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Role of angular correlations on the mechanical properties of 2D packings of cylinders

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Abstract. We have studied the mechanical properties of two-size disc mixtures, in relation to their geometrical structure. These packings present an orientational order: the spatial extent of this order, depending on the composition of the sample, has been measured in terms of a characteristic length ξ . The stress–strain law in an oedometric compression is particularly sensitive to the disorder of contacts between the discs, but also clearly depends on orientational order.

1. Introduction

From a general point of view, the mechanical properties of granular media are described as dependent on density—the denser the packing, the stronger it is—and/or on the mean coordination number—stresses are transmitted only by contacts between grains. These two geometrical characteristics, density and coordination number, are average parameters, and the description of the mechanical properties starting from such quantities often supposes that the medium is homogeneous, i.e. that the representative elementary volume is small compared to the volume of the sample studied. At this large scale, one generally considers the granular medium as continuous, in order to describe its mechanical properties.

In fact, this description is not very accurate. A granular material always presents a disorder of contacts: all the contacts do not play the same role; they can be different geometrically (real contacts or near neighbours) or physically (different surface states, for example). Most of the properties of such materials in the grain space are very sensitive to that disorder (Guyon *et al* 1990). For example, in studying the compression of two-dimensional (2D) models (packings of cylinders with parallel horizontal axes), we have shown (Travers *et al* 1987) that the macroscopic stress–strain characteristic is non-linear, not essentially because of the non-linearity of the microscopic (Hertz-type) stress–strain characteristic at the contact between grains (Mindlin 1954), but due to the disorder of contacts. The same result has been obtained by numerical simulations (Herrmann *et al* 1987): the main results of these studies are given in section 2.

This paper is devoted to the experimental study of the effects of angular correlations on this non-linear behaviour. It is easier to perform this sort of experiment on two-dimensional packings of cylinders rather than on 3D packings of spheres:

(i) The geometry of the packings can be determined from direct observations or photographs. Such a determination in 3D is more difficult and generally indirect.

(ii) Photoelastic experiments can give some information on the intergranular stresses and then allow better understanding of the transmission of a macroscopic stress on the system.

(iii) Moreover, in such systems, it is possible to impose some smooth variations of the correlation length relative to orientational order by introducing progressively larger (or smaller) cylinders in a packing of equal grains (Rubinstein and Nelson 1982), as described below.

We have therefore performed a geometrical study, paying particular attention to the evaluation of short-range effects (section 3). Taking into account the results of this first study, we have studied the compression of the same packings (section 4).

2. Statement of the problem

It is useful to represent a packing by a network in which the nodes are the centres of the grains, and the bonds connect the sites if the corresponding grains are in contact. An 'ideal' representation of two-dimensional disc (or cylinder) packings is one where all the bonds are present: the network is a—generally irregular—triangular one. To take into account the disorder of contacts in real packings, Dodds (1975) has proposed to cut randomly some bonds until one obtains the required mean coordination number. This model is very useful, particularly to describe the geometry of packings with grain size distribution. But in actual packings, it is not possible to assume that such a random dilution is relevant, for two reasons: stability imposes a minimum number of contacts for each grain (two for discs under gravity, for example), and, more important, the building procedure imposes some geometrical correlations. In 2D packings of discs (or cylinders), these correlations can be long range. If the discs are nearly equal, the packing is geometrically ordered: the representative network is a regular triangular lattice, with a disorder of contacts created by the—even weak—fluctuations in the radii of the grains. But if the packing has been built under gravity, the probability for a contact to be real is large following the two directions y and z , and weak following the third one (horizontal x) (see figure 1): so, long connected arms can spread out along the two directions y and z , as can be observed in photoelastic experiments described below. In materials in which orientational order exists at a more or less large scale, such arms may be present whose role in mechanical properties is expected to be important: the length of these arms is in some way a measure of the distance at which there are correlations in the transmission of the stresses.

