Permanent shear localization in dense disordered materials due to microscopic inertia

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Received 9 June 2023 / Accepted 13 October 2023 / Published online 2 November 2023
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Abstract In this work using computer simulations of 3D model of dense disordered solids we show, for the first time, the appearance of shear localization in the stationary flow under homogeneous driving conditions. To rationalize our simulation results we develop a continuum model, that couples the dynamics of the local flow to the evolution of a kinetic temperature field related to the local inertial dynamics. Our model predicts that the coupling of the flow field to this additional destabilizing field appears only as a necessary condition for shear localization, a minimum system size is necessary to accommodate the flow instability. Moreover we show that this size criterion resulting from our continuum description is in quantitative agreement with our particle-based simulation results.

1 Introduction

In honor of Fyl Pincus: It is a great pleasure to dedicate this manuscript to Fyl Pincus, who introduced one of us (JLB) to soft matter physics, and made UCSB such an attractive place for so many young postdocs, especially from France.

Disordered materials, ranging from pharmaceutical, cosmetic and food products to construction components, such as glass or cement, form an integral part of our everyday life. Instabilities formed during the flow of such materials are ubiquitous and have been widely studied in the last few decades [1–3]. These flow instabilities manifest in terms of strong spatial inhomogeneities in the flow, e.g. in form of shear bands, even when the material is homogeneously driven. These flow instabilities can either be transient (although long persisting [4]) and related to an overshoot in the stress–strain curve or permanent and related to a rate weakening effect [2]. For both type of flow instabilities there exist approaches based on auxiliary fields such as local concentration [5–7], local temperature [8–12] or local structure [5,6,13]. Despite these various approaches to understand flow instabilities under homogeneous driving, the origin of permanent shear localization in dense disordered solids is still debated in the literature. In this work, we propose a quantitative theoretical framework for the formation of permanent shear bands in dense disordered solids where the dynamics is influenced by microscopic inertia.

Among the different scenarios leading to permanent shear banding, the case of polymeric systems and wormlike micelles solutions is well understood. In these systems, shear induced structuration leads to the coexistence of regions flowing at different shear rates, even when the system is driven homogeneously [3,5–7,14,15]. In the framework of continuum mechanics, these permanent shear bands have been understood as a consequence of a material instability, e.g. resulting from a non-monotonic constitutive flow curve (macroscopic stress vs. applied shear rate) [16–19]. Shear banding was also reported in the case of dense disordered solids, that exhibit a yield stress [20], such as concentrated emulsions, foams and other dense colloidal suspensions [1,2,21]. Although there is lack of consensus on the origin of shear banding in such materials, in the case of shear history-dependent materials [22–24] and dense hard sphere suspensions [25], theoretical approaches based on coupling flow fields with either the microstructure [26,27] or concentration field [25,28,29] have been successful in predicting permanent shear bands.

The case of soft dense suspensions, where neither significant structural nor volume fraction inhomogeneities are observed [20,30], remains however unclear. The role of attractive or adhesive interactions, proposed to lead to permanent shear banding, is debated in the literature [30–32]. Alternatively, an intrinsic timescale for “restructuration” at the microscopic scale is suggested as a mechanism to induce local weakening leading to shear banding [16,33]. However this mechanism has not yet been evidenced at the microscopic level. Recent works, looking at the role of inertia on the flow behavior of yield stress materials [34–37] have demonstrated...
rate-weakening mechanisms resulting in non-monotonic macroscopic flow curves. This effect has been rationalised by Nicolas et al. [37] in terms of kinetic heating of the system due to inertia. The idea is to use settings in which the motion of the particles is underdamped, so that the external energy input through the macroscopic strain rate is, in part, converted into kinetic energy of the particles - which will eventually dissipate through inelastic shocks or solvent friction. The kinetic energy per particle then defines a local temperature. This idea to define a temperature derived from the local kinetic energy is a well established concept in the framework of sheared granular materials [38–40]. However, although it has been shown that the inertial heating effect on the microscopic scale can indeed lead to non-monotonic flow curves [37], no evidence of shear localization due to inertial effects has been reported in that study.

In this work we show that kinetic heating due to inertia can indeed lead to local softening and hence shear banding. However, the coupling of the mechanical properties to an additional destabilizing field appears only as a necessary condition, as a minimum system size is required to observe a permanent flow instability. This additional requirement has been highlighted already in many of the theoretical works cited above. However, only few works attempt quantitative comparisons with experiments [25] or particle based simulations [29] so far. Here, we propose a continuum model based on a kinetic temperature description that allows for the quantitative prediction of the development of shear instabilities for system sizes exceeding a critical size. We also find that the steady state profiles at different applied shear rates do not form a banded structure following a lever rule, a phenomenon that we can again rationalize using the same continuum description.

