Mechanical noise dependent aging and shear banding behavior of a mesoscopic model of amorphous plasticity

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We discuss aging and localization in a simple "Eshelby" mesoscopic model of amorphous plasticity. Plastic deformation is assumed to occur through a series of local reorganizations. Using a discretization of the mechanical fields on a discrete lattice, local reorganizations are modeled as local slip events. Local yield stresses are randomly distributed in space and invariant in time. Each plastic slip event induces a long-ranged elastic stress redistribution. Mimicking the effect of aging, we focus on the behavior of the model when the initial state is characterized by a distribution of high local yield stress values. A dramatic effect on the localization behavior is obtained: the system first spontaneously self-traps to form a shear band, which then only slowly broadens. The higher the "age" parameter the more localized the plastic strain field. Two-time correlations computed on the stress field show a divergent correlation time with the age parameter. The amplitude of a local slip event (the prefactor of the Eshelby singularity) as compared to the yield stress distribution width acts here as a mechanical effective temperaturelike parameter: the lower the slip increment, the higher the localization and the decorrelation time.

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I. INTRODUCTION

While metals are characterized by a low elastic limit and large deformation before failure, their amorphous counterparts, bulk metallic glasses (BMGs) are known for the exact opposite, high mechanical strength and low ductility. The propensity of plastic deformation in BMGs to localize and form shear bands is the main mechanism leading to mechanical failure. Understanding and thus controlling shear band formation is the main challenge that has so far limited the use of glasses as structural materials.[1,2]

Although plastic deformation may be responsible for significant heat production, recent experimental studies have shown that the origin of nucleation and propagation of shear bands could not be attributed to an adiabatic shear banding instability via local temperature rise.[3] In the absence of such a thermal softening mechanism, Falk, Shi, and collaborators have explored by molecular-dynamics simulations the hypothesis of a structural softening mechanism.[4] They showed in particular that shear banding was facilitated by a high degree of relaxation of the glassy structure.

They proposed an interpretation of this phenomenon in the framework of the shear transformation zones (STZs) theory[5] describing plastic deformation of metallic glasses as resulting of local inelastic transformations.[6] Let us recall that according to STZ theory plastic deformation is assumed to result from a series of local reorganizations occurring within a population of "small" atomic/molecular clusters (zones) through microinstabilities. Plastic deformation directly results from the balance between flips in the positive and negative directions of these shear transformation zones at a rate that depends on an intensive parameter (e.g., free volume or effective structural temperature). Shi and Falk could associate the shear band with a structural signature characterized by an effective temperature, reflecting a higher potential energy in the band than in the still surrounding. In a similar spirit, Manning, Langer, and collaborators[7] proposed an enriched version of the STZ theory able to capture strain localization. The introduction of a relaxation-diffusion equation of the effective structural temperature was in particular shown to induce shear banding in aged structure (low effective structural temperature) and/or high shear-rate conditions.

Independently, starting from the trap model developed by Bouchaud[8] for the glass transition, Sollich, Cates, and Lequeux[9] developed a soft glassy rheology (SGR) model to capture the rheology of complex fluids. In the trap model a landscape of traps of depth E drawn from an exponential distribution $\exp(-E/E_0)$ is assumed. A breakdown of ergodicity naturally emerges at $T_0 = E_0/k$. From this simplified view of the glass transition, Sollich *et al.* introduce the mechanical stress as a bias to the energy landscape. It is important to note that the temperature in their model is not associated to a real thermal bath but is assumed to emerge from some mechanical noise *a priori* related to elastic interactions induced by local reorganizations.

While STZ and SGR models capture part of the rich phenomenology of amorphous visco-plasticity, their mean-field character does not allow them to account for localization unless an additional ingredient is introduced. The latter can be the relaxation/diffusion of a state variable as discussed above and/or the inclusion of anisotropic elastic effect of local plastic events (Eshelby inclusion)[10] in the modeling.

