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## Simulation of disordered systems of cylinders. II. Mechanical behaviour

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**Résumé.** — Nous présentons une simulation numérique utilisant une technique de relaxation non linéaire modélisant le comportement d'un empilement aléatoire de cylindres durs et mous. De plus, les cylindres durs présentent de faibles fluctuations de rayon. La dépendance force-déplacement macroscopique est comparable au comportement microscopique (loi de Hertz) pour des cylindres de même taille. Au contraire, les fluctuations de rayon sont responsables de changements importants du comportement macroscopique. Pour environ 80 % de cylindres durs, nous observons un seuil de « percolation » élastique.

**Abstract.** — A model is simulated, with non-linear relaxation methods close to molecular dynamics, describing the mechanical behavior of a random array of hard and soft parallel cylinders. Moreover, the hard cylinders fluctuate slightly in their radii. The relation between compression and force is about the same for the whole system as it is for two cylinders (Hertz law), if only soft cylinders exist. Instead, the radius fluctuations of the hard cylinders produce drastic deviations between the macroscopic and the microscopic elastic response. For about 80 % of infinitely hard cylinders we observe an elastic « percolation » threshold.

### 1. Introduction.

This second part of our simulation of disordered systems of cylinders studies the compression of this model, introduced in the companion paper [1], of a composite random material under an external force. Many parallel cylinders are packed together; each cylinder is either hard, with probability  $p$ , or soft, with probability  $1 - p$ . The soft cylinders have all the same radius; the radii of the hard cylinders fluctuate by one percent. Cylinders which do not touch each other exert no forces whereas compressed cylinders follow the (non-linear) Hertz law of elastic response. In an experiment [2] the soft cylinders consist of rubber, the hard ones of plexiglass. Now we first describe in detail the model and its numerical solution, then the various results.

### 2. Techniques.

The force  $F$  on a soft cylinder of equilibrium radius  $R$ , exerted by a parallel plane of distance  $r$  from the axis of

the cylinder, is assumed to vary with the microscopic exponent  $\mu$ :

$$F = 0 \quad \text{if } r > R \quad (1a)$$

$$F = (R - r)^\mu \quad \text{if } r < R. \quad (1b)$$

Here  $R = 1/2$  in units of the lattice constant of the triangular lattice formed by undisturbed soft cylinders. Thus the various prefactors from elasticity theory are incorporated into our definition of the dimensionless force. Since the cylinders are supposed not to fluctuate in shape or radius along their axis, we can simply consider the problem to be two-dimensional. The « force » in equation (1) is therefore in reality a force per unit length.

In the simulation of the whole system, we exert opposite and equal forces on the cylinders in the outermost layers; these forces are thought to come from the two missing neighboring cylinders which would be present had we chosen a larger system (see Fig. 1). Thus in our calculation a unit force corresponds actually to a force  $\sqrt{3}$  exerted per unit length on every cylinder in the top and in the bottom layer.

For a pair of hard cylinders, equation (1b) is replaced by  $F = A^\mu (R - r)^\mu$  with a factor  $A$  of proportionality typically equal to 2 in our case, much smaller than the

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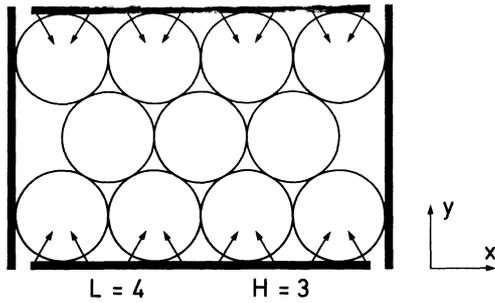


Fig. 1. — Geometric setup of a cylinder lattice of height  $H = 3$  and length  $L = 4$ . Forces are applied to the top and bottom layers, as shown by arrows. Note that  $H$  has to be odd. The heavy lines denotes solid bars.

experimental value. (Our convergence was lost for  $A$  much larger than 10).

The microscopic elastic exponent  $\mu$  defined by equation (1b) is known [3] to be  $3/2$  (« Hertz law ») for spheres and for cylinders whose axes are not exactly parallel. Most of our calculations used this value  $\mu = 3/2$  since experimentally one cannot expect the cylinders to be exactly touching (for zero force) along the whole line. We will show that the choice  $\mu = 1$  does not change much our results. In the analogy with nonlinear electrical resistivity calculations [4] one should regard  $\mu$  as a free parameter. Empirically reference [2] finds  $\mu = 1.8 \pm 0.1$ , for a pair of plexiglass cylinders presumably due to shape imperfections along the axis. Note, however, that even for  $\mu = 1$  our model differs from the usual central force elastic model [5] because we have only repulsive, no attractive forces (« diode effect »). Also, in contrast to some experimental situations, no torques are felt by our cylinders ; one can imagine them to be immersed into an excellent lubricant [2].

