Shear band dynamics from a mesoscopic modeling of plasticity

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Abstract. The ubiquitous appearance of regions of localized deformation (shear bands) in different kinds of disordered materials under shear is studied in the context of a mesoscopic model of plasticity. The model allows us to include relaxational (ageing) effects. In the absence of relaxational effects the model displays a monotonically increasing dependence of stress on strain rate, and stationary shear bands do not occur. However in start-up experiments transient (although long lived) shear bands occur, that widen without bound in time. I investigate this transient effect in detail, reproducing and explaining a $t^{1/2}$ law for the thickness increase of the shear band that has been obtained in atomistic numerical simulations. Relaxation produces a negatively sloped region in the stress versus strain-rate curve that stabilizes the formation of shear bands of a well-defined width, which is a function of strain rate. Simulations at very low strain rates reveal a non-trivial stick–slip dynamics of very thin shear bands that has relevance in the study of seismic phenomena. In addition, other non-stationary processes, such as stop-and-go, or strain-rate inversion situations display a phenomenology that matches very well the results of recent experimental studies.

Keywords: granular matter, slow dynamics and ageing (theory), plasticity (theory)
1. Introduction

The mechanical response of amorphous materials is a mix between solid- and liquid-like behavior. At low applied stresses they typically display recoverable elastic behavior, but they deform plastically when some yield stress is overpassed. The variety of systems that fit into this description is very large, comprising foams and emulsions [1], colloidal suspensions [2], granular matter [3] and metallic glasses [4]. The theory of the flowing state of these materials has developed more slowly than that of the crystalline counterpart, the reason being that, for the crystalline state, there is a clear definition of a reference state onto which defects responsible for plastic flow, namely dislocations, are identified. Thus, for a long time, theories describing the energetics and dynamics of dislocations have been available. For amorphous materials there is no such reference state and there is no obvious definition of the kind of generalized defects that contribute to the plastic behavior.

In the last few years, a theory of the plastic deformation of amorphous materials has become fashionable. This is the shear transformation zone (STZ) theory [5]. It is based in early ideas by Bulatov and Argon [6] that plastic flow can be decomposed by a large amount of local plastic rearrangements that are spatially coupled through the constitutive elastic properties of the material, and that are able to generate large global deformations when summing up their individual contributions. The goal of STZ theory has been to provide rate equations for the temporal evolution of the number of STZs as a function of time, and to show that the results are compatible with many experimental results under a variety of conditions.

One of the most ubiquitous effects in the plastic deformation of amorphous materials is strain localization. In very general terms, it refers to the coexistence of flowing and stacked, or jammed, regions within a single piece of material under the action of an externally imposed stress or deformation rate. This effect is of great experimental importance, and it has been described in most of the realizations of amorphous materials mentioned before: complex fluids [7, 8], metallic glasses [9], granular materials [10]–[12] and foams [13, 14].

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In most of the experiments that have been presented so far, the localization is studied under stationary loading conditions. Yet in this situation the sample is typically not spatially homogeneous, and the question of to what extent the observed strain localization is induced by a non-homogeneous geometry is a very delicate one. A particular geometry is illustrative in this respect. In the so-called split-bottom experiment \cite{11,15}, a Couette cell formed by two concentric cylinders rotating relative to each other is complemented by the inter-annular bottom between the two cylinders being split, with the inner (outer) part being rigidly attached to the inner (outer) cylinder. A granular material placed in the inter-cylinder region then naturally develops a shear band that starts at the position of the split line at the bottom. However, it is observed that the transition region between material moving with the inner or outer cylinder becomes progressively wider as upper layers of material are observed. This widening is, in principle, unbounded, indicating that, in this case, a localized shear band is only induced by the particular boundary conditions by which the system is driven.

Another interesting case of a shear band induced by a ‘boundary effect’ has been observed in the numerical simulations of Lennard-Jones systems by Shi \textit{et al} \cite{16}. In this case, the use of periodic boundary conditions and homogeneous applied deformation makes the system strictly homogeneous, but the analysis of the starting of deformation from a rest situation shows that shear bands appear and become progressively wider at longer times, until they eventually involve the whole system. In this case, strictly speaking, strain localization is a transient phenomenon, although it can last for quite a long time.

In both of the previous examples, the existence of a localized shear band is either a transient effect in time or a localized effect in space. A natural question is thus if there are cases in which a ‘persistent shear band’, i.e. an infinitely long-lived, finite-width shear band, exists in a homogeneous spatial configuration. This question poses from the beginning difficult experimental challenges, since a perfectly homogeneous geometry is not realizable and we have to rely on interpretations of non-homogeneous configurations. For instance, a cylindrical Couette cell tends to localize the strain close to the inner cylinder because of a simple stress reinforcement mechanism due to the geometry of the system. In this case, persistent shear banding has to be searched for in the detailed form of the angular velocity of the material as a function of distance from the center \cite{8}.

Indirect signatures of persistent shear banding can be searched for in the bulk stress versus strain-rate curve of the material. In fact, materials having a part of this curve with a negative slope are known to be unstable under uniform shear, and a phase separation occurs in which the system develops two regions, one of high and another of low shear rate, very much as in the coexistence regime of first-order phase transitions. It is clear that a negative slope in the stress versus strain-rate curve is a sufficient condition for the existence of persistent shear bands. Whether it is also necessary I think is an open question.

Recently, Manning \textit{et al} \cite{17} have shown that the results by Shi \textit{et al} \cite{16} (in particular the time increase of the shear band width) can be well fitted with results from the STZ theory, which thus is capable of describing the existence of transient shear bands. The application of the STZ theory to the case of persistent shear bands has not been done in detail, although it is argued in \cite{18} and \cite{19} that it requires the introduction of relaxation effects that can be incorporated in more than one way \cite{19}.