2 Numerical evidence for a steady state instability

The model disordered solid considered in this work consists of an assembly of polydisperse spheres at a volume fraction \( \phi = 70\% \), interacting via a truncated and shifted Lennard–Jones potential [41]. The initial samples were prepared following standard annealing protocol. These samples are subjected to a shear deformation at a fixed shear rate \( \dot{\gamma} \) using Lees-Edwards boundary conditions (LEBC) and evolved using dissipative particle dynamics (DPD) with a varying contribution from viscous forces. To describe the flow curves obtained from different damping coefficients, we introduce the inertial quality factor \( Q \), similar to Nicolas et al. [37], which is defined as \( Q = \frac{\tau_{\text{damp}}}{\tau_{\text{vib}}} \), where \( \tau_{\text{damp}} = m/\zeta \) and \( \tau_{\text{vib}} = \sqrt{ma^2/\zeta} \), with \( \zeta \) as damping coefficient, \( m \) and \( a \) as mass and average diameter of the particle. For an overdamped system \( Q \leq 1 \) one obtains a monotonic flow curve, well fitted by an Herschel-Bulkley (HB) law \( \sigma(\dot{\gamma}) = \sigma_y + A\dot{\gamma}^n \), with \( \sigma_y \approx 2.5 \) the yield stress, a coefficient \( A \approx 16.5 \) and the HB exponent \( n \approx 0.5 \). As \( Q \) increases the system moves towards an underdamped state where inertial dynamics become relevant and the flow curves exhibit a non-monotonic behaviour [37]. All simulation details are elaborated in Appendix section, and can be found in reference [42].

2.1 Non-monotonic flow curve

We investigate the inertial dynamics of the jammed system under shear by considering the inertial quality factor \( Q = 10^4 \). We perform finite shear rate simulations for a shear rate range of \( 10^{-4} \tau_{\text{vib}} \leq \dot{\gamma} \leq 0.5\tau_{\text{vib}} \) and compute the flow curves for various sizes and geometries (maintaining a constant volume fraction \( \phi = 70\% \)) (see Fig. 1). In all our simulations \([x,y,z]\) dimensions refers to flow, gradient and vorticity directions respectively. For the cubic system \((L_x = L_y = L_z = 42a)\), with around \( 10^6 \) particles, we observe a non-monotonic flow curve which is attributed to the under-damped dynamics [37]. The flow curve has a minimum at \( \dot{\gamma} \approx 0.1\tau_{\text{vib}} \). Hence one could expect a flow instability in the region of shear rates \( \dot{\gamma} < 0.1\tau_{\text{vib}} \), where the flow curve exhibits a negative slope. Similar to the observations of Nicolas et al. [37] we did not find any shear instabilities in the velocity profiles. These results remain unchanged even for a non-cubic geometry, where \( L_x = L_z = 42a; L_y = 120a \). With further increase in \( L_y \) we observe a lowering of the steady state stress for shear rates below \( \dot{\gamma} = 0.1\tau_{\text{vib}} \), while the flow curve remains unchanged in the positive sloped region, suggesting the appearance of a new flow regime for large systems in the regime \( \dot{\gamma} \approx 0.1\tau_{\text{vib}}^{-1} \).

2.2 Permanent shear instabilities

We show, in Fig. 1b, c, for \( L_y = 360a; \dot{\gamma} = 10^{-2}\tau_{\text{vib}} \), that the system exhibits permanent shear heterogeneities along the gradient direction in the flow regime mentioned above. The local shear rates and stresses were computed after the system had been sheared for around \( \dot{\gamma} = 60 \) (or 6000% strain) and averaged over strain window of \( \Delta \dot{\gamma} = 0.20 \). It is clear that the system has reached a steady state both from the load curve (see Appendix) and from the homogeneous stress profile displayed in Fig. 1c. The local shear rate profile in Fig. 1b is clearly showing the feature of steady state shear localization. To our knowledge this is the first time such a formation of shear localization is reported for a dense disordered system without walls (periodic boundary conditions). These set of simulation results indicate that the instability resulting from a negatively sloping flow curve can only be observed above a minimum system size that can accommodate the corresponding instability. While \( L = 360 \) is clearly above this minimum system size, we have not attempted to locate accurately this size, due to the cost this would induce in terms of numerical simulations.

Rather, in the following, we propose a continuum model based on the ideas of ref. [37], in order to predict the minimum length scale required to allow for such an inertia-induced flow instability, and show that our
Fig. 1 a Flow curve showing steady state stress as a function of applied shear rate of athermal underdamped system \((Q = 10^4)\) for different system sizes. b Steady state local shear rate profile as a function of gradient direction, averaged over a strain window of \(\Delta \gamma = 0.2\), computed for a system size \(N = 240731\) and \(L_Y = 360a\) at \(\dot{\gamma} = 10^{-2} \tau_{vib}^{-1}\). c Corresponding stress profile. d 3D rendering of a configuration from simulation trajectory depicting shear localization \((Q = 10^4, N = 240731, L_Y = 360a, \dot{\gamma} = 10^{-2} \tau_{vib}^{-1})\). Hot coloring scheme, based on the kinetic temperature \(\tilde{T}\), varies between white \(\tilde{T} = 0e/k_B\) to black \(V_x = 20e/k_B\). Observations are consistent with this prediction. For the parameters used in this specific simulation, the calculation described below leads to a prediction of a minimum length \(L_c = 336\).