In our first mechanical experiments (Travers *et al* 1987), we have studied short Plexiglass cylinders with the same diameter (4 mm), packed with horizontal parallel axes. The cylinders are arranged according to the regular triangular network, in a U-shaped rigid frame (48 rows of alternately 44 and 45 cylinders) and a force F is applied at the top of the packing. The compression is then oedometric (and not uniaxial) because the vertical walls of the frame are stressed. The length of the cylinders (2.5 cm) was chosen to avoid an overall buckling of the system under compression. In fact, the

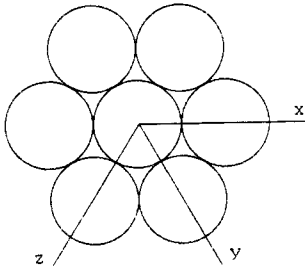


Figure 1. Directions of the contacts in an ordered packing.

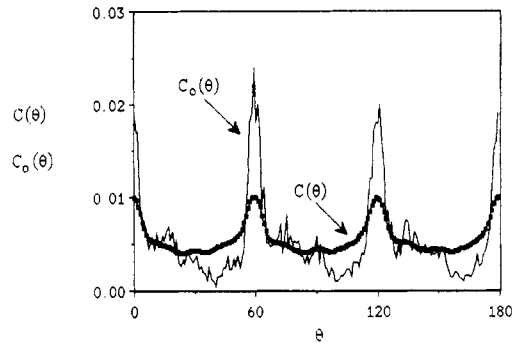


Figure 2. Angular distribution functions $C_0(\theta)$ and $C(\theta)$, as defined in the text, for a packing with 2% of impurities.

cylinders present geometrical defects (diameter fluctuations, ellipticity, bending, etc), essentially due to the annealing necessary to eliminate the residual constraints inconvenient to photoelastic studies. So, the diameter of the cylinders used for these 'ordered' packings is estimated to be 4 ± 0.1 mm: this diameter distribution leads to a disorder of contacts, and the representative network is then a 'dilute' regular triangular lattice.

As mentioned above, we expect a strongly non-linear stress-strain law, which may be written as:

$$F/F_0 = (\Delta h/h_0)^m$$

where h_0 is the initial height of the packing, Δh the deformation, F_0 a prefactor and m the 'macroscopic exponent', depending on the nature of the mechanical contacts—according to Hertz or Mindlin laws (Mindlin 1954)—and on the geometrical and contact disorders of the system (Travers *et al* 1987). m is close to 3.5 for our 'ordered' packings of Plexiglass cylinders. With the same experimental apparatus, we have studied very well defined steel cylinders: taking into account their geometrical defects, their diameter is 4 ± 0.01 mm. The exponent m is found to be smaller, close to 2.2. The difference can be attributed to the difference in the disorder of contact, due to the geometrical defects of the grains. This assumption is confirmed by numerical simulations (Herrmann *et al* 1987), and the effective medium arguments explain the difference between microscopic and macroscopic exponents because of disorder of contact (Roux and Herrmann 1987).

Another effect of this disorder is observed in photoelastic experiments, in which packings of birefringent cylinders (for example, made of Plexiglass), placed between crossed polarizers and submitted to external pressure, are observed along their axes. Such an experiment shows structures of continuous lines of bright—stressed—cylinders, forming a network which becomes progressively richer as more and more cylinders get in good contact. This active mechanical sublattice was first observed by Dantu (1957). The geometry of this sublattice is dependent on the geometry of the sample.

We have performed two experiments to display the dependence of m on the structure of the packing, and to try to connect the non-linearity to the observed photoelastic network. We have shown first (Travers *et al* 1987) that the removal of a fraction of unstressed cylinders (defined by photoelastic observations) does not modify the value of m , whereas m greatly decreases if the stressed cylinders are removed. The second

experiment concerned the mechanical size effects on the same 2D systems (Travers *et al* 1988). These mechanical size effects are first due to friction at the walls of the frame containing the sample, and also to the size itself. Our experimental study, in which the height of the sample is equal to or smaller than its width, has shown that friction does not appreciably modify the mechanical non-linear behaviour of the packings, which depends greatly on the size of the sample: such experiments indicate a characteristic length much larger than the grain size, and which is essentially defined by the geometry of the system. Whilst the role of the contact disorder is clear after these experiments, this is not the case for the role of angular correlations.