For the hard cylinders, we assumed mostly a distribution of radii homogeneous between 0.49 and 0.51 (« continuous distribution »), but we will also give results with a bimodal distribution where each cylinder has either the radius 0.49 or, with equal probability, the radius 0.51. In that bimodal case, both hard and soft cylinders fluctuated in their radius. Finally, to estimate a rigidity threshold  $p_R$  of cylinder mixtures with infinite force ratio  $A$ , we used the same radius for all cylinders, hard and soft.

The force between two cylinders of radius  $R_1$  and  $R_2$  and distance  $r < R_1 + R_2$  between the cylinder axes is thus

$$F = (R_1 + R_2 - r)^\mu / (1 - a(1 - 1/A))^\mu \quad (2)$$

with  $a = 0, 1/2$  and  $1$  for soft-soft, soft-hard and hard-hard contacts. For a given external force, typically of order 0.001, we then calculated by an iteration procedure the equilibrium position of the cylinders. We started with a triangular lattice and then let the

cylinders move continuously in the direction of the force until the forces and the movements become negligibly small. If the total force exerted in  $x$ -direction on a cylinder is  $F_x$ , then its centre is shifted by  $\omega F_x$  into the  $x$ -direction, with  $\omega$  chosen typically as about  $1/2$ . The same  $\omega$  applies for the analogous shift in  $y$ -direction. Our model thus is not a lattice approximation ; instead it has similarity to a molecular dynamics simulation on a continuum. (To simplify the calculation, we took the  $x$ - and  $y$ -components of a force calculated from equation (2) always as  $\pm 1/2$  and  $\pm \sqrt{3}/2$  of that force, since our distortions from the original lattice structure amount only to a few percent or less. For much larger deformations also equations (1), (2) would have to be modified).

Once a cylinder has been shifted in the direction of the force applied on it, we go to its neighbor in positive  $x$ -direction, and apply the same procedure to it. Thus our program went through the lattice like a typewriter. After having gone through the lattice once, the next iteration starts in the upper left corner, and so on.  $10^2$  to  $10^4$  iterations were made to find a good equilibrium, mostly of systems of length  $L = 50$  and height  $H = 5$ . (For larger  $H$  one needs much more iterations ; for larger  $L$  the probability for numerical instabilities is enhanced).

The  $y$ -coordinates of the cylinders in the bottom row were kept fixed, as well as the  $x$ -coordinates of the rightmost and leftmost column of cylinders. The  $y$ -coordinates of the cylinders in the top row were all forced to be equal. We then calculated the relative compression  $\delta$  as

$$\delta = 1 - y_{\text{top}} / (H^* \sqrt{3}/2) \quad (3)$$

where  $y_{\text{top}}$  is the  $y$ -coordinate of the top row. Equation (3) is true only for the case of zero fluctuations in the radius since this  $\delta$  measures the compression relative to the height  $H^* \sqrt{3}/2$  for the undisturbed triangular lattice. If the radii are not all the same, then even for zero force the coordinate  $y_{\text{top}}(F = 0)$  is no longer  $H^* \sqrt{3}/2$  but larger. We thus have to find by extrapolation the (negative) compression

$$\delta_0 = 1 - y_{\text{top}}(F = 0) / (H^* \sqrt{3}/2) \quad (4a)$$

for zero external force, and define the compression  $\delta$  with external force as

$$\delta = 1 - \delta_0 - y_{\text{top}} / (H^* \sqrt{3}/2) \propto y_{\text{top}}(F = 0) - y_{\text{top}} \quad (4b)$$

We cannot use the zero-force expansion calculated in reference [1] for our purposes here since it depends strongly on the length  $L$  of the system and since it was calculated by building up the system row by row, and not through the different zero-force limit of our iteration.

3. Results.

Now we present, mostly in graphical form, the results of our simulations.