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An alternative (or perhaps complementary) theoretical description of the plastic flow of amorphous materials has been proposed in [20]. In that work, I used a mesoscopic approach that (in its unrelaxed version) is conceptually similar to the original Bulatov and Argon ideas [6], and more recent extensions, such as that due to Baret et al [21,22]. The system is modeled as a collection of mesoscopic pieces that evolve in a disordered energy landscape with many equilibrium configurations. All pieces have to fit together to satisfy strain compatibility, and this generates an additional elastic energy in the system and long range elastic correlations. Upon the external shearing, pieces of material jump between different minima of its potential energy landscape, affecting in this process the elastic state of neighboring pieces, due to the compatibility condition. With this model I have been able to describe, for instance, the flowing properties of a granular material placed in the split-bottom Couette cell geometry [23]. However, the point that really motivated the presentation of the model in [20] was the possibility to introduce, in a simplified but fully consistent manner, structural relaxation (or ageing) in the system. This was introduced as a mechanism that dynamically tends to make stresses uniform within the system. It was shown in [20] that the introduction of this mechanism of structural relaxation generates a region of negative slope in the stress versus strain-rate curve, and that persistent shear bands appear naturally in the model.

In this paper I extend the use of this alternative approach to describe the plasticity of an amorphous material to show that this modeling is able to reproduce most of the phenomenology of shear bands described in the previous introduction. In particular, after a self-contained description of the model in section 2, I show in section 3 that, in the absence of relaxation, the model describes the existence of transient shear bands that widen in time as $t^{1/2}$, and I discuss the conditions for this effect to be observable. In section 4, I present results for finite relaxation in the limit of very low applied strain rates, focusing on the appearance of stick-slip dynamics that is relevant for geological applications. In section 5, I describe some non-stationary effects associated mainly with the rapid inversion of the stress applied to the system, showing that also in this case the results compare very well with the outcome of recently presented experiments. Finally, in section 6, I summarize and conclude the presentation.

2. Details of the model

For the convenience of the reader, I give here a self-contained presentation of the model, based on [20] (additional information can be found there). I model a (two-dimensional) amorphous material at a mesoscopic level using the (symmetric) linear strain tensor

$$\epsilon_{ij} = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2,$$

with $u_i$ ($i = x, y$) being the components of the two-dimensional displacement field. For convenience I introduce the three independent variables $e_1 = (\epsilon_{11} + \epsilon_{22})/2$, $e_2 = (\epsilon_{11} - \epsilon_{22})/2$ and $e_3 = \epsilon_{12}$ in such a way that $e_1$ is related to volume changes, while $e_2$ and $e_3$ are the two independent shear distortions.

The three variables $e_1$, $e_2$ and $e_3$ are not independent; instead they are related by a so-called compatibility condition that can be written as

$$(\partial_x^2 + \partial_y^2)e_1 - (\partial_x^2 - \partial_y^2)e_2 - 2\partial_x\partial_y e_3 = 0. \quad (1)$$

This constraint is responsible for generating long range elastic interactions in the model.
In addition to the elastic compatibility condition, the response of the system is dictated by the form of the local free energy \( f(e_1, e_2, e_3) \), from which the total free energy \( F \) is calculated by spatial integration. To model plasticity I have used a form for \( f \) with minima at a set of positions in the plane \((e_2, e_3)\). This means that there is a set of discrete deformations at which the system is locally relaxed. The jump between different minima as the system is driven externally by shear will be the elemental plastic events of the model. Specifically, \( f \) will have the form
\[
 f = f_0(e_2, e_3) + B e_1^2. \tag{2}
\]
The dependence of \( f \) on \( e_1 \) has been assumed to be simply quadratic, since the plastic effects I am interested in are associated with shear, and not to volume changes. The function \( f_0 \) describes the energy landscape in the \((e_2, e_3)\) plane, which should have minima in different positions. The scheme adopted in [20] and also used here, consists in choosing \( f_0 \) as a sum of harmonically oscillating terms with different wavevectors and phases in the \((e_2, e_3)\) plane. The exact form of the function \( f_0 \) can be seen in [20]. As the locations of the minima in the \((e_2, e_3)\) plane do not coincide in different spatial positions of the system, due to the compatibility condition (equation (1)), spatial fluctuations in the local stresses will typically be present.

The dynamical evolution of the strains is assumed to be overdamped. This is reasonable for sufficiently slow external variations of the control parameters, particularly the strain rate. To be concrete, defining the local principal stresses \( \sigma_i \) as
\[
 \sigma_i(x, y) = -\frac{\delta F}{\delta e_i(x, y)}, \tag{3}
\]
the dynamical evolution of the strain is obtained through a first-order temporal evolution equation of the form
\[
 \frac{\partial e_i(x, y)}{\partial t} = \eta \sigma_i(x, y) + \Lambda_i(x, y, e_i, t), \tag{4}
\]
where \( \Lambda_i \) is a Lagrange multiplier chosen to enforce the compatibility constraint and \( \eta \) sets the timescale. In equilibrium \( (\partial e_i(x, y)/\partial t = 0) \), this equation reduces to the standard elastic equilibrium equations, namely \( \partial / \partial x_i (\delta F / \delta e_{ij}) = 0 \).

Structural relaxation, which is a key ingredient in the model, is introduced as an additional mechanism of free energy minimization in the system. In the present model, structural relaxation is a relative shift of the local energy landscapes at different spatial points, which tends to reduce the total free energy. We may think that in a real system this kind of mechanism should exist as a consequence of thermal fluctuations, which allow different parts of the system to adapt dynamically, through activated processes, and reach more stable global configurations.