Building on the latter grounds several authors have developed "Eshelby" mesoscopic models to study plasticity of amorphous materials.[11–17] Except in the case of Ref. 15 where a state variable is implemented or of Ref. 13 where the presence of walls traps plastic deformation, in such models, localization appears to be only transient and complex spatiotemporal correlations very similar to those observed in atomistic simulations emerge from the competition between diffusion and localization.[17,18]

Recently Fielding and collaborators[19,20] investigated an age-dependent transient shear banding behavior in different models where the shear banding was not triggered by an elastic or viscous softening constitutive law, but rather through an aging/rejuvenation behavior where the diffusive character of an internal variable would dictate the widening and progressive vanishing of an initial shear band. The introduction of such a mechanism in a variant of the SGR model results in a very slow ("glassy") spreading of such shear bands.

This age dependence of shear banding and its fast or glassy relaxation motivates us to reassess the question of the connection to be made between the glass theory inspired SGR model and the STZ model built from the identification of the microscopic mechanism of plasticity in amorphous materials. In particular, it has remained so far difficult to give a microscopic justification to the effective mechanical temperature defined in the SGR model.[4,21]

In the following we present results about aging and localization obtained with the original mesoscopic model of plasticity presented in details in Ref. 17. We discuss in particular the effect of two parameters of the model, which will appear to respectively mimic the age of the system before shearing and a mechanical effective temperature.

II. DEFINITION OF THE MODEL

Let us briefly recall the definition of the model (see Ref. 17 for more details). The mechanical fields are discretized on a square lattice with a mesh size significantly larger than the typical scale of a plastic reorganization. Periodic boundary conditions are considered. The material is assumed to be elastically homogeneous, so that stresses and elastic moduli are scaled so that the steady-state local yield stress is unity. A local criterion of plasticity is considered. The initial distribution of local yield stress is denoted $P_i(\sigma_c)$. Every time a local plastic criterion is satisfied at point $\boldsymbol{x}_0$, a local slip $\Delta\varepsilon_p$ occurs (we assume here that local plastic strains obey the same symmetry as the external loading, pure shear in the present case, so that a simple scalar yield criterion can be chosen) with a random amplitude d drawn from a statistical distribution $Q(d)$, $\Delta\varepsilon_p(\boldsymbol{x}) = d\delta_D(\boldsymbol{x}-\boldsymbol{x}_0)$ where δ_D is the Dirac distribution. Note that d is the product of the mean plastic strain by the "volume" of the transformation zone. This local slip d induces a long-range redistribution of elastic stress with a quadrupolar symmetry (see Refs. 17 and 22 for analytical and numerical details about this elastic propagator) $\Delta\sigma_{el}(\boldsymbol{x}) = dG(\boldsymbol{x}-\boldsymbol{x}_0)$ with $G(r,\theta) \approx Ad\cos 4\theta/r^2$ where A is the dimensionless elastic constant, r and θ the polar coordinates. The slip amplitude d is drawn from a uniform distribution in the range $[0;d_0]$.

After slip, the microstructure of the flipping zone has changed and a new value of the local yield stress is drawn from a distribution $P_S(\sigma_c)$. The system is driven with an extremal dynamics so that only one site at a time is experiencing slip. The originality of the present depinning models relies in the anisotropic elastic interaction. Within this framework of dynamic phase transition, the choice of extremal dynamics ensures to drive the system at the verge of criticality: the macroscopic yield stress is given by the critical threshold.

The above model may be seen as a depinning model for amorphous plasticity with a peculiar (anisotropic) elastic interaction. While the richness of the physics of the depinning models mainly relies on the competition between elasticity and disorder, we see here that the anisotropic character and the abundance of soft modes in the elastic interaction, which characterize the present model of amorphous plasticity, naturally induce an additional competition between localization and disorder.

