Absence of ‘fragility’ and mechanical response of jammed granular materials

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Abstract We perform molecular dynamic (MD) simulations of frictional non-thermal particles driven by an externally applied shear stress. After the system jams following a transient flow, we probe its mechanical response in order to clarify whether the resulting solid is ‘fragile’. We find the system to respond elastically and isotropically to small perturbations of the shear stress, suggesting absence of fragility. These results are interpreted in terms of the energy landscape of dissipative systems. For the same values of the control parameters, we check the behaviour of the system during a stress cycle. Increasing the maximum stress value, a crossover from a visco-elastic to a plastic regime is observed.

Keywords jamming · kinetic arrest · granular materials · rheology · phase diagrams

1 Introduction

Among the peculiarities of granular systems [1], there are jamming processes consisting in a sudden transition from a flowing to a solid state [2,3]. In particular, if submitted to an anisotropic stress, a granular material can jam after a transient flow. This transition is observed neither at low densities, where granular materials behave like fluids, nor at very high densities, where they behave as disordered solids. The jammed solids obtained under these conditions, are so unconventional that it has been claimed to represent an absolutely new state of matter, which have been termed ‘fragile matter’ [4]. Fragility is based on the idea that during the flow particles rearrange until they find a configuration able to balance the external stress. It is speculated that the force chains sustaining this configuration are strictly related to the flow-generating stress, so that they can support incremental stress oriented as the former (compatible stress). By contrast, the may not sustain a stress applied in a different direction (incompatible stress), which may allow the system to restart flowing. This resembles the case of a pile of sands obtained in the presence gravity. The pile responds as a solids to stress directed as the weight, but it falls down under the action, for example, of a shear stress.

A more precise statement of the idea of fragility has been provided in the limit of hard spheres [4,5,6]. Consider, for example, a system jammed in the presence of a constant shear stress $\sigma_{zx}$: in this framework compatible stress variations, $\sigma' = a\sigma_{zx}$ with $a > 1$, lead to an elastic response. Conversely incompatible stresses, such as $\sigma' = a\sigma_{zx} + b\sigma_{zy}$ restore flow, also for infinitesimal values of $b$. In this sense, these systems are ‘fragile’ and strongly differ from any ordinary visco-elastic or elasto-plastic material.

Previous results suggest that, in the presence of a shear stress, a fragile behavior can only be observed in frictional granular systems [7,8,9,10,11,12,13,14,15]. Indeed, as reported in Refs. [7,8], flowing frictionless systems have never been observed to spontaneously select a microscopic state able to sustain the applied stress, while, conversely, in the presence of friction a much more complex phenomenology has been found [9,10,11,12,13,14,15,16]. In particular, in recent works [14,16] reporting molecular dynamics (MD) simulations of soft frictional grains at constant volume and applied shear stress, it was observed the phenomenology who
inspired the idea of ‘fragile matter’ [17]. Indeed, for some values of the control parameters, the system was found to select a configuration able to sustain the applied stress after a small slip, or even after very large strains at constant rate [18].

Under these conditions, whether the mechanical response of the system is peculiar or rather similar to that of other amorphous and soft materials [19] is still an open question. In particular it is not clear to what extent fragility can capture the physics of these systems. In more concrete terms, can small incompatible stresses restore the flow?

In this paper, we investigate via MD simulations the mechanical response of frictional granular systems jammed in the presence of a shear stress. After shortly reviewing the numerical model and the overall phenomenology (Sec. 2), we discuss the limit of validity of the concept of ‘fragile matter’ (Sec. 3). We find that our system is not fragile but it responds as an elastic and isotropic solid to small incompatible stresses. Anisotropy and macroscopic rearrangements only emerge in the response to strong stress variations. In Sec. 4, we will focus on the stress-strain curves during a stress cycle, in order to check analogies with ordinary rheological behaviours. Increasing the maximum stress reached during the cycle, we find a crossover from a visco-elastic to a plastic regime.