To obtain this effect, a couple of additional fields \( e_2^0(x, y) \) and \( e_3^0(x, y) \) are introduced in order to get a rigid relative displacement of the energy landscapes in different spatial positions by changing the function \( f_0 \) according to
\[
 f_0(e_2, e_3) \rightarrow f_0(e_2 - e_2^0, e_3 - e_3^0). \tag{5}
\]
The tendency towards more relaxed configurations will be modeled by the dynamical evolution of $e^0_2$ and $e^0_3$. In the simplest possible approach this evolution will be chosen to be

$$\frac{\partial e^0_i(x, y)}{\partial t} = \lambda \nabla^2 \delta F \delta e^0_i(x, y) \quad (i = 2, 3).$$

The dynamics of the $e^0_i$ will be assumed to be much slower than that of the $e_i$s. In a situation in which externally applied strains are fixed in time and uniform in space, evolution through (4) and (6) produces eventually a configuration in which the principal stresses $\sigma_i$ (and also the usual stress tensor of the system) become uniform throughout the system. In this state the system has reached its most relaxed configuration locally available.

The results to be presented were obtained in system periodic boundary conditions, upon the constraints that $\bar{e}_1 = \bar{e}_3 = 0, \bar{e}_2 \equiv \varepsilon$ (where the bar denotes spatial averages over the system), except in section 4, where for convenience I use $\bar{e}_1 = \bar{e}_2 = 0, \bar{e}_3 \equiv \varepsilon$. Then $\varepsilon$ is the main control parameter, which represents a shear strain (I will call it simply ‘strain’ from now on). The reported stress $\sigma$ is defined as $\sigma \equiv \bar{\sigma}_2$. Dimensionless units are used for all quantities by choosing $B = 1.5, \eta = 1$, and measuring lengths in units of the numerical cell size, which is denoted $a_0$. When necessary, the shear strain rate $\gamma$ is defined in such a way that $\varepsilon = \gamma t$. Now I will apply this model to some particular cases.

3. Nucleation and widening of shear bands in the absence of relaxation

In this section I concentrate on some properties of the model obtained in the absence of relaxation. In this case, the equilibrium stress versus strain-rate curve is monotonically increasing (see [20], figure 3, for instance) and persistent shear bands under homogeneous spatial conditions do not occur. However, there is still room for interesting and experimentally very relevant phenomena associated with the presence of transient (although typically long lived) shear bands. In fact, shear bands can appear in the first stages after a strain rate is applied, depending on the initial conditions of the sample. For an amorphous material, sample preparation may involve the quench from a melt at some cooling rate. The characteristics of the sample obtained are thus dependent on this cooling rate. Typically, lower cooling rates give the system more time to reach a more relaxed configuration which makes it more reluctant to shear. In fact, we will see that a relaxed initial configuration produces a yield stress peak in the stress versus strain relation. In the language of our model, in order to get an initial configuration with different degrees of relaxation, I will prepare the starting sample by choosing an initially random configuration and letting the relaxation term act during some time $t_w$, before shear is applied. Once the sample is prepared in this way, I set the relaxation parameter $\lambda$ to zero in equation (6), apply a strain rate $\gamma$ and observe the evolution of the system. An example of the type of curves that are obtained is shown in figure 1. The applied strain in this case is of type $e_2$, corresponding to a combination of shear distortions at $45^\circ$ on the coordinate axis. The stress reported in figure 1 is the one corresponding to this symmetry. Note that a very similar phenomenology has already been obtained by Bulatov and Argon [6] when starting their simulation on more ordered initial configurations. They also showed how
Figure 1. Stress–strain relation for an unrelaxed sample and for a sample allowed to relax during a time $t_w = 5000$ under a relaxation parameter $\lambda = 0.01$. The strain is increased linearly in time, as $\varepsilon = \gamma t$, with $\gamma = 2 \times 10^{-4}$. System size is $128 \times 128$; other parameters as in [20].

plastic deformation starts around the maximum of the stress versus strain curve and how shear bands develop as the stress tends towards its asymptotic value. However, they did not follow in detail the widening of shear bands upon deformation.

I discuss now the development of plastic deformation in the system for the unrelaxed starting sample and for the relaxed one. Let us concentrate first on the unrelaxed curve in figure 1. This curve does not present a stress peak. Plots of the spatial distribution of the strain deformation (figure 2) show how the plastic deformation occurs throughout the whole sample on average. However, note that in the small strain intervals plotted in figure 2 the plastic deformation looks correlated and this might be taken as a signature of strain localization. This interpretation has been given, for instance, in [22] but I think it is not correct. The signatures of localization shown in figure 2 can possibly be considered as precursors of a localization that, however, does not take place. To observe localization (although still transient) we have to analyze the corresponding results for the relaxed initial sample. Spatial distribution of plastic deformation is seen for this case in figure 3. It is observed that plastic deformation initiates close to the maximum of the stress curve and that the spatial regions in which plastic deformation occurs are well defined and conserved during a large strain interval.