3 Rationalising numerical results using a continuum model

3.1 Kinetic temperature due to inertia

If we consider that inertia is introducing a kinetic temperature \(\tilde{T}\) to the athermal dynamics, quantified through an excess of kinetic energy \([35, 37, 40]\), one can interpret the non-monotonic flow rheology of athermally driven inertial systems \(\sigma(\dot{\gamma}; Q, T = 0)\) effectively as an over-damped rheology at a finite shear-rate dependent temperature \(\sigma(\dot{\gamma}; Q = 1, \tilde{T}(\dot{\gamma}))\). In Fig. 2a we show flow curves (solid lines) obtained for \(Q = 1\) at different \(T\) values as well as the flow curve for \(Q = 10^4\) at \(T = 0\) (filled red circles). The stress values of underdamped flow curves at different shear rates corresponds to stress values of overdamped flow curves at different \(T\). We know that in over-damped situations the athermal flow rheology of simple yield stress fluids is usually well described by a Herschel-Bulkley type monotonous relationship between the shear stress and the applied shear rate \(\sigma_0(\dot{\gamma}) = \sigma(\dot{\gamma}; T = 0) = \sigma_y + A \dot{\gamma}^n\) with \(n \approx 0.5\). In Fig. 2b we show the temperature dependence of yield stress \(\sigma_y\), the prefactor \(A\) and H.B exponent \(n\). We find that the temperature dependence of \(A\)
and $n$ can be neglected and hence $A(T) \approx A(T = 0)$ and $n(T) \approx n(T = 0)$. The functional form of the first correcting term in the macroscopic flow curve for small but finite temperatures has been worked out in previous works but is valid only at large enough shear rates [43,44]. Lacking a specific form of the temperature dependence of the flow curve, that can be sensitive to the details of the modeling and the interaction potentials, we only assume a formal dependence of the local stress on the local kinetic temperature to derive the most general form of a continuum description.

### 3.2 Continuum model

Starting from the hypothesis developed above, that the shear stress $\sigma = \sigma(\dot{\gamma}, \dot{T})$ is not solely depending on the shear rate $\dot{\gamma}$ but also on the kinetic temperature $\dot{T}$ accounting for inertial effects, we aim for a derivation of continuum equations describing the evolution of the local shear rate and the local kinetic temperature. To fix the notations we assume in the following a specific driving protocol at a fixed externally applied shear rate $\dot{\gamma} = \partial v_x / \partial y$ in a 3d planar geometry (flow direction $x$, gradient direction $y$, and vorticity direction $z$). Using the continuity equations for momentum and energy, we derive the time evolution equations for the shear component of the velocity $v_x(y, t)$ and the kinetic temperature $\dot{T}(y, t)$ as [12]:

$$
\rho \frac{\partial v_x}{\partial t} = \frac{\partial \sigma}{\partial y} = \frac{\partial \sigma}{\partial \dot{T}} \frac{\partial \dot{\gamma}}{\partial y} + \frac{\partial \sigma}{\partial \dot{\gamma}} \frac{\partial^2 v_x}{\partial \dot{\gamma} \partial y^2}, \quad (1)
$$

$$
c_V \frac{\partial \dot{T}}{\partial t} = \gamma T + \frac{\partial v_x}{\partial y} \dot{\gamma} \left( \frac{\partial v_x}{\partial y} \dot{T} \right) - \frac{c_V}{\tau} \dot{T}. \quad (2)
$$

where $\rho$ is the system density, $c_V$ the volumetric heat capacity, $\lambda_T$ the thermal conductivity and $\tau$ the typical time to remove the kinetic energy (originating from the external shear) by the thermostat (at zero temperature). In the above model equations, the second term in Eq. 1 is the usual expression obtained from momentum conservation in systems with a simple flow curve relation solely depending on the shear rate. The really interesting new part in Eq. 1 is the first term that is introduced through the dependence of the shear stress on the kinetic temperature. The derivative in this expression will be negative accounting for a local shear weakening effect introduced by the local heating, which we expect to be the source of our shear instability. The second Eq. 2 simply describes the heat evolution as a diffusive process together with a source term given by the driving, where a dissipative stress opposes flow in steady states with a fixed strain rate $\dot{\gamma}$, and a sink term given by the thermostating at zero temperature.

As a test of our continuum model we first obtain from the above equations the relation between temperature and shear rate in the stationary state ($\partial \sigma / \partial t = 0; \partial \sigma / \partial y = 0; \partial \dot{T} / \partial t = 0; \partial \dot{T} / \partial y = 0$) and uniform flow limit ($\partial \dot{\gamma} / \partial y = 0$), given by

$$
\dot{T} = \frac{\tau}{c_V} \sigma(\dot{\gamma}, \dot{T}(\dot{\gamma})) \dot{\gamma} \quad (3)
$$

In simulations one can measure $\lambda_T$ and $c_V$, which are system properties fixed by the interaction potential and $\tau$ is fixed by the dissipation coefficient $\zeta$. For $Q = 10^4$ and $L_x = L_y = L_z = 42a$ we measure, as a function of $\dot{\gamma}$, the kinetic temperature, which is obtained as $\dot{T} = (1/N) \sum_i (m/2k_B)(V_z^i)^2$, where $N$ is the total number of particles in the system, $V_z$ is the velocity of a particle in the neutral vorticity direction, which is not influenced by the affine flow. At each shear rate, after the system reaches a steady state flow, $\dot{T}$ is obtained by averaging over a strain window of $\Delta \dot{\gamma} = 0.2$. In Fig. 2c, we show $\dot{T}$ measured from simulations as well as the one obtained from Eq. (3). We find a good match between the measured and predicted temperatures, showing that the kinetic temperature emerging from the continuum model is well describing the simulations in the homogeneous flow regime.
3.3 Stability analysis and system size dependence

