is the area of the sample) to the plastic dissipation of energy

\[
Q_{\text{sum}} = \int_A Q \, dA
\]

(11)

for three different values of \( \epsilon_0 \). All three simulations were strained at a rate of \( D_{\text{tot}} = 10^{-4} \). Each of the three
graphs on the left displays three curves, of which the solid represents the rate of work done on the system at the grip,

\[ P_{\text{external}} = F v_y = (X^1 - X^0) \sigma_{yy} v_y. \]  

(12)

\( F \) is the force applied to the end of the material, and \( \sigma_{yy}, \ v_y, \ X^0, \ \) and \( X^1 \) were all evaluated at \( y = Y(t) \). Since the upper boundary was kept flat and moved perpendicular to its surface, only the \( y \)-component of the stress was needed. \( P_{\text{external}} \) is thus the rate at which energy flowed into the system.

The middle curve in all three graphs shows \( Q_{\text{sum}} \), the rate of energy dissipated due to plastic deformation summed over the whole material. The axis on the left side displays the values for both this curve and that of \( P_{\text{external}} \), although they were multiplied by \( 10^3 \) to reduce clutter (the interval is really \([0, 0.0004]\)). The axis on the right sets the scale for the third curve, \( \Lambda_{\text{avg}} \), which represents the density of STZs averaged over the whole sample.

The two density plots to the right of each of the graphs show the final distributions of \( \Lambda \) and \( Q \) when the systems had reached 7% strain. In the density plots for \( \Lambda \), the shading was scaled so that the interval \([0, 1]\) went from white to black. With \( Q \), the gray scale was mapped onto the interval \([0, 0.003]\), with white again representing zero. In the latter density plots there were occasional points that exceeded 0.003 (these were just painted black as well), but choosing a larger interval would have erased most of the structure seen in the pictures.

In the simulation where \( \epsilon_0 = 0.003 \), \( \Lambda_{\text{avg}} \) quickly rose to one while \( Q_{\text{sum}} \) grew equal to \( P_{\text{external}} \) once the stress reached yield. The latter meant that all the energy provided at the grips was dissipated through plastic deformation, and none was stored, after the material reached about 2% strain. In the \( \epsilon_0 = 0.3 \) simulations, \( \Lambda_{\text{avg}} \) never even reached a value of 0.15, and the plastic rate of dissipation grew a lot slower. In fact, looking at the density plot shows that the density of STZs only saturated along one band, and the plot for \( Q \) shows that this was where most of the plastic dissipation took place as well. The fact that \( \Lambda \) so quickly reached its equilibrium value everywhere in the material for small \( \epsilon_0 \) meant that the initial value of \( \Lambda_0 = 0.01 \) had little effect in this case.

Although the density plots of \( Q \) and \( \Lambda \) both were snapshots, the latter in some ways gave a cumulative look at what had happened since the start, since \( \Lambda \) could not decay (this is not true in other versions of the STZ theory that incorporate thermal relaxation [22, 23]). In contrast, the density plot of \( Q \) is more appropriate when examining the instantaneous dynamics, since it highlights the current rate of plastic deformation in the different areas of the material.

In the simulation with \( \epsilon_0 = 0.3 \), the rate at which energy flowed into the system, \( P_{\text{external}} \), started decaying towards the end. This is because the stress at the grip began to drop due to the increased plastic flow along the shear band. The high value of \( \epsilon_0 \) allowed the material to deform enough in the small area of this band to account for all the strain imposed by the grip, thus inducing inhomogeneous flow and perhaps cause the material to break at a later time.

B. Comparing Pre-Annealed and Worked Materials

Fig. 12 compares a pre-annealed and a worked material, having initial conditions of \( \Lambda_0 = 0.01 \) and \( \Lambda_0 = 1 \), respectively. The two curves in the center show the true stress-strain curves of these two materials as they were strained beyond yield and toward failure (the materials would eventually grow extremely thin somewhere in the center). The density plots of \( Q \) on either side were arbitrarily chosen some time after the materials had yielded, with the stress at the grips being the same in the two snapshots. Although the two density plots look different, their initial geometries were identical to each other and to all the other simulations in this section.

The only comparison shown here is that of the simulations with \( \epsilon_0 = 0.3 \). Although no less important, the pre-annealed materials with a lower \( \epsilon_0 \) would have \( \Lambda \) rise to one everywhere so quickly that the results were essentially the same as for the worked materials; this effect was seen in Fig. 11.

A high value of \( \epsilon_0 \) allowed the stresses to grow more slowly, permitting some areas to reach \( \bar{s} > 1 \) while others remained at \( \bar{s} < 1 \). This is because \( \Lambda \) only rise to one everywhere so quickly that the results were essentially the same for the worked materials; this effect was seen in Fig. 11.