With only soft cylinders,  $p = 0$ , all having the same radius, the macroscopic and the microscopic behaviour are about the same. That means we assume  $\mu = 3/2$  for the force between two cylinders, and then get

$$\text{force} \propto (\text{compression})^{3/2} \quad (5)$$

for the force needed to compress the whole system. This result agrees with the experiments for rubber cylinders [2]. Only for very large forces, when the compression  $\delta$  is more than just a few percent, do we find slight deviations due to lattice distortion ; thus  $\delta$  should be restricted to  $\delta \leq 0.1$  in this work.

When hard cylinders are added with concentration  $p$ , we first try to determine a rigidity threshold  $p_R$  for the case of all hard cylinders also having the same radius. Geometrically, for all concentrations  $p > p_c = 1/2$  the hard cylinders form an infinite network [5] connected by nearest-neighbour distances (site percolation on a triangular lattice). But the rigidity threshold  $p_R$  can be larger [5, 6] than this percolation threshold  $p_c$ . To find it we let  $A$  (i.e. the ratio of forces needed to compress a hard and a soft cylinder by the same amount) go to infinity and check from which concentration  $p_R$  on we find no compression at all (see Fig. 2).

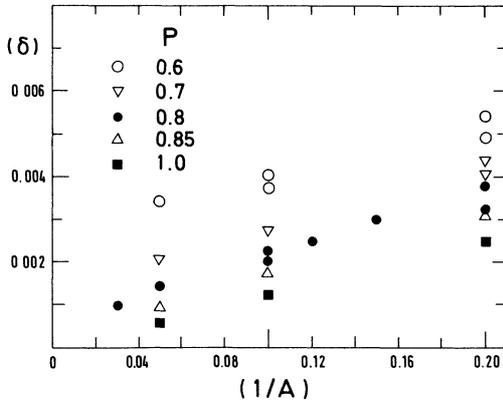


Fig. 2. — Search for rigidity threshold, without radius fluctuations ( $\mu = 1.5$ , force = 0.001). The compression  $\delta$  is plotted linearly versus  $1/A$ , the ratio of soft versus hard microscopic elastic response. For  $A = \infty$  we estimate a phase transition at  $p = 0.8$  (one fifth soft cylinders) where the extrapolated macroscopic response vanishes.

Figure 2 suggests that in this limit for  $p < 0.8$  one finds a finite compression whereas for  $p > 0.8$  the compression approaches zero if  $1/A$  goes to zero. Thus, for this limited system size, the rigidity threshold is

$$p_R = 0.8 \quad (6)$$

for our model, roughly compatible with the experimental [2] estimate 0.7. The bond percolation

threshold 0.655 of references [5] and [6] corresponds, to first order in  $1 - p_R$ , to a site percolation threshold  $1 - p_R = \frac{1}{2}(1 - 0.65)$ , thus  $p_R \approx 0.825$  compatible with equation (6). However, in contrast to references [5] and [6], our forces are zero if the cylinders do not touch. For  $p = p_R$  one expects a nontrivial power law relating compression and force ratio  $A$ ; but our  $5 \times 50$  systems are not large enough to estimate reliably the corresponding critical exponent.

For a bimodal radius distribution,  $R = 0.5 \pm 0.01$  for both hard and soft cylinders, we see in figure 3 already what is seen later for the more realistic continuous distribution. The compression  $\delta$  is a complicated function of force. Small forces allow the system to expand compared to the original triangular lattice ; the amount of expansion,  $-\delta_0$ , in the limit of zero force should be extrapolated such that a power law behaviour is found. We see that with an expansion of about 4 % we get a reasonable straight line in our log-log plot for small forces :

$$\text{force} \propto \delta^m \quad (7)$$

with a macroscopic elastic exponent  $m$  near 4, close to the experimental value [2] for pure plexiglass ( $p = 1$ ). Instead, for intermediate forces near 0.01 in our units, the system crosses over to the trivial behaviour of equation (5) observed without fluctuations in the radius, as also shown in this figure. (Except where otherwise noted we work with force ratio  $A = 2$ , height  $H = 5$ , and length  $L = 50$ ).