3. Geometrical study of disordered packings

To create disorder, we use the idea of Rubinstein and Nelson (1982) by progressively introducing impurities (cylinders of 6 mm diameter) in the ordered packing described above. The diameter of these impurities has been chosen to allow smooth variations of the translational and orientational orders.

The disordered mixtures are built grain by grain, the diameter of the grain to be added to the system being determined from a pseudo-random-number generator program. Whatever the composition of the mixtures, the area of the packing is kept constant, and equal to that of the ordered 'monosize' packings. We define the concentration s of impurities as

$$s = S_i / (S_c + S_i)$$

where S_i is the surface occupied by the impurities and S_c the surface occupied by the 4 mm cylinders. s does not exceed 45%.

Rubinstein and Nelson (1982) have studied the phase diagram of a packing of discs of radius R_1 as a function both of the number of impurities (discs with radius $R_2 \neq R_1$) and of the ratio R_2/R_1 . Their samples were built numerically according to Bennett's (1972) algorithm: each new disc is added to the system at the place nearest to the centre of the system and with at least two contacts with it. Rubinstein and Nelson showed the existence of a hexatic phase characterized by orientational order, between the domains of existence of the crystalline and amorphous phases: in other words, the correlation length ξ_6 relative to orientational order (six because of local six-fold crystallographic axes) is always greater than ξ_T , the translational correlation length. Our building procedure is different, but we expect the same smooth variations of the scale of the orientational (or angular) correlations.

One of the main problems in this sort of experiment is the presence of the walls of the rigid frame necessary for the mechanical study. Because they are compatible with the triangular order characteristic of 2D dense equal disc packings, these plane walls impose some correlations—relative to translational and orientational order—at distances which can be larger than the sample size in the case of packings with a low number of impurities. The structures used by Rubinstein and Nelson are also very dependent on their seed.

To try to minimize these wall effects, especially those created from the bottom, we have used the following building procedure. The frame is put upside down. The first half of the piling is built between the lateral walls of the frame, starting from the lower horizontal plate. Its 'surface' is slightly corrugated, because of the grain size distribution. It is then pushed up until its top comes in contact with the upper horizontal wall of the

frame. Thus, we minimize the order due to this wall. The frame is then given back its normal position and the rest of the packing is built above the cylinders already in position. However, we shall see below that some wall correlations remain.

We have made two photographs of each packing to characterize its geometry; the first is a 'natural' one, and for the second, the packing is placed between crossed polarizers in order to study the photoelastic properties of the samples. From the first, we use a digitizer table to create a file giving the centre of each grain, thus defining a lattice whose sites are these centres, and with bonds linking two nearest-neighbours centres in the Voronoï tessellation. Such a network is a completely triangulated one, with no gaps. Because it is too difficult to distinguish between real and not real contacts in 2D packings of cylinders, we have chosen to use this network to characterize our samples.

Starting from this file, our goal is to measure the orientational correlations, with particular attention to short-range ones. We are mainly interested in short range order, in fact at distances less than $40 R_1$ from the centre of a given site (R_1 is the mean radius of the small cylinders). On the other hand, the finite size of our samples (approximately 2000 cylinders) does not allow us to neglect the wall effects, even if they have been reduced by our building procedure. Figure 2 illustrates the problems we have met in 'measuring' the orientational order. It shows two different 'angular distribution functions' for the same sample with a concentration of 2% of impurities; these functions both give the probability for a given bond between two small cylinders to have an angle θ with a given direction. The first function, $C_0(\theta)$, is obtained with the horizontal direction, i.e. one of the imposed directions of the sample, taken as the reference for measuring the angles.

For the second function, $C(\theta)$, we change the reference axis at every site i (small cylinder): by choosing one of the bonds of the site i as the angular reference, the same calculation as for $C_0(\theta)$ leads to $c_i(\theta)$ at each site i , and, doing that for all the N small cylinders of the sample, we obtain:

$$C(\theta) = \frac{1}{N} \sum_i c_i(\theta).$$

Two reasons can be invoked to explain the difference observed. The first comes from the fact that $C(\theta)$ is a mean value, so the height of the peaks is reduced. The second is a physical one: $C_0(\theta)$ takes into account the correlations arising from the walls, which impose the orientation of a more or less important zone of the sample. So, the height of the peak can be partly explained, as can the fact that we observe secondary peaks, corresponding to domains of order with other principal orientations.