An implicit assumption used in our model is that the statistical distribution $P_S(\sigma_c)$ used to renew the local plastic threshold under shear (i.e., after local slip) is the very same as the distribution of plastic thresholds in the initial configuration $P_i(\sigma_c)$. This hypothesis may be questioned. Indeed, various experimental and numerical results obtained in friction or in shearing granular material or complex fluids[4,23,24] seem to indicate an effect of the preparation of the material upon its behavior under shear. One may think, for instance, of the effect of density of granular material: a loose (dense) packing tends to exhibit hardening (softening) while under shear the density progressively evolves toward a so-called "critical" value.

In order to test the effect of our hypothesis we give in the following a bias to the initial threshold's distribution and try to test its consequences. Practically speaking, the yield stress distributions $P_i(\sigma_c)$ (initial state) and $P_S(\sigma_c)$ (under shear) are chosen as uniform in the ranges $[\delta;1+\delta]$ and $[0;1]$, respectively. A positive (negative) value of δ is expected to induce some softening (hardening) behavior since all threshold values above unity (below zero) should eventually be replaced by thresholds within the interval $[0,1]$.

We focus in the following discussion on the effect of these two parameters, d_0 and δ. In the view developed by Sollich *et al.*,[9] the parameter d_0, which gives the amplitude of the mechanical noise induced by the elastic interactions, may be thought of as analogous to the effective mechanical temperature x in the SGR model. However, it is to be emphasized that this mechanical "noise" is strongly inhomogeneous in space and displays strong temporal and spatial correlations, absent from the SGR model. The second parameter δ measures the shift between the initial yield stress distribution, that uniform in $[\delta;1+\delta]$, and the distribution of new local yield stress under shear, uniform in the range $[0;1]$ may be related to the initial state of the system prior to shearing. Indeed it is expected that the older the glassy system, the more stable and the more difficult it is to shear. This effect is described here through a mere penalty in the initial yield stress. High mean values of the plastic thresholds should thus be associated with aged configurations of the glass. As discussed in Ref. 25, a logarithmic increase of the yield stress with the age of the system is often observed in glassy materials: $\delta \approx s_0(T)\ln(t_w/t_0)$ where t_0 is a microscopic time scale. According to this perspective, the age of the system would simply be related to the bias δ through an exponential dependence. Yet another interpretation would consist of relating the parameter δ to a structural temperature as discussed in Refs. 4,7, and 26. The two quantities are expected to vary in opposite ways when the structure relaxes. The more relaxed the glass, the higher the δ and the lower the structural temperature. We now test these simple ideas against numerical simulations.