We thus conclude that small fluctuations in the radius can drastically influence the elastic response because they lead to an expansion of the system in the limit of zero force. A small external pressure then first has to counteract against this initial expansion, and it does so with an effective macroscopic exponent  $m$ , equation (7), much larger than the microscopic exponent  $\mu = 3/2$ . Once the influence of this initial expansion has become negligible, the trivial result  $m = \mu$  is recovered. Before the compression many cylinders do

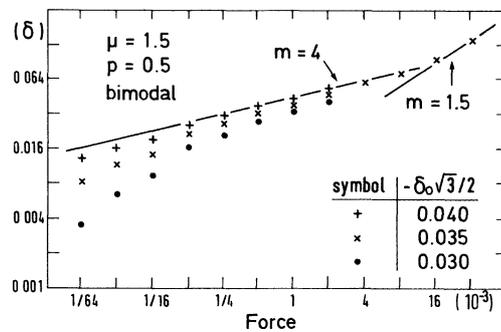


Fig. 3. — Log-log plot of compression versus force for bimodal distribution of radii at  $p = 0.5$  and  $\mu = 3/2$ . Several assumptions for the zero-force expansion are tested. The triangles give the « trivial » result  $m = \mu$  found when all radii were identical.

not touch (thus the initial expansion). During the compression more and more contacts are being made. These contacts enhance the rigidity of the system so much that  $m > \mu$ .

This conclusion is confirmed by our more realistic simulations with a continuous distribution of radii between 0.49 and 0.51, for the hard cylinders only. We find about the same result, whether we use only hard cylinders ( $p = 1$ , Fig. 4), a 50% mixture (Fig. 5), or mostly soft cylinders ( $p = 0.2$ , Fig. 6, and  $p = 0.05$ , Fig. 7). Experimentally a continuous variation of  $m$  with concentration  $p$  was observed in reference [2], in contrast to our simulations at  $p = 0.05, 0.2, 0.5$  and  $1$ .

The elastic exponents  $\mu$  and  $m$  for the microscopic and the macroscopic relation between force and compression are not critical exponents in the sense of phase

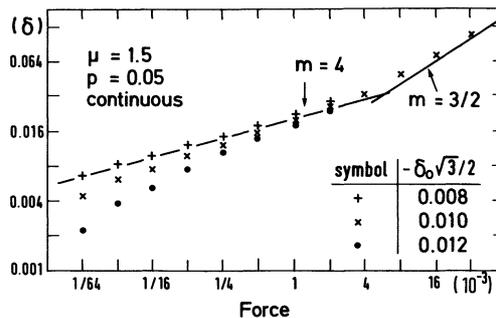


Fig. 7. — As figure 6 but for  $p = 0.05$ .

transitions. Therefore our rather small systems seem sufficient. Figure 8 shows that neither an increase in length  $L$  to 500, nor in height  $H$  up to 51, changes the result appreciably.

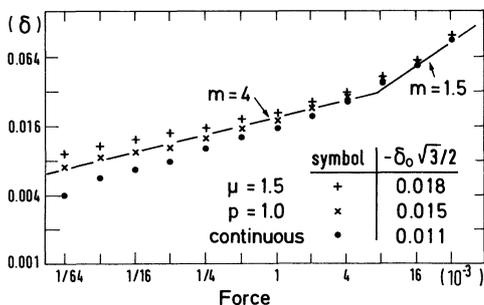


Fig. 4. — As figure 3 but for  $p = 1$  and with continuous distribution of radii between 0.49 and 0.51 lattice constants.

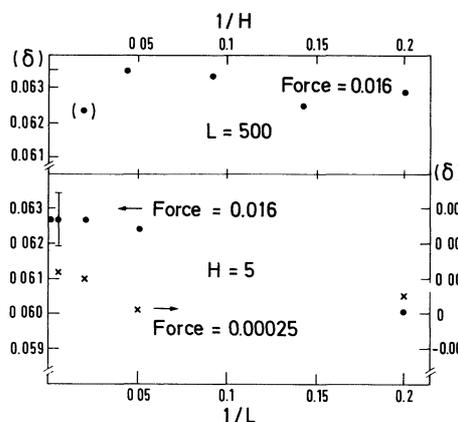


Fig. 8. — Search for finite-size effects. In the top part we plot the expansion versus reciprocal lattice height, in the bottom part versus reciprocal lattice length, for two different vertical forces ( $\mu = 1.5, p = 0$ , continuous).

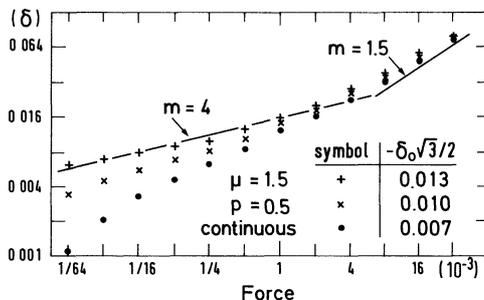


Fig. 5. — As figure 4 but for  $p = 0.5$ ; only the radii of the hard cylinders fluctuate.