Next we perform a linear stability analysis for small perturbations of the homogeneous flow solution \( v_\infty(y, t) = \gamma y + \delta v_\infty(y, t) \) and of the constant kinetic temperature field \( T(y, t) = T_0 + \delta T(y, t) \), using the ansatz \( \delta v_\infty(y, t) = v \exp(\lambda t) \exp(-i k y) \) and \( \delta T(y, t) = T \exp(\lambda t) \exp(-i k y) \). Linearizing the set of Eqs. (1) and (2) and solving for the characteristic polynomial, the product of the eigenvalues \( \lambda_1 \) and \( \lambda_2 \) yields

\[
\lambda_1 \lambda_2 = \frac{\lambda_T}{\rho c_v} \frac{\partial \sigma}{\partial \gamma} k^4 + \frac{1}{\rho c_v} \left( \frac{\partial \sigma}{\tau} + \frac{c_v}{\tau} \frac{\partial \sigma}{\partial T} \right) k^2
\]

\[
\lambda_1 + \lambda_2 = -\left( \frac{1}{\rho \frac{\partial \sigma}{\partial \gamma}} + \frac{\lambda_T}{c_v} \right) k^2 - \frac{1}{\tau} + \frac{1}{\tau} \frac{\partial \sigma}{\partial \dot{\gamma}}
\]

The expression in Eq. (5) for the sum of the eigenvalues being strictly negative tells us that at least one eigenvalue is negative. For the homogeneous flow to be stable we need both eigenvalues to be negative and thus the expression in Eq. (4) to be positive. The first term on the right hand side in Eq. (4) is indeed positive and thus stabilizing, since we started from a monotonic flow curve assumption in the over-damped limit. The sign of the second term will however depend on the competition of two contributions, one stabilizing related to the efficiency of the thermostat and one destabilizing related to the sensitivity of the flow curve to the increase in kinetic temperature. When this last term becomes predominant in the case of weakly damped systems, we expect the homogeneous flow solution to become unstable for large wavelength perturbations. In that case the exact expression for the critical wavelength \( \ell_c = 2\pi/k_c \) associated with the onset of instability (given by a positive eigenvalue of the Eqs. (4) and (5)) can be expressed as

\[
\ell_c = 2\pi \sqrt{\lambda_T} \left( -\frac{\partial \sigma}{\partial \gamma} \sigma - \frac{c_v}{\tau} \right)^{-\frac{1}{2}}
\]

\[
= 2\pi \sqrt{\lambda_T} \left( \sigma \frac{1}{\partial_{\dot{\gamma}} T} - \frac{c_v}{\tau} \right)^{-\frac{1}{2}}
\]

where we used a simplified notation for the partial derivative operator \( \partial_{\bullet} f = \partial f / \partial \bullet \).

Equations (6) and (7) indicate the existence of a critical system size \( \ell_c \), above which a shear instability can develop in our continuum model. We would thus expect an instability to occur in simulations for system sizes \( L_y > \ell_c \) along the gradient dimension larger than this critical length, \( L_y > \ell_c \).

From the expression in Eq. (7) one can clearly identify the reason for the linear instability that arises from a competition of a stabilising term related to the thermostattoing at zero temperature and a destabilising local heating effect, quantified through the kinetic temperature change caused by the change of the local shear rate. In the case where this heating effect becomes negligible, as is the case for overdamped dynamics, the value of \( \ell_c \) becomes infinite and the flow remains stable for any system size as expected.

Additionally we can show that the increasing part of the constitutive relation leads to a stable flow giving us an estimation for the limiting shear rate \( \dot{\gamma}_{\min} \) above which the dynamics become stable again. In the upriser part of the constitutive curve we know that

\[
\frac{\partial \sigma}{\partial T} \frac{dT}{d\dot{\gamma}} + \frac{\partial \sigma}{\partial \dot{\gamma}} > 0.
\]

We can obtain the derivative \( dT/d\dot{\gamma} \) from Eq. (3) and insert the solution in Eq. (8) yielding

\[
\frac{c_v}{\tau} \frac{\partial \sigma}{\partial \dot{\gamma}} + \frac{\partial \sigma}{\partial T} > 0.
\]

From Eqs. (4) and (5) follows that both eigenvalues need to be negative and thus the solution of an homogeneously flowing state remains stable beyond the minimum of the constitutive curve at \( \dot{\gamma}_{\min} \).

In the following we compute \( \ell_c \) using Eq. (6) inputting the values of numerically measured parameters as well as estimates of \( \partial_{\gamma} \sigma \) and \( \partial_{\dot{\gamma}} \sigma \) from the simulations (details in the Appendix). In the parametric plot of Fig. 3, we show the system size along the gradient dimension \( L_y \) as a function of \( \dot{\gamma} \). The system size \( L_y = \ell_c \) computed from Eq. 6 separates two different flow regimes. The small system regime (\( L_y < \ell_c \), red shaded area) corresponds to the homogeneous flow being stable, which becomes unstable for large systems (\( L_y > \ell_c \), blue shaded area). The symbols represent numerical simulations data (for an underdamped system with \( Q = 10^4 \)) where we find either an homogeneous flow (red triangles) or a localised flow (blue circles). We find a good match between the prediction for the system size at which an instability emerges \( \ell_c \) from the continuum model and the system size at which shear bands are observed in numerical simulations. These result indicate that our model can predict quantitatively the onset of the flow instability observed in microscopic simulations. Note however, that in order to make a quantitative comparison with the predictions from the continuum model, it is necessary to obtain numerically the derivatives of the stress with respect to temperature and shear rates. As described in the appendix, these derivatives are obtained from the flow curves of homogeneously flowing systems. They are, however, difficult to obtain numerically, especially in the vicinity of the minimum of the curve or at small strain rates. For this reason, the theoretically calculated boundary is affected by large uncertainties (indicated by error bars) in these two regions. In the vicinity of the minimum (\( \dot{\gamma}_{\min} \)), Eq. 7 clearly shows that \( L_c \) has to diverge. As we cannot compute this divergence accurately, we have indicated it schematically by a vertical line. In the small strain rate region, the apparent increase is related to these large uncertainties. In fact,
if the same calculation is done with a simple analytical representation of the flow curves such as the one given in Eq. 10, no such increase is observed at small strain rate [45].