The qualitative difference between the two cases produced by the initial relaxation has to be emphasized. Remember that the relaxation mechanism acts by trying to make uniform the values of the stress through the sample. For a relaxed starting sample, the yield stress is larger than the flowing stress. When the strain is such that the stress on the sample is reaching the yield stress value, some part of the sample fails and starts to flow. This flowing part creates a shear band\(^1\) in the system, and now the stress decays to the flowing value throughout the sample due to a condition of mechanical equilibrium. This

\(^1\) The appearance of one or more shear bands in the system in this case seems to depend on particular conditions associated with the fluctuations of stresses across the whole sample. The expectation is that a larger stress rate will produce, on average, more shear bands.
Figure 2. Local accumulated strain, in the strain intervals indicated on top of each plot, for the unrelaxed initial state. Each plot shows the local accumulated values $\Delta \varepsilon(x, y)$ according to the grayscale on the right. Although there is evidence of correlated plastic rearrangements, there is no evidence of shear banding, since on average the full system participates equally in the total plastic deformation.

includes the regions that did not start to flow (thus, that retain the high yield stress of the initial sample), implying that the sample separates into a part that is flowing and a part that is jammed and that has a yield stress higher than the actual stress. This image is consistent with an analysis of stress in the relaxed and unrelaxed cases (figure 4). The local stress in the starting relaxed samples is much more uniform than in unrelaxed samples (remember I described relaxation precisely as tending to make stress uniform across the system), and this indicates a higher yield stress. Once the shear band has formed, stress acquires large fluctuations within the shear band, but remains smooth outside it, i.e. the region outside the shear band maintains the high yield stress of the starting sample, whereas the band is shearing at the lower flowing value of the stress. In these conditions it seems that the jammed part should be persistent in time, the shearing occurring only in the spatially limited shear band. In fact we observe the plastic deformation to be spatially localized for a rather large deformation range. However, eventually the flowing regions take over the whole sample. The evolution between localized and homogeneous flow seen in figure 3 occurs by a mechanism consisting of a progressive widening of the shearing regions in time. This is a very interesting effect that was observed unambiguously in atomistic simulations in Lennard-Jones systems [16]. Note that in that case a peak in the
stress versus strain curve was, in fact, observed (originating in the way the sample was prepared) so the phenomenon is probably similar to the one we are observing here.

In principle, mechanical equilibrium is compatible with any width of the shear band. The reason for shear band widening seems to be a dynamical effect at the interface between shearing and jammed regions. Below I will provide some qualitative arguments for the origin of this effect. Assuming by now that the effect exists, it is remarkable that the functional dependence of shear band width with time can be predicted on very general arguments. Consider a sample in which a shear band of width \( w_0 \) exists at \( t = 0 \), and in which an average strain rate \( \gamma \) is being externally applied. The problem that is being considered is athermal, and for a sufficiently low strain rate the evolution is quasistatic, implying in particular that there is no internal timescale set by the system itself. This means that the velocity \( v \) at which the border of the shear band advances (i.e. half the rate at which its width \( w \) increases) must be dependent only on the local state of the interface between flowing and non-flowing regions. The only dynamic parameter that can be unambiguously defined around this interface is the local strain rate \( \gamma_{\text{loc}} \) within the shear band, which is given by \( \gamma_{\text{loc}} = \gamma D/w \), where \( D \) is the total width of the sample.
Figure 4. Grayscale plot of the spatial stress distribution $\sigma(x, y)$ (calculated using equation (3), with $i = 2$) for two different values of strain, for the unrelaxed (upper panels) and relaxed (lower panels) initial configurations. The effect of relaxation in the initial configuration ($\varepsilon = 0$) is clearly seen by the uniformization of the stress across the system. The relaxed state has a larger yield stress than the unrelaxed state, where much larger stress fluctuations exist. For the flowing configuration ($\varepsilon = 5$), stress fluctuations occur everywhere for the unrelaxed sample, whereas they remain low outside the shear band for the relaxed sample (compare the last panel with the corresponding plot of strains in the previous figure).

Thus, dimensional arguments indicate that $dw/dt$ is proportional to $\gamma_{\text{loc}}$ (no other dependence can be constructed in the absence of additional parameters), i.e. we get

$$\frac{dw}{dt} = AD\gamma/w,$$

where a proportionality constant $A$ has been introduced. By integrating we obtain

$$w = \sqrt{w_0^2 + 2AD\gamma t},$$

where I have set $w = w_0$ for $t = 0$. The product $\gamma t$ is the average strain $\varepsilon$ applied to the sample, i.e.

$$w = \sqrt{w_0^2 + 2AD\varepsilon}.$$
The constant $A$ is a length that characterizes the material. We should expect $A$ to be a typical length in our system. The only such value in the present case is related to the typical size of the particles (or the mesh size, in the simulations), that I called $a_0$. In addition, the appearance of the strain $\varepsilon$ in equation (9) is not totally satisfactory, as the strain scale can be easily modified in the model. This is particularly obvious in the equations of the mesoscopic model, where it is seen that the only sensible values for the strain are those measured with respect to $\varepsilon_0$, which is the typical strain at which plastic events start to occur ($\varepsilon_0$ can be defined as the value at which the peak in the stress–strain dependence is observed). This means that we can conveniently set the value of $A$ to

$$A = B a_0 / 2 \varepsilon_0$$

(10)

where $B$ is a non-dimensional numerical constant, expected to be of order one.

From equation (10) we see that, given a shear band with some initial width $w_0$, the additional shear strain needed to increase its width by an amount $a_0$ is $\Delta \varepsilon \sim \varepsilon_0 w_0 / D$, i.e. an additional shear strain of order $\varepsilon_0$ needs to be applied inside the shear band for this to thicken by the order of one particle diameter. It is clear that this widening rate may be hardly observable experimentally for shear bands that are already much wider than the atomic size $a_0$.