All these calculations were made for  $\mu = 3/2$ . Figure 9 indicates that even with  $\mu = 1$  one finds the same qualitative behaviour. The effective exponent  $m > \mu$  is dominated by the expansion  $\delta_0$  in zero force and its influence on the collective elastic response, whereas the microscopic force law ( $\mu$ ) between two cylinders is less important for small forces. The case

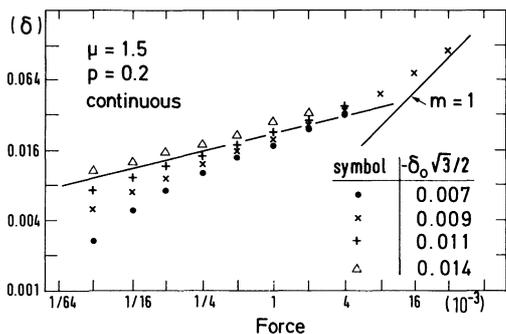


Fig. 6. — As figure 5 but for  $p = 0.2$ .

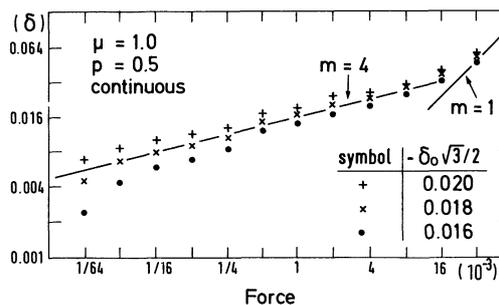


Fig. 9. — As figure 5 but with microscopic exponent  $\mu = 1$ .

$\mu = 1$  is the most sensitive to variations in  $\delta_0$  so that it is the best for a precise determination of  $\delta_0$ . With  $\mu = 3$  again the same effective exponent  $m \gg 1$  is found in figure 10 ; but since now  $m$  is nearly equal to  $\mu$  one does not see anymore the crossover at force near 0.01 for  $\mu = 1$  and  $= 3/2$ .

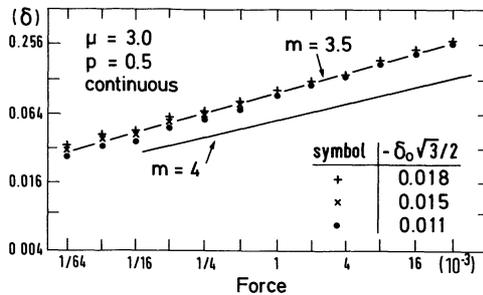


Fig. 10. — As figure 9 but with  $\mu = 3$ .

This absence of a clear crossover allows perhaps for  $\mu = 3$  a more accurate determination than for our smaller  $\mu$  values of the effective exponent  $m$ . Figure 10 suggests

$$m = 3.5 \quad (8)$$

and  $\delta_0 = -0.015$ ; the same  $\delta_0$  should then be used in the cases of figures 5 and 9 since the zero-force expansion must be independent of  $\mu$ . Indeed these two other cases are roughly compatible with such  $\delta_0$ .

Simulations of an analogous but numerically simpler resistivity problem allowed a direct determination of  $\delta_0$  and at very small currents again the macroscopic

exponent  $m$  became equal to  $\mu$  [7]. This throws doubt on our extrapolations for  $\delta_0$ . Nevertheless it confirmed our main result  $m \gg 1$ .

In contrast to some experimental observations it seems that most of the nearest-neighbour pairs of cylinders are exerting forces on each other. Also, the horizontal forces trying to push the side walls out is not very small; for  $p = 0.5$ ,  $\mu = 3/2$  and  $A = 2$  this horizontal pressure is about 1/3 of the external vertical pressure which causes the contraction of the system. Since our vertical boundaries were fixed a measurement of the Poisson ratio is meaningless. No hysteresis in the elastic response was found (for large forces).

#### 4. Summary.

Our simulations have given qualitative agreement with experiment [2]: for a mixture of hard and soft cylinders the macroscopic exponent  $m$  relating force to compression is appreciably different from the microscopic exponent  $\mu$ . We actually found it independent of  $\mu$  and dominated by the disorder from small fluctuations in the radius of the hard cylinders. In contrast to experiment, our effective exponent  $m$  near 3.5 is roughly independent of the mixing ratio  $p$  for  $p \geq 0.05$ . Only for zero fraction  $p$  of fluctuating hard cylinders do we get the smaller exponent  $m = \mu$ .

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