4 Steady state flow profile

4.1 Lack of lever rule

We now discuss the dependence of the flow profiles on the applied shear rate. In usual shear banding scenarios [3], if the average stress is homogeneous in the system, one generally expects the maximum shear rate achieved in the system to be independent of the applied shear rate, as well as an increasing band width with an increase in shear rate, so as to conserve the applied shear rate (so called 'lever rule'). In Fig. 4a, we show the local shear rate profiles obtained from molecular simulations for different applied shear rates for a given system size (with $L_y > \ell_\gamma(\dot{\gamma})$). The profiles show that, even though the width of the band increases with an increase in shear rate, there is a clear absence of one chosen maximum shear rate. Instead, the profiles exhibit a continuous interface, without a clear plateau associated with the flowing region. Similar features are observed in the flow profiles computed from the model (Fig. 4b). To obtain the flow profiles of Fig. 4b we integrate the continuum model in steady state (Eq. (2) with LHS term equal to 0) using the shooting method for single-banded profiles. In practice, we look for periodic steady state solutions of Eq. (2) for a given value of stress, with a spatial period equal to the system size $L$. The problem is thus reduced to finding the boundary conditions $\tilde{T}(0)$ that satisfy the above constrains, which is done using a minimization procedure.

To this aim, we assume a simple constitutive relationship relating the shear stress to the shear rate and kinetic temperature, based on a Herschel-Bulkley description at a given temperature:

$$\sigma = \sigma_y + A\dot{\gamma}^n - B\tilde{T}^\alpha$$

where $A$ and $n$ are fitting parameters for the molecular simulation data at zero temperature, $B = 2.3$ and $\alpha = 0.3$ describe the decrease in stress with kinetic temperature. Using Eq. (3), relating $T$ to $\dot{\gamma}$ for an homogeneous flow, one can solve the implicit equation given by Eq. (10), which leads to a non-monotonic constitutive flow curve (see Appendix). This expression is not the best fit to the MD data but constitutes the simplest form to qualitatively reproduce the main features of the flow curve, with a minimum located at $(\dot{\gamma}_\text{min}, \sigma_\text{min})$ close to the values of MD simulation.

4.2 Rationalizing the flow profiles

A stationary localised flow corresponds to a situation of coexistence between flowing and nearly immobile regions, with a homogeneous stress profile.

The determination of the flow profile is analogous to the determination of interfacial profiles in phase coexistence problems, and can be described using a classical mechanical analogy [46,47]. The steady state temperature $T(y)$ obeys Eq. (2) with $\partial_1 \tilde{T} = 0$, and this equation can be interpreted as describing the trajectory $\tilde{T}(y)$ of a fictitious particle in an external potential, in one dimension:

$$\lambda_T \frac{d^2 \tilde{T}}{dy^2} = -\frac{dU(\tilde{T})}{dT}.$$  (11)

In this mechanical analogy, $\tilde{T}$ corresponds to the position of the particle and $y$ to time.

This effective potential is computed by integrating the last two terms of Eq. (2) in the steady state with respect to $\tilde{T}$ at a fixed value of the stress $\sigma$: $U(\tilde{T}) = \sigma \int_0^{\tilde{T}} \dot{\gamma}(\sigma, T')dT' - c_v T^2 / 2\tau$, where the function $\dot{\gamma}$ is expressed using the flow curve given in Eq. (10) as

$$\dot{\gamma}(\sigma, \tilde{T}) = A^{-1/n}(\sigma - \sigma_y + B\tilde{T}^\alpha)^{1/n} \text{ if } \sigma > \sigma_y - B\tilde{T}^\alpha;$$

$$\dot{\gamma}(\sigma, \tilde{T}) = 0 \text{ otherwise}$$  (12)  (13)

The resulting potential is displayed in Fig. 5a for various values of the stress, and will define four different regimes for the possible trajectories. The temperature and flow profiles associated with these different regimes are shown in Fig. 5c–g. We first note that, by construction, extrema of the effective potential correspond to temperatures (and shear rates) that are solution of the set of Eqs. (3) and (10), which describe homogeneous flow. Note that, as in the molecular simulations, we are only interested in periodic solutions with a period equal to the system size, $L$.

For stress values above the yield stress, $\sigma > \sigma_y$ (Fig. 5c), $U(\tilde{T})$ exhibits a single maximum at high temperature and has a finite, positive slope at $\tilde{T} = 0$. This maximum corresponds to homogeneous flow in the high shear rate, high stress regime.
Another simple regime corresponds to the low stress case, when \( \sigma < \sigma_{\min} \), with \( \sigma_{\min} \) corresponding to the minimum of the actual flow curve. In this case, the only extremum is obtained for \( \dot{T} = 0 \), which implies \( \dot{\gamma} = 0 \). This situation is depicted by the brown solid line in Fig. 5a and in Fig. 5g. For \( \sigma < \sigma_{\min} \), no flow is possible.