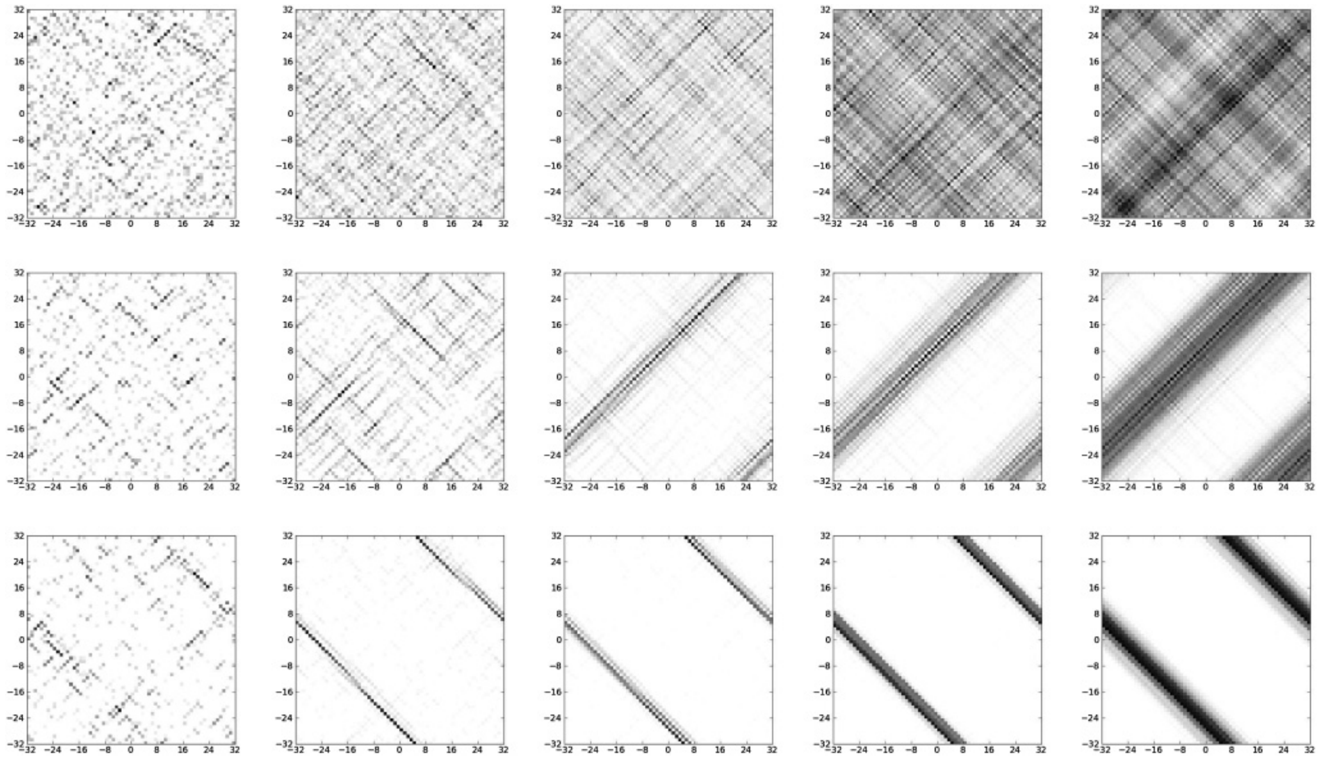

FIG. 1. Maps of plastic strain obtained from left to right at $\langle \varepsilon_p \rangle = 1/16$, 1/4, 1, 4, and 16 and from top to bottom with a bias value $\delta = 0$, 0.5, and 0.7 with a slip increment $d = 0.3$.

III. MAPS OF PLASTIC ACTIVITY

In Figs. 1 and 2 the evolution of the spatial distribution of plastic strain under shear is shown for different values of the agelike parameter δ (Fig. 1) and of the temperaturelike parameter d_0. We show snapshots of the plastic strain field taken at $\langle \varepsilon_p \rangle = 1/16$, 1/4, 1, 4, 16. The value of the local strain is represented with a gray scale (the darker, the larger the plastic strain).

In Fig. 1, the values $d_0 = 0.3$ of the slip increment has been used. The first row corresponds to the value $\delta = 0$. When using this unaged initial configuration, we see that plastic strain first self-organizes along shear bands at $\pm\pi/4$, i.e., according to the maximum shear directions. This localization is, however, not persistent and after a transient, these shear bands diffuse throughout the system. The evolution obtained with a bias value $\delta = 0.5$ (second row) is markedly different. Again plastic deformation first tends to form shear bands according to directions at $\pm\pi/4$, but remains essentially trapped in a strongly localized state. The formed shear band only slowly widens with "time" (mean plastic strain). The evolution obtained with a bias value $\delta = 0.7$ (third row) is very similar: formation of a persistent shear band before an apparent diffusive widening of the band. Localization appears to be more intense and widening slower with this higher value of the agelike parameter δ.

Let us only note here that the way the plastic activity gets localized along a band is somewhat reminiscent of the behavior of an earlier model proposed by Torok and Roux.[27] In this study, the authors made evidence for a weak breaking of ergodicity, which they relate to the progressive building in the threshold's landscape of a valley (along the shear band) surrounded by ridges elevating significantly above the base level. Plastic activity thus tends to be confined in the valley and can no longer fully explore the disordered landscape.