In the present mesoscopic plastic model, the shear band widening occurs precisely in the way just sketched. This widening is observed, for instance, in figure 3. However, to quantitatively check the prediction contained in equation (10), we face the problem that, when the shear bands initially form, there may be a number of them and the time evolution of the width is not accurately defined. To overcome this situation, and in order to check quantitatively the widening law, I rely upon the following trick. A shear band of a well-defined width can be stabilized if the structural relaxation applied to generate the initial configuration does not act in a certain region in which we expect to create the shear band. I thus act with the structural relaxation mechanism during some time $t_w$ in the absence of any strain, to set up the starting configuration, and after that, relaxation is set to zero and the strain rate is applied. Figure 5 shows the time evolution of the shear band width for two different values of the time $t_w$ during which relaxation acted during the preparation stage. The linear trend in time of $w^2$ is a verification of equation (10). The same kind of temporal dependence can be extracted from the data presented in [16], figure 3. The numerical value of $B$ turns out to be slightly dependent on $t_w$, corresponding to a more rapid widening for the case of lesser relaxation, i.e. a slightly more rapid widening for a less relaxed sample, which is a reasonable effect.

The previous arguments suggest that, assuming the shear band widening effect exists, it has to follow the previous analytical expressions. But the question remains of why the effect exists at all. In fact, by definition the flowing region in the material has a stress which is the flowing stress value and this region can in principle be in mechanical equilibrium with a non-shearing and more relaxed region, loaded at the flowing stress value, which is slower than the yield stress. I can only speculate that the reason for widening lies in some sort of fluctuations occurring in the interface of the flowing and non-flowing regions: if because of some fluctuation in the dynamical state of the system some part of the flowing region becomes temporarily stuck, it can immediately resume flow when the fluctuations in the conditions vanish. On the other hand, if some part of the non-flowing region starts

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Figure 5. Evolution of the shear band width with time in a sample that has been relaxed initially during a time \( t_w \), as indicated, with a relaxation coefficient \( \lambda = 0.01 \). After this preparation step, the strain rate applied is \( \dot{\gamma} = 2 \times 10^{-4} \). The evolution follows accurately the theoretical expectation contained in equation (10). The value of the coefficient \( B \) used to fit the dependence in equation (10) shows a slight decrease when \( t_w \) increases.

to flow because of the fluctuation, it loses its high yield stress and is likely to continue flowing even if the fluctuations that originated it vanish.

While the theoretical description given here of the shear band widening effect is compatible with the numerical simulations presented, and with the findings in [16] using atomistic simulations, I am not aware of experimental situations where this widening has been observed. As I mentioned above, the rather small rate of shear band widening for bands already much wider than some atomic distance may produce that the effect is difficult to be experimentally observed, and more careful investigations are needed.

4. Thin shear bands: stick–slip dynamics in the presence of relaxation

I have emphasized the crucial role played by a negatively sloped stress versus strain-rate curve in producing a persistent shear band in the system. In addition, geophysicists have known for a long time [24, 25] that this negatively sloped curve is a fundamental ingredient for the seismic processes that occur when two tectonic plates slide against one another. In fact, they call this effect ‘velocity weakening’ and take it as a necessary condition for the instabilities that produce earthquakes. What is the relation between persistent shear bands occurring in velocity weakening systems and the earthquake phenomenon? In this section I will discuss the scenario that emerges from the present model. Note that a similar analysis on the basis of STZ theory has been made in [26] and that a model based on the ideas of structural relaxation presented here has been devised and applied specifically to seismic phenomena in [27] and [28].

It was indicated that the mesoscopic model in the presence of relaxation produces a stress versus strain-rate curve with a region of negative slope. The mechanical instability associated with this negative slope produces the rupture of spatial homogeneity in the
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system and the appearance of persistent shear bands, as was described in [20]. In the presence of this shear band, the global stress versus strain-rate behavior of the system acquires a plateau, in which a change in strain rate does not produce a change in stress, but it is accommodated through a change in the shear band width. This mechanism is very much in parallel with the coexistence of liquid and gas phases upon a change of volume when crossing the liquid–gas first-order phase transition. In this way the mechanical stability of the system is regained and the shear band width adjusts to the value of the externally imposed strain rate. In addition, the sliding is smooth, in the sense that stress fluctuations during sliding do not scale with system size and are associated with the individual plastic arrangements of the system constituents. However, this picture breaks down at sufficiently low strain rates, as we will now see.

In fact, if the applied strain rate diminishes, the mechanical equilibrium conditions indicate that the width of the shear band has to decrease accordingly. But there is a limit to this possible decrease. Experimentally, a shear band cannot be thinner than a few diameters of the constituent particles in the system. In the mesoscopic model itself, the minimum width cannot be lower than a few cell sizes of the numerical mesh. In any case, when this limit is reached, the uniformly sliding solution must break down. The route that the system follows in these conditions is the following [20]: at very low strain rates the thickness of the shear band saturates to a small fixed value and sliding proceeds as a sequence of stick-and-slip events. Clear evidence of this stick–slip regime has been obtained in atomistic numerical simulations in [29]. One of the macroscopic manifestations of this qualitative change is the fact that stress fluctuations in the system become progressively larger as the strain rate diminishes.

Before showing the concrete results in the case of the present mesoscopic model, let me point out that I choose in this section to work with a system that is not square, but rectangular, and in a case in which the external deformation applied corresponds to a deformation of type $e_3$. This, in principle, generates shear bands that run horizontally or vertically, and due to the non-equivalency created by the rectangular geometry they systematically appear along the shortest length, in our case the horizontal direction. This simplifies the presentation of the results a bit, and is more convenient for a description in which a friction process (in the limit of very thin shear bands) is the main concern.