A richer situation is observed for intermediate stresses, \( \sigma_{\min} < \sigma < \sigma^* \). Here \( U(\dot{T}) \) has three extrema: a maximum at \( \dot{T} = 0 \), a second maximum at \( \dot{T}_{\max} \), and an intermediate minimum at \( 0 < \dot{T}_{\min} < \dot{T}_{\max} \). Possible interfacial profiles correspond to oscillations of \( \dot{T} \) around the minimum, with the “period” of the oscillation being equal to the size of the system. Here, two cases must be distinguished, and we focus first on the one that corresponds to the profiles effectively observed in simulations, with \( U(\dot{T}_{\max}) > U(0) \), as illustrated by the blue curve in Fig. 5a and in Fig. 5d. In this case, an oscillation can be obtained for values of the potential energy \( U \) between \( U(\dot{T}_{\min}) \) and \( U(0) \). The period of the oscillation will have a value that starts from a minimum, nonzero value for the smallest energies in the vicinity of \( U(\dot{T}_{\min}) \), where the oscillation is harmonic. This minimum period defines the critical system size, below which no interface can be observed and the system remains in an homogeneous state. We have checked that the corresponding analytical expression of \( \ell_c \) obtained from this analysis coincides with the one obtained from the linear stability analysis in Eq. (6).

As the value of the energy increases towards \( U(0) \), the period of oscillation increases and becomes infinite at \( U(0) \), where the trajectory spends a short time at a finite temperature and most of the time near \( \dot{T} = 0 \). This corresponds to a narrow sheared layer coexisting within a broad non-flowing part (Fig. 5d, middle and left panels). The blue dot in Fig. 5a (constructed from the intercept between the horizontal dashed line corresponding to \( U(\dot{T}) = 0 \) and the \( U(\dot{T}) \) curve) marks the maximum temperature \( \dot{T}_{\max} \) inside the sheared region.

Figure 5b depicts the stress as a function of temperature in steady state. The black line represents the constitutive temperature-stress curve (which is directly related to the constitutive stress-strain rate curve for an homogeneous flow, see Appendix). The solid part of the black line corresponds to a stable homogeneous flow and is constructed from the loci of the high temperature maximum \( (\dot{T}_{\max}) \) of \( U(\dot{T}) \) when varying \( \sigma \). The dashed part of the black line, constructed from the loci of the minimum of \( U(\dot{T}) \) \( (\dot{T}_{\min}) \), corresponds to unstable homogeneous flow leading to coexistence of various temperatures in the system if the system size \( L \) exceeds the critical size \( L_c \).

The blue solid line in Fig. 5b represents the maximum temperature \( \dot{T}_{\max} \) that can coexist in the system (in the limit of an infinite system), and corresponds to the solution of \( U(\dot{T}_{\max}) = 0 \) with \( \dot{T}_{\max} \neq 0 \) (blue dot in Fig. 5a). The shaded blue region thus corresponds to the values of temperatures that can exist within the profile. Clearly the value of \( \dot{T}_{\max} \), which can be defined by \( U(\dot{T}_{\max}) = U(0) \), depends on the applied stress. As
a result, no lever rule is expected: the total shear rate increases as stress increases not only by broadening the sheared region, but also by increasing temperature and strain rate inside the flowing region.

The above described regime, which accounts well for the observations made in the atomistic simulations, is observed for values of the stress $\sigma^* < \sigma < \sigma_y$. At $\sigma^*$, $U(T_{\text{flow}}^{\text{max}}) = U(0) = U(T_{\text{max}})$ (Fig. 5e), and for $\sigma_{\text{min}} < \sigma < \sigma^*$, $U(T_{\text{min}}^{\text{flow}}) < U(0)$ (Fig. 5f). As a result, oscillating trajectories will exist between a small temperature ($T_{\text{flow}}^{\text{min}}$ in the limit of an infinite system) and $T_{\text{max}}$, with most of the “time” being spent in the vicinity of $T_{\text{max}}$, the second maximum of $U(T)$. This situation is illustrated with the magenta line in Fig. 5a and would correspond to a broad region at high shear rates coexisting with a narrower immobile layer, as shown by the corresponding profile in Fig. 5f.

We have not observed this situation in the molecular dynamics simulations: this is not surprising, as it corresponds to a very narrow range of stresses approaching the minimum of the flow curve (see Appendix, Fig. 8), where the critical size for the flow instability to develop becomes increasingly large (see Fig. 3).

5 Conclusions

The aim of this work is to show how permanent shear bands in soft amorphous solids emerge from a simple change in the microscopic dynamics, from overdamped to underdamped, as measured by the dimensionless parameter $Q$. Such a change does not modify any of the structural, static properties of the system. Note that the value of $Q$ involves a combination of the interaction potential between particles and of the friction mechanism. Qualitatively, $Q$ is expected to increase as particle size decreases, and to decrease if the viscosity of the solvent increases. However, the use of a simple Lennard-Jones potential for describing the interaction precludes a quantitative comparison with real granular media.