In Fig. 2, the values $\delta = 0.5$ of the agelike parameter has been used. From top to left, the evolution of the plastic strain field is shown for values of the slip increment $d_0 = 0.03$, 0.1, 0.3. A similar behavior as above is obtained. We see that the higher the value of the temperaturelike parameter d_0, the less intense the localization and the faster the subsequent widening process. Age and mechanical temperaturelike parameters δ and d_0 thus seem to behave as could be expected, at least phenomenologically.

IV. SLOW RELAXATION OF SHEAR BANDING

The residual stress field is the self-balanced stress field, which results from the local slip events taking place from the initial (stress free) state. The latter has a zero volume average. It allows one (in conjunction with the local random yield threshold) to characterize the propensity of a site to undergo a plastic slip. This motivates the recourse to standard tools used for aging behavior characterization. Two-point correlation functions based on the residual stress field are proposed:

$$C_\sigma(\varepsilon_w,\varepsilon_p) = \frac{\langle \sigma_{\text{res}}(\varepsilon_w,x)\sigma_{\text{res}}(\varepsilon_p,x)\rangle_x}{[\langle \sigma_{\text{res}}(\varepsilon_w,x)\sigma_{\text{res}}(\varepsilon_w,x)\rangle_x \langle \sigma_{\text{res}}(\varepsilon_p,x)\sigma_{\text{res}}(\varepsilon_p,x)\rangle_x]^{1/2}} \quad (1)$$