2 Investigated System

We perform MD simulations along the line of Refs [13, 16, 18]. Monodisperse spherical grains of mass \( m \) and diameter \( D \) are enclosed in a box of dimension \( l_x = l_y = 16D \), and \( l_z = 8D \). Periodic boundary conditions are used along \( x \) and \( y \), while the size of the vertical dimension is fixed and chosen to be comparable to that of recent experiments [20, 21]. The upper and lower boundary surfaces of the box are disordered collections of particles that move as a rigid object. The bottom plate has an infinite mass, and is therefore fixed, while the top one has a mass equal to the sum of the masses of its particles (roughly \( l_x l_y \)). We impose a shear stress \( \sigma_{xz} = \sigma \) to the system, applying a force to the top plate.

Grains interact via the standard linear spring-dashpot model. Two particles \( i \) and \( j \), in positions \( \mathbf{r}_i \) and \( \mathbf{r}_j \), with linear velocities \( \mathbf{v}_i \) and \( \mathbf{v}_j \), and angular velocities \( \omega_i \) and \( \omega_j \), interact if in contact, i.e., if the quantity \( \delta_{ij} = D - |\mathbf{r}_{ij}| \) is positive. \( \delta_{ij} \) is called the penetration length, and \( \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j \) is the distance between particles \( i \) and \( j \). The interaction force has a normal component \( \mathbf{F}_{n_{ij}} \) and a tangential one \( \mathbf{F}_{t_{ij}} \):

\[
\mathbf{F}_{n_{ij}} = -k_n \delta_{ij} \mathbf{n}_{ij} - \gamma_n m_{eff} \mathbf{v}_{n_{ij}}
\]

Here \( k_n \) and \( k_t \) are elastic moduli, \( \mathbf{n}_{ij} = \mathbf{r}_{ij}/|\mathbf{r}_{ij}| \), \( v_{n_{ij}} = [v_i - v_j] \cdot \mathbf{n}_{ij} \), \( v_{t_{ij}} = v_i - v_j \), \( m_{eff} \) is the reduced mass, and \( \gamma_n \) accounts for dissipative character of the normal component. \( \mathbf{u}_{k_{ij}} \), set to zero at the beginning of a contact, measures the shear displacement during the lifetime of a contact. Its time evolution is fixed by \( \mathbf{v}_{k_{ij}} \) and \( \omega_i \) and \( \omega_j \), as described in Ref. [22]. The presence of tangential forces implies the presence of torques, \( \tau_{ij} = -1/2 \mathbf{r}_{ij} \times \mathbf{F}_{t_{ij}} \). We use the value of the parameters of [22]: \( k_n = 2 \times 10^5 \), \( k_t/k_n = 2/7 \), \( \gamma_n = 50 \). Length, masses and times are expressed in units of \( D \), \( m \) and \( \sqrt{m/k_n} \). We vary the volume fraction \( \phi \), which represents the volume occupied by the grains divided by the volume of the container, by changing the number of particles. The initial state is prepared setting to zero the friction coefficient [25], randomly placing small particles into the system, and then inflating them until the desired volume fraction is obtained; such a protocol is a short-cut of experimental procedures with which it is possible to generate very dense disordered states of frictional systems, such as oscillations of high frequency and small amplitude [26].

We have recently investigated the jamming properties of this system [16] as \( \phi, \sigma, \) and \( \mu \) are varied, and summarize our findings below. Confirming previous results [7], in the frictionless case the system is either found in a flow or in a jammed phase, a single line marking the transition between these two phase in the \( \phi - \sigma (\mu = 0) \) plane. By contrasts, at a finite value of the friction coefficient, more complex rheological regimes are found, corresponding to four distinct regions in the \( \phi - \sigma (\mu > 0) \) plane, as illustrated in the schematic jamming phase diagram reported in Fig. 1.