The main results of this section are contained in figures 6 and 7, that correspond respectively to a larger and a slower value of the applied strain rate. For the case of the larger strain rate (figure 6), we observe the existence of a relatively thick shear band. The stress $\sigma$ in the system as a function of time (lower panel) is rather smooth in this case. I also plot in figure 6 the value $\delta \dot{\varepsilon} \equiv \langle \dot{\varepsilon}(x, y) - \gamma \rangle^2$ (the bar indicates spatial average) of the spatial fluctuation of the instantaneous strain rate for a case of uniform sliding. This quantity should be almost constant in time, and this is in fact what is observed.

For the case of a much lower strain rate, the corresponding results are presented in figure 7. Now the stress in the system acquires a larger temporal fluctuation, with periods of consistent increase and others of sharp decreases, namely a typical stick–slip pattern. In fact, the intervals of linear increase of stress are correlated with periods in which spatial strain-rate fluctuations are almost absent (indicating a rigid deformation of the whole sample), whereas abrupt stress decreases correlate with large spatial strain fluctuations (corresponding to the coexistence of regions that flow and others that do not). This is also qualitatively seen in the plots of accumulated deformation (the snapshots) in figure 7.
Figure 6. Four snapshots of the local accumulated deformation $\Delta \varepsilon(x, y)$ in the system for four different strain intervals (indicated in the lower panel) for a simulation with relaxation parameter $\lambda = 0.005$ and a strain rate $\gamma = 0.01$. We observe the existence of a persistent shear band of a rather well-defined width, which however wanders around the system as a function of time. The instantaneous stress $\sigma$ and the instantaneous spatial fluctuation of strain rate $\delta \dot{\varepsilon}$ are shown in the last panel. System size is $64 \times 128$.

A remarkable characteristic to be noticed in the dynamics of the system is the fact that the average spatial location of the shear band is not constant over time, but tends to diffuse in the system. This is seen in the plots of accumulated strain in figures 6 and 7. In the case in which the shear band is thick and the sliding uniform (figure 6), this movement is, in fact, a sort of diffusion of the mean position of the shear band. Runs at doi:10.1088/1742-5468/2010/12/P12025
Figure 7. Same as the previous figure for a lower value of the applied strain rate, namely $\gamma = 0.002$. A typical pattern of stick–slip dynamics is apparent, with periods in which the system is almost completely blocked (in the ‘B’ interval, for instance) and others with rapid, localized deformation. Note also how these localized slips do not occur necessarily at the same spatial position, but can jump between different places (compare ‘C’ and ‘D’, for instance).

different strain rates indicate that the tendency to diffuse becomes stronger as the shear band becomes thinner. In the case of stick–slip motion, the shear band movement can involve a more drastic situation. In fact, it is systematically observed that subsequent slip events can occur at well-separated spatial positions (compare, for instance, snapshots ‘C’ and ‘D’ in figure 7). In [26], Daub et al showed how strain localization (within the context of STZ theory) can induce the failing of geological gouge in a typical thickness much thinner than the gouge thickness itself. Here I am obtaining the same qualitative
results (the sample here can be considered to be the gouge material), with the additional indication that successive failures of the gouge can occur in different spatial positions. This could possibly be a relevant phenomenon to consider in the dynamic rupture process during earthquakes.

The results of this section show that the velocity weakening characteristic of the stress versus strain-rate response in the presence of relaxation manifests itself very differently for the case of larger or smaller strain rate: when the strain rate is relatively large, in such a way that the equilibrium width of the shear band is much larger than the mesh size (or particle size, for an experimental situation), the sliding is smooth, the expected instability of a velocity weakening system being cured in this case by the possibility to adjust the width of the shear band to the externally imposed strain rate. When the imposed strain rate becomes very small, in such a way that the equilibrium width of the shear band would nominally be smaller than the mesh size, the system enters a stick–slip regime as usually expected for systems with velocity weakening. The transition between the two regimes is seen not to be abrupt; instead, a smooth crossover is observed. In the limit of small strain rate in which the dynamics becomes stick–slip, the very thin resulting shear band can be treated essentially as two-dimensional and a specific model for this case has been devised and analyzed in [27] and [28]. It was obtained that this limit of the model reproduces many features of friction phenomena that were previously described by the so-called rate- and-state model of friction [24, 30]. This is encouraging, as in the rate-and-state formalism the relaxation mechanism is introduced in a purely phenomenological way, whereas for the present model, the ageing mechanism is based on a very general physical prescription of energy minimization as given by equation (6). More details on the frictional properties of the model and a comparison with the rate-and-state equations are contained in [27, 28].

Before closing this section, it may be useful to mention an apparently very different experimental problem with some similar phenomenology: the so-called Portevin–Le Chatelier effect in crystalline materials (mainly metals), in which dislocations may be temporarily pinned by impurities (see, for instance, [31] and references therein). The crystal separates into deforming and non-deforming phases, and the deforming bands may evolve in three different ways: (i) smooth propagation, (ii) periodic jumps on a well-defined distance or (iii) generation of new bands at random in the crystal which resembles in some way the behavior of shear bands observed here. The similarity is not by chance. The dislocation movement in the Portevin–Le Chatelier effect can be described by the same kind of ‘relaxational term’ that is included in the present model. A description of the Portevin–Le Chatelier effect using the present modeling is left for future work.

5. Application to shear reversal experiments

In recent times there has been some interest in analyzing the response of amorphous or granular materials to non-stationary stressing conditions. One particular case corresponds to an externally imposed flow condition that is stopped and then re-initiated, in the same or in the opposite direction. Asymmetries between the two cases are clearly detected experimentally [10, 32]. If the flow is stopped and re-initiated in the same direction, stress recovers immediately to the value prior to the flow stop. However, if flow is started in the opposite direction, there is a typical strain interval in which the stress increases smoothly before reaching the steady state value. Here I will show that these results are obtained
in the present model of plasticity, and also give a very simple description in terms of a mean-field analysis. In all this section, structural relaxation is set to zero, which means in particular that only transient strain localization phenomena can occur, but no persistent shear banding.