In general, the linear instabilities in the steady state rheology of complex fluids can be induced by spatial fluctuations of a field coupled to the flow (e.g. local concentration [5–7], local temperature [8,12] or local microstructure [5,6]). Although this picture appears very general, there is still a lack of quantitative models especially in the framework of yield-stress materials, that could be directly compared to experiments or simulations. In this work we single out a specific destabilizing field that couples with the stress dynamics to produce permanent shear bands. In this context we propose a truly quantitative description by inferring all parameters of our proposed continuum model from particle based simulations.

We show that a small change in the dynamics induced by microscopic inertia, can lead to a local increase of kinetic temperature which promotes local shear weakening. We recognize this process as the leading cause for the phenomenon of shear-localization. Hence in the continuum model, we define a destabilizing field in terms of a local kinetic temperature. Contrary to effective fields, or parameters that enter former continuum descriptions [2,9–11], the kinetic temperature has the advantage of having a clear microscopic definition, and is thus easily measurable in particle based simulations (as shown in Fig. 1d) and experiments [40]. We quantitatively predict the appearance of shear localization for systems larger than a critical size $\ell_c$. To go beyond the linear stability analysis, we show that the qualitative features in the stationary profiles match well between particle simulations and the continuum model. Notably, the our description allows to understand why the stationary profiles do not exhibit a simple band but a more complex continuous profile, leading to a lack of lever rule. Given an exact analytical expression for the effect of temperature on rheological flow curves, our model provides a prediction for the overall dynamics including coarsening dynamics and stationary profiles. We note indeed that in large systems, we have observed in MD simulation the formation of several bands that merge into a single one. However, comparing such transient phenomena between the continuum and microscopic description is quite difficult computationally, and is beyond the scope of the present study.

In many inertial systems the role of the kinetic temperature and its shear weakening effect is often ignored. This is, for example true in the case of granular materials where flow instabilities have been attributed to lubrication of frictional contacts [17,19]. The emergence of hysteresis and shear bands in these systems could result from a complex interplay between the different mechanisms involved in the dynamics. Following a similar approach as the one suggested in the present work, a complete continuum description should couple the stress dynamics to several destabilizing fields, including the local kinetic temperature.

Acknowledgements J.-L. B. and V. V. V. acknowledge financial support from ERC grant ADG20110209 (GLASS-DEF). K. M. acknowledges financial support from ANR Grant No. ANR-14-CE32-0005 (FAPRES) and CEFIPRA Grant No. 5604-1 (AMORPHOUS-MULTISCALE). Simulations on the CURIE and IRENE hybrid cluster at TGCC were possible thanks to the Grand Equipement National de Calcul Intensif Project No. A0070910286. Further we would like to thank Peter Olmsted, Guillaume Ovarlez and Romain Mari for fruitful discussions.

Declarations

Data availability The MD data were generated using a modified version of the LAMMPS code, accommodating polydispersity. The code and the scripts needed to generate the trajectory will be made available upon reasonable request.

Authors contributions VV. performed the molecular dynamics simulations. The continuum model was developed
A Appendix

A.1 Simulation details

The model disordered system is characterised by an interaction potential defined by $U(r) = 4\epsilon \left[ (a_{ij}/r_{ij})^{12} - (a_{ij}/r_{ij})^6 \right] + \epsilon$, for $r_{ij} \leq 2^{1/6}a_{ij}$, else $U(r_{ij}) = 0$. Here $a_{ij} = (a_i + a_j)/2$ defines the distance between the center of particles $i$ (with diameter $a_i$) and $j$ (with diameter $a_j$) at contact and the unit energy $\epsilon = 1$ for all particles. The diameters of the particles are drawn from a Gaussian distribution with a variance of $10\%$. The initial configurations are prepared by quenching a equilibrated liquid configuration at a volume fraction $\phi = 0.70$, with a chosen set of simulation box dimensions $(L_x, L_y$ and $L_z)$. The quench rate used here is $\Gamma = 5 \times 10^{-3}/(k_BT_0)$ and we find that the steady state flow features do not depend on preparation protocol. Before subjecting the sample to shear, we take the system to the zero temperature limit using conjugate gradient energy minimisation technique. Samples so prepared is subjected to zero temperature limit using conjugate gradient energy minimisation technique. Before subjecting the sample to shear, we take the system to the zero temperature limit using conjugate gradient energy minimisation technique. Samples so prepared is subjected to shear deformation at a finite shear rate using Lees-Edwards boundary condition and evolving the system by solving the Dissipative Particle Dynamics (DPD) equation of motion given by

$$
\frac{d^2\mathbf{r}_i}{dt^2} = -\zeta \sum_{j \neq i} \omega(r_{ij})(\mathbf{r}_{ij} \cdot \mathbf{v}_{ij})\dot{r}_{ij} - \nabla r_i U
$$

where the first term in the right hand side (RHS) is the damping force which depends on the damping coefficient $\zeta$ and $m$ is the mass of the particle. The relative velocity $\mathbf{v}_{ij} = \mathbf{v}_j - \mathbf{v}_i$ is computed over a cut-off distance $r_{ij} \leq 2.5a_{ij}$, with the weight factor $\omega(r_{ij}) = 1$. The second term in the RHS is the force due to interactions between particles. As a measure of the extent of over damping, we define an inertial quality factor $Q = \tau_{\text{damp}}/\tau_{\text{vib}}$, where $\tau_{\text{damp}} = m/\zeta$ is the viscous timescale and $\tau_{\text{vib}} = \sqrt{ma^2/\epsilon}$ defines an elastic timescale. The inertial quality factor measures the number of inertial oscillation within the damping time. The shear rate in our simulations is defined in the units $\tau_{\text{vib}}^{-1}$.