On increasing the volume fraction the system visits the following regimes: Flow, Flow & Jam, Slip & Jam, Jam. In each of these regime the system exhibits

![Fig. 1](Color online) Jamming phase diagram in the density-shear stress \( (\phi - \sigma) \) space at a fixed value of the friction, \( \mu = 0.8 \). Three transition lines bound the different regions.
a different response to the applied shear stress $\sigma$, as illustrated in Fig. 2 where we show the time evolution of the velocity of the shearing top plate. The different regimes can be characterized as follows:

**Flow**: the system flows with a steady velocity reached after a transient.

**Flow & Jam**: the system reaches a steady velocity after a transient. However, after flowing for a time, $t_{jam}$, it suddenly jams.

**Slip & Jam**: the system jams after a small inelastic displacement of the top plate. Steady flow is never observed.

**Jam**: the system responds as an elastic solid.

The value of the volume fraction ($\phi_{j1}$, $\phi_{j2}$, and $\phi_{j3}$) marking the transition between the different regimes depend both on $\sigma$ and $\mu$, and their identification [16] allow to describe the overall phenomenology in a three-dimensional jamming phase diagram in the $\phi, \sigma, \mu$ space. In the limit $\sigma \rightarrow 0$ the transition from the ‘Flow & Jam’ to the ‘Jam’ regime appears to occur at a volume fraction identifiable with random–close packing volume fraction, if one neglects its protocol dependence [23]. We prefer not to associate the other transitions volume fraction to the random loose volume fraction, considering that this has been introduced using a different protocol (pouring), and that this is also expected to be protocol dependent [24].

We have previously investigated the dynamical and geometrical properties in the different regimes [15]. For example, we find that in the ‘Flow & Jam’ region the average value of $t_{jam}$ diverges on approaching the ‘Flow’ regime, thus allowing to identify the transition line $\phi_{j1}$ between ‘Flow’ and ‘Flow & Jam’ region. In addition, the $t_{jam}$ distribution is found to be extremely broad. Moreover, for each value of the friction, $\mu$, we find the mean contact number $Z$ to be constant across the ‘Flow & Jam’ and the ‘Slip & Jam’ regimes. This is in agreement with Ref. [25], even though we also found the constant value of $Z$ to depend on the applied shear stress. We described in Ref. [15] the rheology of the system and living in a sea of spectators [4,5,6]. We show the network of all forces of a system jammed under the action of a constant shear stress. Each segment marks the direction of the force acting between a pair of grains in contact. A color scale is used to represent the force intensities. b) The picture only shows the strongest contacts (10% of all contacts) of the network.

### 3 Mechanical response of jammed states

A minimal model for the structure of fragile systems consists in a series of force chains directed along the strongest stress direction, supporting the applied stress and living in a sea of spectators [15,26]. We show the network of all forces of a system jammed under the action of a shear stress in Fig. 3a. A percolating cluster of contacting particles furnishes the support for the network of force. Finite clusters, except few single particles, called rattlers, are not allowed, since, due to repulsive force acting between particles in contact, a cluster not hold by the confining plates breaks. The network may be also explored investigating how it changes as a function of a threshold on the inter–particle force one may introduce to define the bonds. For instance, in Fig. 3b we show the network of the strongest forces, obtained using a threshold which allow to pick–up roughly
δσ

(b) shows the response at ϕ = 10 the inside, | is small, being values of the perturbing stress (from the inside, σ shear stress. Panel (a) shows the response at Response of a jammed system to a small perturbing shear stress. The non-zero components of this perturbing shear stress are δσzz and δσzy, we fix in such a way that δσz2 + δσ2y = δσ2. The perturbing shear stress is therefore conveniently expressed in terms of δσ and of θ = arctan(δσy/δσx).

Figure 4 shows the displacement δr = (δx, δy) of the top plate position for different values of the volume fraction (from 0 to 2π). While the network of existing shear stress, σzz = σ, by superimposing a perturbing shear stress. The non-zero components of this perturbing stress are δσzz and δσzy, we fix in such a way that δσz2 + δσ2y = δσ2. The perturbing shear stress is therefore conveniently expressed in terms of δσ and of θ = arctan(δσy/δσx).