One can define a short-range orientational order parameter X from $C(\theta)$ by the expression:

$$X = (h - h_0)/h$$

where h is the mean height of the peaks at 0° , 60° , 120° , and h_0 is that of the background. Figure 3 gives the variations of X versus s . One can observe that orientational order subsists for relatively large concentrations (as large as or larger than 20%) of impurities.

It is interesting to measure the spatial extent of that orientational order. We have then defined a new function $Y(r)$, in the same way as X , but taking only into account in the determination of $c_i(\theta)$ the sites which are at a distance less than r from the site i . Moreover, in order to minimize the wall effects, the sites i on which the measurements

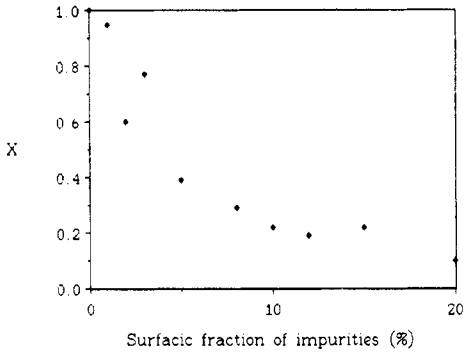


Figure 3. Variation of the orientational order parameter X with s , the concentration of impurities (diameter 6 mm) in a packing of equal cylinders (diameter 4 mm).

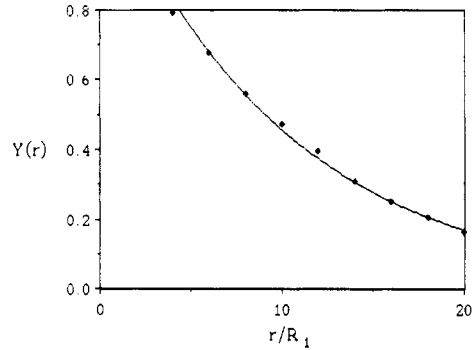


Figure 4. Variation with the distance r of the orientational order parameter Y for a 25% impurity concentration. The experimental points are well fitted (full line) by the law, $Y(r) = 1.235 \exp(-r/10R_1)$, where R_1 is the radius of the small cylinders.

are done are situated at a distance larger than r from the walls. Figure 4 gives the variations with r of $Y(r)$ for a packing with a concentration of 25% of impurities. One can think that these variations, which are of the form $\exp(-r/\xi)$, allow us to define a correlation length relative to orientational order. Such experimental behaviour is expected for large r in the case of translational order, leading to the definition of the correlation length, but not for the orientational order (Halperin and Nelson 1978). Nevertheless, we can consider that we obtain a length ξ characteristic of the angular correlations in our samples. Such a length is an *a priori* measure of the correlations in the 'stress propagation', as indicated above. The variation of ξ with the concentration of impurities is given in figure 5; the fluctuations of these variations are due to the finite size of the samples: in particular, for concentrations smaller than 10%, the correlation length is larger than the sample.

4. Mechanical study

The experiments are performed on an Instron 1175 universal testing machine. The range of forces F applied to the sample runs from 0 to 2000 N, so that the overall displacement Δh is small, and the local deformations remain elastic. About 20 pressure cycles are necessary to obtain a reproducible (non-linear) macroscopic response.

The first step of our mechanical experiments is to visualize, by photoelastic experiments, the spatial distribution of the stresses in our packings. Figure 6 gives a photoelastic view of a packing containing 5% of impurities (6 mm diameter discs), and submitted to the maximum force $F = 2000$ N: the long bright arms we observe are clearly a proof of the existence of angular correlations in the transmission of the stresses, and it is also clear that the photoelastic network is a subnetwork of the geometrical one.