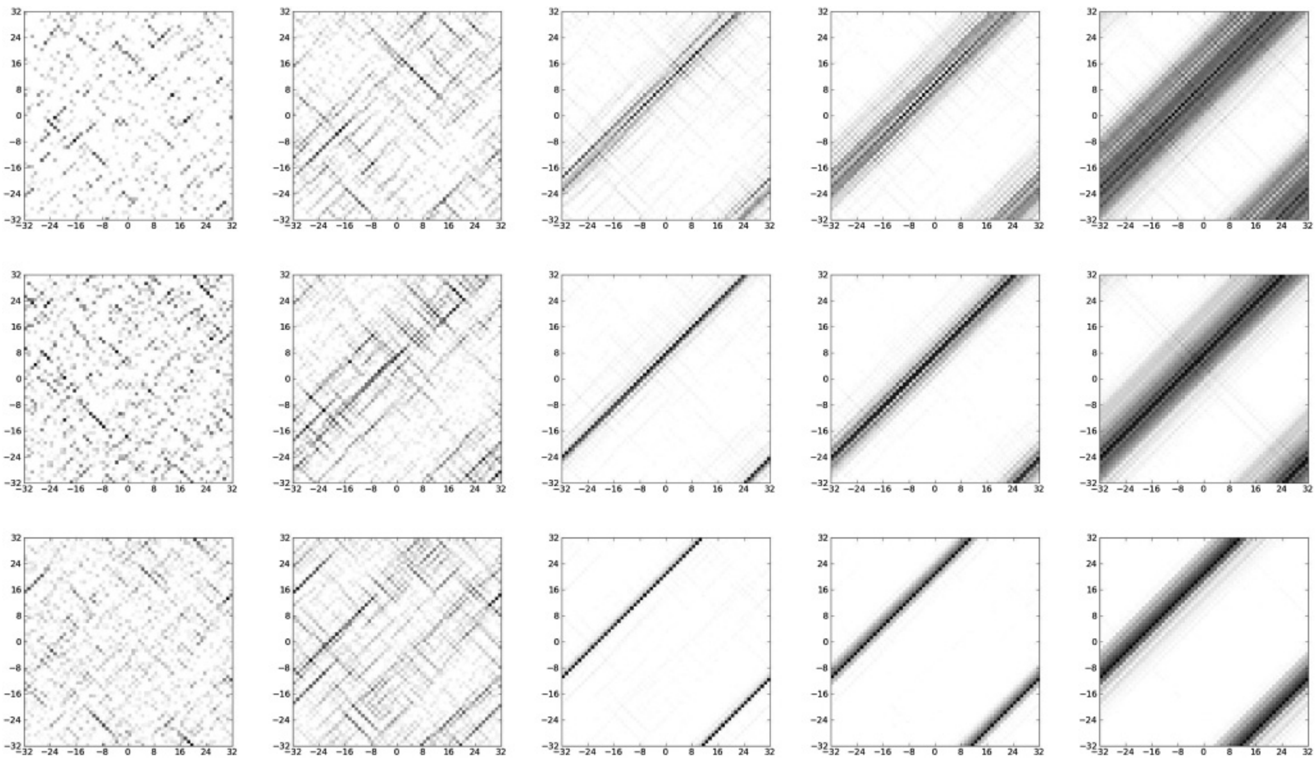

FIG. 2. Maps of plastic strain obtained from left to right at $\langle \varepsilon_p \rangle = 1/16$, 1/4, 1, 4, and 16 with a bias value $\delta = 0.5$, and from top to bottom with a slip increment $d_0 = 0.3$, 0.1, and 0.03.

where the symbol $\langle \cdots \rangle_x$ designates a spatial average over x. Note that the model does not depend on time as such; the global plastic strain plays the role of an evolution parameter.

Such two-point correlation functions can be used to follow the formation and the subsequent relaxation of shear banding.[28] In the following we only discuss the relaxation stage after the initial transient and full formation of the shear band. In Fig. 3 we present the dependence of the stress correlation for $\varepsilon_w = 1$; at this deformation level, which corresponds to the typical amplitude of the local plastic threshold, localization (if any) is fully set.

The left panel of Fig. 3 shows the effect of the "age" parameter, with $\delta = 0$, 0.2, 0.4, 0.6, 0.8, and $d_0 = 0.2$. In the unaged configuration ($\delta = 0$), the system decorrelates after a typical plastic strain $\varepsilon_p = d_0^{0.5}$. This reflects the nonpersistence of localization in the standard unaged case. In the case of an aged initial configuration we obtain significantly different results. The systems appears to decorrelate only after a plastic deformation growing exponentially with the parameter δ. Moreover, when fitting data with a simple stretched exponential, the exponent can be shown to transit from values slightly below unity in the unaged case to values close to or below 1/2 in the more aged configurations. The shear banding persistence thus seems to directly depend on the age.

Pursuing the above discussed analogy we now show in the center panel of Fig. 3 the correlation functions obtained with a fixed age parameter $\delta = 0.6$ for values of the slip increment