Fig. 4 Response of a jammed system to a small perturbing shear stress. Panel (a) shows the response at σ = 10−2 , and δσ = 10−4 for different values of the volume fraction (from the inside, φ = 0.655, 0.630, 0.617, 0.613 and 0.610). Panel (b) shows the response at φ = 0.617, σ = 10−2, for different values of the perturbing stress (from the inside, δσ = 10−3, 5 10−3, 10−2, 2.5 10−2, 5 10−2, 7.5 10−2, 10−1).

10% of all forces (strongest ones). While the network of Fig. 3a appears to be isotropic, that of Fig. 3b appears highly anisotropic, with force chains lying in the direction of the strongest stress, and resembles that mentioned by Cates et al. If the response to external perturbations is dominated by these strong forces, one may therefore expected a ‘fragile’ behavior.

In order to check this point, we probed the elastic properties of a system jammed under the action of the existing shear stress, σzz = σ, by superimposing a perturbing shear stress. The non-zero components of this perturbing stress are δσzz and δσzy, we fix in such a way that δσz2 + δσ2y = δσ2. The perturbing shear stress is therefore conveniently expressed in terms of δσ and of θ = arctan(δσy/δσx).

Figure 4 shows the displacement δr = (δx, δy) of the top plate position for different values of the volume fraction at fixed σ and δσ (left), and for different values of δσ at fixed σ and φ (right). Each curve is obtained applying a perturbing shear stress with (θ = 0), and then increasing θ from 0 to 2π. While open path were expected for restored flow, we find that each curve describes a close path, which implies that the system responds elastically to the applied force. Moreover, this path is to a good approximation a circle (|δr| ≃ const), which implies that the elastic response is the same for all values of θ. An estimation of the degree of anisotropy in the response if obtained by measuring the parameter

\[ \xi(θ) = \left[ \frac{δx^2(θ) + δy^2(θ)}{g} \right]^{1/2} - \overline{δr}, \]

where \( \overline{δr} = \left[ \frac{δx^2(θ) + δy^2(θ)}{g} \right]^{1/2} \).

As illustrated in Fig. 5, the anisotropy of the system is small, being |\( \xi(θ) \)| < 4% and does not reveal any particular pattern.

Fig. 5 (Color online) Anisotropy in the response to a small perturbing shear stress of a system jammed under the action of a large shear stress. Different curves refer to different values of the volume fraction. Using the same protocol of Fig. 4, response of a jammed system at φ = 0.606, σ = 10−2 to a perturbation δσ = 10−4. The open path signals the presence of restored flow.

Being the response to small δσ elastic (the strain is proportional to the stress) and to a good approximation isotropic (the strain does not depend on θ), as clarified by Fig. 4 and Fig. 5, the system is characterized by a well defined shear modulus G = limδσ→0 δσ/ε, where ε = δr/Lz is the shear strain induced by δσ. As a further characterization of the mechanical properties of the system, we have studied the Hessian along the line of Ref. [28], only finding zero eigenvalues (expected due to the presence of rattlers), and negative ones, while positive values are expected for fragile solids.

This analysis clarify that frictional granular systems jammed at constant volume and applied shear stress are not fragile, as they respond elastically to small perturbations, regardless to their orientation. The absence of fragility can be rationalized in terms of the properties of the energy landscape of the system. Indeed, fragile jammed systems can be associated with saddle points, as their elastic energy may increase or decrease, depending on the direction of the perturbation, respectively leading to an elastic response or to an instability.