Comparing the stress-strain curves in Fig. 12 the pre-annealed material plateaued before breaking. It almost seemed like it was riding along an unstable equilibrium before it increased the density of STZs in one location and then deformed and broke there. In comparison, the worked material would deform substantially more before reaching yield stress, and then “ooze” apart (rather than “break”).

It is tempting, although perhaps somewhat speculative, to compare the necking on the left side of Fig. 12 to fracture. Some of the simulations, including this one, had extremely concentrated stresses and narrow necks, and the deformations behaved in many ways similar to brittle cracks. The simulations have shown that there is an interplay between the STZs, the geometry, and stress concentrations. Naturally, the geometry of the numerical grid in these simulations was quite restricted, the single-valued boundaries forcing the “crack” to run horizontally rather than following the 45° shear bands as seen in experiments [36, 57]. Also, the resolution was too low to make any good quantitative arguments. Nevertheless, this behavior suggests that the STZ description might be capturing some of the dynamics that is present in fracture (for more information on fracture in brittle amorphous materials, see the review by Fineberg and...
FIG. 11: Three pre-annealed simulations with $\Lambda_0 = 0.01$ were run for $\varepsilon_0 = 0.003$, $\varepsilon_0 = 0.03$, and $\varepsilon_0 = 0.3$, all with a strain rate of $D^\text{tot} = 10^{-4}$. The graphs on the left show $P_\text{external}$, the rate of work done at the grips, $Q_\text{sum}$, the rate of dissipated plastic energy summed over the whole material, and $\Lambda_\text{avg}$, the average density of STZs. The left vertical axis shows the range for $P_\text{external}$ and $Q_\text{sum}$ (the interval is $[0, 0.004]$), while the right vertical axis displays the scale for $\Lambda_\text{avg}$. The density plots on the right show $\Lambda$ and $Q$ at 7% strain.
FIG. 12: The true stress-strain curves for two materials, one with $\Lambda = 0.01$ and one with $\Lambda = 1$. The density plots show the plastic rate of dissipation at some arbitrary time after yield, with the stress at the grips being the same in the left and right snapshots. ($D^{\text{tot}} = 10^{-3}, \epsilon_0 = 0.3$)

Marder [38].

C. Strain-Rate Dependent Localization

When comparing the results of the simulations from both the current and previous sections, the shear bands at a given strain were more pronounced for smaller strain rates. Comparing two identical materials that were strained to $7\%$ at rates of $D^{\text{tot}} = 10^{-4}$ and $D^{\text{tot}} = 10^{-3}$, the former would not only be stretched ten times slower, it would also have ten times as long to relax and deform. Could it be that it was not the difference in speed, but the difference in relaxation time that allowed the shear bands to form in the slow case?

Fig. 13 shows density plots of $\Lambda$ at $7\%$ strain where the materials had been strained at the rates mentioned above, with both $\epsilon_0 = 0.03$ and $\epsilon_0 = 0.3$. The system that had been strained at the slower rate, $D^{\text{tot}} = 10^{-4}$, reached $7\%$ at time $t = 700$, while the faster system with a rate of $D^{\text{tot}} = 10^{-3}$ was stopped around $t = 70$ (the snapshot was taken at $t = 75$ to make sure the material had come to a complete stop, reaching its full $7\%$; in order to stop the material at this exact strain, it was necessary to start slowing it down already at $t = 65$). After stopping the fast system, it was held fixed until $t = 700$, the same amount of time it took the slow system to reach $7\%$ strain.

It turned out that there was practically no change in the quickly-strained material after the grips had come to a halt (this was the case both for $\epsilon_0 = 0.03$ and $\epsilon_0 = 0.3$, although the former ended up with a higher $\Lambda_{\text{avg}}$). This means that all the deformation took place instantly, not allowing any of the stored energy to escape later.

This does not preclude a situation where a more irregular geometry might induce a stress concentration, allowing both stored plastic and elastic energy to be released, perhaps even driving a necking instability; this kind of behavior was seen in the previous section. It does mean, though, that the shear bands were created without the need of instability mechanisms. In fact, the bands of STZs were more pronounced when energy flowed into the system at a slower rate.

The previous section speculated that the STZ theory could perhaps contribute to explain fracture dynamics. The current section seems to contradict this somewhat, at least at first glance. From experience, a material strained at a higher rate seems more brittle, implying that it should have sharper stress concentrations, and more localized shear bands. How could such behavior be compatible with the results shown above?

It was briefly mentioned earlier that the thermal relaxation is being incorporated into some versions of the STZ theory [22, 23]. With that mechanism included, $\Lambda$ can decrease as STZs are annihilated over time, and this might suppress the creation of localized bands of STZs as the strain rate drops. The model used in this paper did not allow $\Lambda$ to decrease, which might be interpreted as running the simulations close to zero temperature.