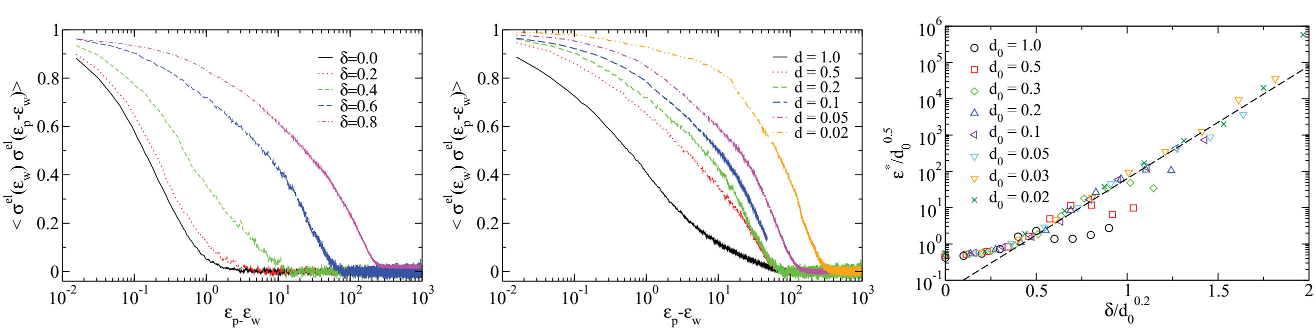

FIG. 3. (Color online) Effect of the agelike parameter δ (left) and of the mechanical noise amplitude d_0 (center) on the two-point stress correlation function with $\varepsilon_w = 1$. Right: Dependence on δ and d_0 of the typical plastic deformation ε^* needed to relax shear banding. After rescaling data can be reasonably collapsed onto a single master curve; the dashed line indicates an exponential behavior accounting for the glassiness of shear banding at high δ–low d_0.

parameter varying from $d_0 = 0.02$ to $d_0 = 1$ (computations were performed on lattices of size 64×64 with 20–200 realizations). As could be anticipated from the above displayed maps of plastic deformation, the shear banding persistence tends to increase inversely with the slip increment parameter, the lower the d_0 the higher the decorrelation time. The slip increment parameter d_0 thus seems reasonably to act as the amplitude of a mechanical noise allowing the system to escape its trapped state. In other words, d_0, which stands here for the product of the volume of a flipping zone times its typical plastic strain, seems to be a good candidate for the elusive effective mechanical temperature discussed in the SGR model.[9]

We try to rationalize in the right panel of Fig. 3 the age and mechanical noise dependence of the shear banding persistence. Exploring the two-dimensional space of parameters δ and d_0, using a simple stretched exponential fitting procedure, we extracted the typical plastic strain ε^* associated with stress decorrelation after shear banding formation ($\varepsilon_w = 1$ in the above notations). This allows us to propose a reasonable scaling dependence:

$$\varepsilon^* = d_0^a \varphi\left(\frac{\delta}{d_0^b}\right), \tag{2}$$

where

$$\varphi(x \to 0) \approx A \quad \text{and} \quad \varphi(x \to \infty) \approx Ce^{Bx}.$$

The choice $a = 0.5$ and $b = 0.2$ allowed us to obtain a reasonable collapse of the data collected for $d_0 \in [0.02, 0.03, 0.05, 0.1, 0.2, 0.5, 1]$ and $\delta \in [0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9]$. In Fig. 3 an indicative exponential curve is shown to account for the high age and/or low mechanical noise shear banding slow relaxation behavior.

V. CONCLUSION

To summarize, we showed that our simple Eshelby-like mesoscopic model of amorphous plasticity exhibits a striking dependence on initial conditions. The introduction of a simple bias to shift the initial distribution of local yield stress values from its counterpart used to renew the yield stress after local reorganization has a remarkable consequence: the system self-traps in a localized state to form a shear band and remains so for a longer and longer "time" when the bias value increases. This bias can thus be interpreted as an estimator of the age of the system before shearing or be related to some effective structural temperature.[26]

Moreover, we show that the ratio of the typical slip increment (more rigorously in the formalism of the Eshelby inclusion, the volume of a reorganizing zone times its typical plastic strain) on the typical plastic yield stress acts as an effective mechanical temperature in the sense proposed in the SGR model of Sollich *et al.*[9] This parameter indeed gives the amplitude of the mechanical noise induced by successive reorganizations. The lower this amplitude, the longer the systems gets trapped and the slower the widening of the shear bands.

In conclusion, the present depinning model of amorphous plasticity appears to reproduce shear banding, a crucial feature of the phenomenology of metallic glasses. The nucleation step of the shear band is followed by a slow broadening step of the band. The latter is quantitatively characterized by a slow relaxation of the stress-stress correlation. Note that this slow dynamics spontaneously emerges in the absence of any prescribed internal relaxation time scale.

The behavior of the model is controlled by two parameters that can be associated to a *structural* effective temperature[26] and a *mechanical* effective temperature,[9] respectively. This model may thus contribute to clarify the respective effects of structural relaxation and mechanical noise induced by local reorganizations in the plastic behavior of amorphous materials.

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