Since dissipative systems do not spontaneously arrest in an unstable point of their energy landscape, we ex-
expect them to arrest in a true energy minimum. Systems that jam under the action of an applied stress are, therefore, not expected to be fragile. Of course, restored flow predicted by fragility, may appear in response to large stress variations, which are able to carry the system away from an energy minimum. Indeed, at higher \( \delta \sigma \), we find that curves like those in Fig. 4 become more and more elliptic, signaling the emergence of anisotropy.

At a threshold \( \delta \sigma \), these curves turn in open paths, such as the spiral shown in Fig. 5, which evidence the presence of restored flow. The value of the threshold depends on the volume fraction, \( \delta \sigma_c = \delta \sigma_c(\phi) \) as well as on the applied shear stress. In the explored rage of volume fractions, we have never observed a fragile behavior when the relative variation of the shear stress is \( \delta \sigma_c / \sigma < 10^{-3} \).

These results suggest that in the response to small perturbations the systems probes the roughly isotropic network of all forces of Fig. 3, rather than the strong network of Fig. 5.

4 Stress cycle

As discussed in the previous section, the mechanical response of jammed grains in the investigated range of control parameters resembles that of other elastic solids. However, granular systems are also expected to exhibit a plastic response, as other disordered systems. We have investigated this possibility probing the response of the system to stress-strain cycles. In Fig. 6 we have used this approach to locate the line separating the ‘Slip & Jam’ and the ‘Jam’ region in the jamming phase diagram of Fig. 1. Here we focus on the degree of plasticity emerging in the solid response for increasing value of the shear stress.

We have measured stress-strain curves when the system undergoes a stress-cycle for values of the control parameters which span from the ‘Flow & Jam’ to the the ‘Jam’ region. Precisely, after preparing the system, we slowly increase the shear stress \( \sigma \) up to a maximum value \( \sigma_m \), and then decrease it to zero. After each stress cycle we measure the residual strain \( \epsilon = \Delta L / L_z \), where \( \Delta L \) is the displacement of the top plate.

At low volume fraction, in the ‘Flow & Jam’ regime, the initial state of the system is not jammed, and accordingly we expect a finite residual strain at the end of the cycle, \( \epsilon_r > 0 \). Conversely, at higher volume fraction the system has a solid response, we expect to be elastic (\( \epsilon_r = 0 \)) at small \( \sigma_m \), and plastic (\( \epsilon_r > 0 \)) for \( \sigma_m \) overcoming the yield stress. Figure 7 shows the strain as a function of the shear stress for a small value of the maximum stress, \( \sigma_m = 10^{-4} \), and different volume fractions. Accordingly to the expectations, the residual strain becomes smaller as the density increases, and appears to critically vanish at \( \phi_j \), which has been determined via a numerical fit, as shown in Fig. 8. On increasing \( \sigma_m \), a finite residual strain \( \epsilon_r > 0 \) is also found at higher volume fractions. This is shown in Fig. 8 where we observe that \( \epsilon_r \) vanishes on increasing \( \phi \) at small \( \sigma_m \), while it decreases and then bends at larger \( \sigma_m \).

The crossover in the behavior of \( \epsilon_r \) can be related to a change from a visco–elastic to a plastic regime, and may be explained focusing on the increase of the number of contacts that break as the strain increases. At small stress, the strain of the system is small, contacts do not break and the system responds elastically. At higher stress, the strain of the system is large, and contacts break. This is the microscopic origin of the plastic response, as the system looses memory of the tangential force of the contacts reaching the Coulomb threshold.
5 Conclusion

We have investigated the mechanical response to small perturbations of systems jammed under the action of an applied shear stress, and found this to be elastic and isotropic, and therefore not consistent with the expectation of a ‘fragile’ state. This result is explained considering that the response to small perturbations see the cooperation of all contact forces, which are isotropically distributed in the systems. Conversely, the response to large perturbation is due to the strongest forces, which are not isotropic. Accordingly, we have found that large perturbations lead either to an anisotropic response, or to unjamming. The investigation of the response of the system to stress–cycle, also allowed to observe the transition from an elastic to a plastic response as the maximum applied stress increases.

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