We have measured the variations of the exponent m with s (from 0 to 45%). First, for a given concentration of impurities, the value of m fluctuates greatly from sample to sample. The smaller is the concentration, the larger are the fluctuations. It is clear that this effect is due to the finite size of our samples; the correlation length is then of the

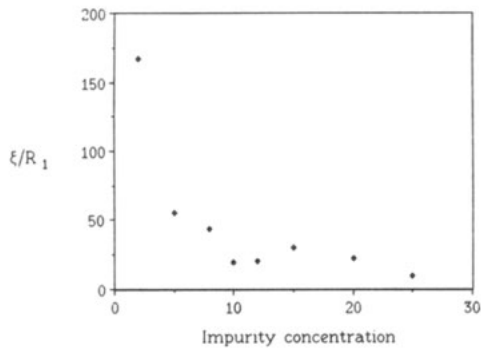


Figure 5. Variation of the correlation length ξ with the concentration of impurities.

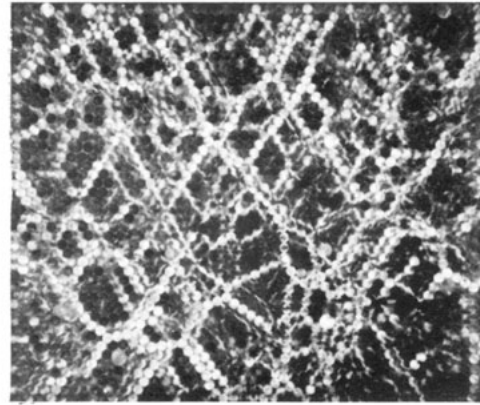


Figure 6. Photoelastic view of a packing with 5% of impurities and a compression vertical force $F = 2000$ N.

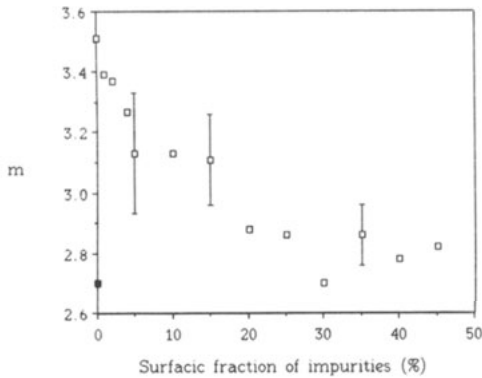


Figure 7. Variation of the exponent m of the macroscopic stress–deformation law with s .

order of the size of the samples. The complete results are given in figure 7: the value of m is an average, obtained from measurements on three different samples with the same composition.

We observe a decrease in m from 3.5 (for a geometrically ordered packing) to a value close to 2.7, which is also the value obtained with a disordered packing of equal (4 mm diameter) cylinders: in this case, the disorder is obtained by placing a small number of large cylinders at the walls of the sample. On the other hand, as expected, the variations in m are comparable to those in X : it is clear that for concentrations of impurities larger than 5%, no translational order is present in our sample, whereas angular correlations are still present for concentrations larger than 20% (see figure 3).

5. Conclusion

Plexiglas cylinders, which are not precision manufactured objects, are in fact good tools for the analysis of the different parameters responsible for the strong non-linearity of

the stress–strain law. Clearly, the macroscopic deformation law in our models of packings is very sensitive to two types of disorder:

(i) Angular correlations in transmission of the stresses, due to the ‘orientational order’ in the packing, are very important in the structure of the observed photoelastic sublattice: the length of the observed bright arms depends essentially on them. It is clear that they modify the macroscopic behaviour of the packing, i.e. the exponent m . However, with 4 mm diameter Plexiglas cylinders, it has not been possible to obtain values of m smaller than 2.7, a value much larger than that expected (1.5–1.8) according to Hertz or Mindlin microscopic law (at the scale of the contact between grains).

(ii) Thus we must conclude that the most important dependence is related to contact disorder which is responsible for the gap between the microscopic (1.5) and macroscopic (2.7) exponents.

An open question is how can we determine more accurately the exact part of the finite size effects on the behaviour observed.

Acknowledgments

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