A.2 Steady state flow

We make sure that a sample has indeed reached a steady state flow, by monitoring the macroscopic load curve as well as the microscopic flow profiles ($V_x$ vs. $Y$) and stress profiles. Reaching steady state, the macroscopic shear stress fluctuates around a mean stress value. Similarly the flow profiles as well as the distribution of local stresses do not evolve any longer with time (strain) (Fig. 7).

A.3 Minimum length to accommodate an instability in molecular simulations

In order to obtain the minimum length scale to accommodate the flow instability, using the Eq. (6), one needs to compute the thermal conductivity $\lambda_T$, heat capacity $c_v$, the time associated with the relaxation of kinetic energy $\tau$, along with the derivative of stress with respect to temperature $\partial_T \sigma$ and to shear rate $\partial_\gamma \sigma$. We compute $\lambda_T$, for a system size of $N = 10^5$, using the reverse non-equilibrium molecular dynamics method introduced by Muller-Plathe (JCP 106, 6082 (1997)) and its value is $\lambda_T = 30$ (LJ units). We have performed a slow quenching run to prepare the initial sample. From this data we compute the heat capacity as the

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by ML, KM and JLB. All authors contributed to the data analysis and manuscript writing.
slope of total energy vs. temperature. To compute $\ell_c$, we use $c_V = 3.0$ (LJ units). To compute the relaxation time associated with the kinetic energy, we monitor the dissipation of kinetic energy with time at a fixed dissipation constant corresponding to $Q = 10^4$ and we find $\tau_{KE} \equiv \tau \approx 350 \tau_{Vib}$. The partial derivative of stress w.r.t. temperature ($\partial_T \sigma$) should be obtained by measuring, at a given shear rate, the stress in the finite temperature simulations in overdamped conditions ($Q = 1$). However it turns out that for the data quality we are able to reach at this stage the error bars within this method are too large to come to a conclusive result for the critical length. This is especially true in the low shear rate limit. This is why we opted for a different method to approximate this term through another measurement. We measure for a given shear rate in an underdamped simulation the critical length. This is especially true in the low shear rate limit. This is why we opted for a different method to approximate this term through another measurement.

A.4 Herschel-Bulkley fitting parameters

To obtain the Herschel-Bulkley (HB) fitting parameters for a finite temperature, over-damped system ($Q = 1$), we have performed molecular simulations, over shear rates ranging between $\dot{\gamma} = 10^{-5} \tau_{Vib}^{-1}$ to $\dot{\gamma} = 10^{-1}$, of a system of $10^4$ particles keeping all other parameters the same as the underdamped simulations. In order to extract over-damped HB parameters ($\sigma_y$, $A$ and $n$) at finite temperature we make sure that at each temperature (ranging between $T = 0 \epsilon/k_B$ to $T = 7.5 \epsilon/k_B$), the system has reached a steady state.

A.5 Flow curve for the continuum description

The assumed local constitutive relation used in the continuum description with the chosen model parameters is displayed in Fig. 8.

A.6 A remark on shear-concentration coupling effects

To be sure that in our case it is really the local heating effect that plays the role for the instability to occur we also provide additional measurements to disentangle potential mass migration effects from local kinetic temperature effects. To do so we measure alongside the local shear rate profile also the steady state density profiles in the unstable region, shown in Fig. 9a and b. The question is whether these variations in the local volume fraction could as well explain the instability. To answer this question we also measured the yield stress dependence on density. We estimate the yield stress values for the range of different packing fractions that we observed in the density profiles of the simulations. And indeed we find that these are all above the actual homogeneous stress value, as shown in Fig. 9. This means that the change of local volume fraction cannot induce an instability in our dynamics. However, the change of the local yield stress due to a finite kinetic temperature is much more drastic within the temperature range that we measure in the profiles. Therefore temperature is indeed inducing an instability to make the system flow in the high kinetic temperature regions where the temperature dependent yield stress is smaller than the homogeneous stress value. This is for us is a proof that the observed migration is not the source of the instability but rather a consequence of another type of instability induced by the heating effect.

![Fig. 8 Assumed constitutive relation for the analytical model obtained from solving Eqs. (3) and (10), using the implicit expression: $\sigma = \sigma_y + A \dot{\gamma}^n - B (\frac{\dot{\gamma}}{c_V})^n$ with the following parameters (in LJ units): $c_V = 3$, $\rho = 1.337$, $\tau = 350$, $\sigma_y = 2.7$, $A = 12$, $B = 2.3$, $n = 0.5$, and $\alpha = 0.3$. Since there is no general form of the temperature dependence of the flow-curve we implement the most simple form that reproduces the minimum in the flow-curve, $\dot{\gamma}_{min} \approx 5.10^{-2}$ and $\sigma_{min} \approx 1.21$. The red line indicates $\sigma^* \approx 1.2374$.](image1)

![Fig. 9 Steady state measurement of a Local shear rate, b Local volume fraction and c Local stress and yield stress for a underdamped system ($Q=10^4$) with a system size $L_y = 360a$, sheared at $\dot{\gamma} = 10^{-2} \tau_{Vib}^{-1}$.](image2)
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