I will first consider a spatially homogeneous situation of uniform flow under a constant applied strain rate. Let us suppose that in these conditions the applied strain rate is suddenly reversed during some time. Upon this inversion the stress in the system has to revert eventually to minus its original value (the system is symmetric upon a change of sign of strain). However, the response of the system is not instantaneous. In figure 8 we see the evolution of stress upon this process, in two different cases. In the first case strain rate is inverted only up to point C where stress becomes zero, and then is re-initiated again in the original direction. In this case the system responds elastically, the strain reduces almost linearly with the decreasing strain, and recovers also linearly up to the original strain value when strain is increased again. Once at the original point, upon a further strain increase the stress continues at the same constant level it had prior to inversion. This kind of behavior can reasonably be termed ‘immediate recovery’ upon reloading. The second case corresponds to a permanent flow reversion. We see in this case how the stress reaches the asymptotic value (equal to minus the original one) rather smoothly, instead of what would be an immediate response, as indicated by the dotted line in figure 8. This kind of result, that has been interpreted in [32] in terms of ‘chain forces’ that are present in the system and that take some time to be rebuilt upon stress inversion, can be qualitatively understood using a simplified mean-field description of the model studied here, that I will now present.

Figure 8. Stress in the system in the absence of relaxation and under spatially homogeneous flow, upon inversion of the strain rate. For a reversion to a state of zero stress, and reloading in the same direction, the recovery of the original configuration is instantaneous beyond an elastic unloading–reloading effect. When the flow is reverted during a long time the stress reaches the negative of the original value following a smooth evolution (compared to an immediate recovery, as indicated by the dotted line), indicating that the system takes some finite strain interval to accommodate to the new flowing conditions.
Shear band dynamics from a mesoscopic modeling of plasticity

The mesoscopic plastic description of the present paper assumes a disordered energy landscape, independently chosen for every point of the system in the plane of the two shear distortions that are called $e_2$ and $e_3$. Let me now think in a simplified description in which we concentrate on a single type of distortion (I call it simply $\varepsilon$, for definition) and assume each elemental piece of the system behaves as an ideal plastic element as indicated in figure 9(a), i.e. the stress at each element increases linearly upon strain increase until a maximum stress $\sigma_0$ is reached, in which case a further increase of $\varepsilon$ does not increase the value of $\sigma$. Upon strain-rate inversion, stress goes down linearly to $-\sigma_0$ and remains there. Different spatial positions are assumed to have different values of $\sigma_0$.

Driving the system (through the mean value of $\varepsilon$, namely $\varepsilon_m = \langle \varepsilon \rangle$) produces a stress that is obtained as the spatial average of the local values, i.e. $\sigma = \langle \sigma \rangle$. The typical form of $\sigma$ versus $\varepsilon_m$ curve can be seen in figure 9(b). The smooth increase of $\sigma$ is due to the broad distribution of values of $\sigma_0$. If the driving is stopped (at point B of figure 9(b)) and strain reduced to the point of zero stress (C), the system retains a memory of the sense in which it was flowing, which produces the asymmetric response upon resuming deformation in the same or opposite direction. This is most clearly seen in the plots in figure 9(c), where the value of deformation of each element with respect to the mean value is plotted against its flowing stress value $\sigma_0$ (for simplicity, here I assume a uniform distribution of the values of $\sigma_0$ between $\sigma_0^{\text{min}}$ and $\sigma_0^{\text{max}}$). For a flowing state in one direction, the elements with larger values of $\sigma_0$ are lagged with respect to those with the smaller values, and this produces the anisotropy. When the flow is reversed, there is a transient in which this situation has to be rebuilt for the new flowing direction. There would not be any asymmetry if all elements have the same $\sigma_0$ value. This justifies the asymmetry observed in the simulations using the mesoscopic plasticity model, as in figure 8.

Another observation that has been made concerning flow inversion experiments is the fact that regions that are jammed during forward flow become more mobile during a transient period after inversion [10,32]. For instance, in [32] the case of the flow of a granular material in a Couette cell was analyzed. In a stationary regime, the angular velocity of the material is maximum at the inner cylinder and decays rapidly with radial distance (the external cylinder is at rest). Upon flow inversion, and during some time, the decay of angular velocity with radial distance is much slower and regions that were at rest participate in the flow, until the stationary situation sets in. Again this phenomenology is consistent with the present findings if we admit that we can represent the system as a collection of pieces having a stress versus strain ratio like that in figure 9(b) that are located at different distances $r$ from the center. We can analyze the response in the following way. Consider that the inner and outer cylinders are located at radial distances $r_1$ and $r_2$, and the angular velocity is fixed at them as $\omega$, and 0, respectively. Mechanical equilibrium implies that the product $r \sigma$ has to be constant across the system at every time, i.e. $r \sigma = C(t)$. According to the assumptions made, the value of $\sigma$ is a function (the one plotted in figure 8(b)) of the strain at the appropriate value of $r$. Noting that the strain can be written (up to a constant factor) as $r d\theta/dr$, we get