VI. CONCLUSION

The goal of this paper has been to explore the STZ theory in a spatially extended geometry. In addition to showing that a two-dimensional implementation is capable of describing shear localization, a wide range of parameter values were used to expose the different types of behavior inherent in the model. The geometry, energy flow, and internal state of the material all contributed to the rheology through effects such as jamming and plastic flow, annealing, strain softening, necking, and shear banding.
Amorphous metals have two modes of deformation: Homogeneous and inhomogeneous flow \[11, 26, 39\]. Homogeneous flow is typical for low stresses and high temperatures, and under uniaxial tension a material sample will deform uniformly throughout the specimen. In inhomogeneous flow, the deformation is usually localized in narrow shear bands that run at a 45° angle with respect to the tensile axis \[36, 37\] (some studies show that the angle of the shear bands deviate under large isotropic pressures \[40, 41\]). The cross-section of the material decreases as slip, and eventually fracture, occurs along these shear bands \[36, 37\]. At low temperatures, the shear-localization instability sets in right after yield, making the material behave in a seemingly brittle manner; there is no hardening due to strain in metallic glasses, although physical aging decreases the plastic response \[27\].

Section IV looked at how the strain rate, the strainability of STZs \(\varepsilon_0\), and the geometry affected flow and deformation during necking. It was especially striking how sharp shear bands and narrow necks were formed at low strain rates and high \(\varepsilon_0\), respectively. The former of these two trends appeared to contradict experimental evidence: An amorphous metal displays increased brittle behavior as it is strained at a higher rate \[29\], while the opposite seemed true for the simulated materials. The discrepancy probably stems from the lack of temperature in the current STZ model. There was no mechanism once the simulation had started, apart from plastic deformation, to annihilate existing STZs. In the experiments, the non-zero temperature allowed the molecules in the most strained areas to relax if given enough time. This resulted in more homogeneous flow as the material was strained at lower rates. Efforts have been made to incorporate thermal relaxation into the model \[22, 23\].

Section V considered pre-annealed amorphous solids, starting with a lower initial relative density of STZs \(\Lambda_0\). Experiments have shown that amorphous metals become more brittle when annealed, even though no crystallization is detected \[30, 31, 32, 33, 34, 35\]. Rather, the embrittlement correlates with structural relaxation, leaving the more closely packed molecules less room to move. In the simulations, the lower \(\Lambda_0\) enhanced the localization of the strain, especially for higher values of \(\varepsilon_0\) when most of the stored energy was in the form of flipped STZs (rather than elastic strain). Compared to either virgin as-quenched or worked samples, the pre-annealed materials behaved in a more brittle manner with narrower shear bands and something resembling a cleavage fracture. The latter observation should be approached with caution since the implementation was not designed to handle such extreme deformations; the numerical grid forced the “crack” to run horizontally through the material, while a diagonal path running at 45° would seem more natural \[44\]. Nevertheless, the similarities between the dynamics of the STZ theory at low \(\Lambda_0\) and empirically annealed solids were strong enough to warrant further investigation.

As mentioned, an increased value of \(\varepsilon_0\) would result in more of the applied work being stored as flipped STZs rather than elastic strain. This was particularly apparent for the virgin materials \(\Lambda_0 = 1\), where an increased \(\varepsilon_0\) meant that the material would reach yield stress at a much larger total strain. On the one hand, it is possible that the large values of \(\varepsilon_0\), which were needed to produce interesting dynamics in the simulations, exaggerated the strain caused by flipped STZs. On the other hand, \(\Lambda_0 \ll 1\) would restrict the plastic strain (and thus the stored plastic energy) to narrow shear bands, causing a mostly elastic behavior before yield and more brittle dynamics at failure. It is possible that the sharp bands of inhomogeneous flow in experimentally deforming amorphous solids are due to an internal structure corresponding to low initial values of \(\Lambda\); unless the materials were quenched extremely rapidly and to very low temperatures, chances are that some structural relaxation would occur. Incorporating the earlier mentioned thermal relaxation into the STZ model could help lower the value of \(\Lambda\) throughout the simulation and yield better agreement with the experimental results.

This work was supported primarily by the Research Council of Norway. It was supported in part by the National Science Foundation Materials Research Science and Engineering Centers (NSF MRSEC) program (DMR96-32716), due to Jim Langer’s gracious and surprising decision to assist me financially when my main grant ended. This work made use of the computing facility of the Cornell Center for Materials Research (CCMR) with support from the NSF MRSEC program (DMR0079992), and computing facilities at UC Santa Barbara sponsored by a grant from the Keck Foundation for Interdisciplinary Research in Seismology and Materials Science. Additional support came from the NSF-KDI program (DMR-9873214) and the U.S. Department of Energy (DE-FG03-99ER45762). I would like to thank Jim Langer for his advice and support, as well as Leonid Pechenik, Craig Maloney, Anthony Foglia, and Michael Falk for stimulating discussions.

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