$$\sigma \left( r \frac{d\theta}{dr} \right) = \frac{C(t)}{r}$$

(11)
Figure 9. A mean-field interpretation of the flow inversion experiments. A collection of individual plastic elements with the stress versus strain characteristic shown in (a) is considered. The values of the flowing stress values $\sigma_0$ are broadly distributed for different elements. In (b) we see the average stress as a function of the average strain for a collection of elements as in (a). The stress increase is smooth due to the broad distribution of $\sigma_0$ in (a). In (c) the distribution of strains of the different elements $\varepsilon_i$ minus the average value $\varepsilon_m$ as a function of its flowing stress value is plotted for different points in (b). Note in particular how the distribution corresponding to point C keeps a memory of the flowing state prior to the flow stop: elements with smaller (larger) $\sigma_0$ have strain values larger (smaller) than the average. This justifies the asymmetry of the response upon resuming flowing in the original or in the opposite direction.
Figure 10. Angular velocity as a function of time at different radial positions in the Couette cell experiment, after inversion of rotation direction. The cylinder ratios are \( r_1 \) and \( r_2 = 2r_1 \). The curves were obtained assuming a local stress versus strain that is plotted in the inset (following the law \( \sigma(z) \propto z/(1 + z) \), \( z \equiv r(d\theta/dr) \)) and requiring mechanical equilibrium to hold. Note that, as \( t \to \infty \), the shear band becomes singularly localized at the inner cylinder.

so the instantaneous value of \( \theta(r) \) can be obtained by solving this equation for \( \theta \), which gives

\[
\theta(r) = \int_{r}^{r_2} \sigma^{-1}(C/r) \, dr/r
\]

where \( \sigma^{-1} \) is the inverse function of \( \sigma \). The time dependence of the \( C \) value is implicitly determined by the fact that the inner cylinder is rotated at an angular velocity \( \omega \), i.e.

\[
\omega t = \int_{r_1}^{r_2} \sigma^{-1}(C/r) \, dr/r.
\]

In figure 10 I show the result of solving the previous two equations for a particular form of the function \( \sigma(r \, d\theta/dr) \) (namely \( \sigma \equiv z/(1 + z) \), \( z \equiv r \, d\theta/dr \)) which is just a simple analytical possibility with the appropriate qualitative form, and we see how a transient of enhanced mobility is observed upon flow reversion. After this transient, velocity of all points except the inner cylinder decay to zero, as in this description the equilibrium shear band is singularly localized in the point of maximum stress\(^2\).

6. Conclusions

In this paper I have presented results that indicate that a mesoscopic theory of plasticity complemented, if necessary, with the inclusion of relaxational (ageing) terms is able to

\(^2\) Note that in the experiments in \([32]\) an equilibrium non-singular profile is obtained. This is associated with a material that has a stress that increases with strain rate. In the simple mean-field description given here stress does not depend on strain rate and the shear becomes singularly localized at the inner cylinder for long times.
reproduce much of the available phenomenology associated with plasticity in different kinds of amorphous materials. A summary of the different possibilities that have been described is the following. First of all, it has been argued that a persistent shear band (i.e. one whose formation is not associated with inhomogeneities of the experimental set-up, and that persists indefinitely with a well-defined width) can only exist for materials that have a part of the stress versus strain-rate curve with a negative slope. In my modeling, this condition is fulfilled only in the presence of structural relaxation. Under this condition a shear band forms in the system satisfying formally a sort of ‘Maxwell construction’, as occurs in coexistence regions of first-order phase transitions. In the present case the stress plays the role of the pressure (thus remaining constant at coexistence) and the shear band width plays the role of the relative fraction of the two coexistent phases. In this situation sliding is smooth. However, if the strain rate is so low that equilibrium shear band width would be smaller than some atomic length in the model, the sliding becomes of the stick–slip type. In this limit the model provides an interesting conceptual tool to study the characteristics of seismic phenomena [27, 28].

In all cases in which structural relaxation is absent and the stress versus strain-rate curve is monotonically increasing, a shear band can exist at most as a transient phenomenon or induced by particular inhomogeneous boundary conditions. I have discussed cases of these two possibilities: in one case, namely the split-bottom Couette flow configuration, the shear is stationary in time and the shear band is induced to appear at the split line in the bottom of the container. The width of the shear band increases as layers progressively away from the bottom are observed. The second case is a perfectly homogeneous spatial situation (obtained by the use of periodic boundary conditions) and a flow that is initiated at some fixed time. There are two possibilities in this case. If the initial configuration of the system was unrelaxed, regions of plastic deformation appear throughout the sample, the stress versus strain curve grows continuously to the asymptotic value and no sign of spatial strain localization appears. However, in the case in which the starting sample was relaxed, the stress versus strain curve develops a peak (the yield stress) and plastic deformation is localized in space, forming a shear band. This shear band, however, widens in time with a $t^{1/2}$ law that was explained in terms of the athermal and quasistatic nature of the process. Eventually, for very long times, the shear band broadens sufficiently to involve the whole system and deformation becomes spatially uniform. If in this homogeneous and stationary state, external deformation is stopped and then re-initiated in the same original direction, the stress recovers its original value almost instantaneously (beyond some elastic unloading–reloading stage). However, if deformation is re-initiated in the opposite direction, there is a reaccommodation stage during which the stress in the system grows smoothly before reaching its asymptotic value. This behavior was interpreted in terms of a simplified version of the mesoscopic plasticity model.

On a general perspective, I think that the present kind of modeling is an interesting alternative to other more microscopic approaches (such as, for instance, STZ theory) to study the different possibilities of the plastic deformation of amorphous materials. On the one hand, the results in the absence of relaxation have been shown to be compatible with different equilibrium and nonequilibrium phenomena, as the shear band widening described in [16] and the stress inversion experiments in [32]. On the other hand, the inclusion of relaxation terms opens new routes in the study of physical
properties of systems with velocity weakening features, in particular related to the seismic phenomena [27, 28].

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