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Random Close Packings of Regular Polygons

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Abstract. — We study by numerical simulation the progressive densification of assemblies of equal regular polygons (pentagons and heptagons). We follow the evolution of the packing fraction, of the coordination numbers and of the void space structure during the densification. At high packing fraction ($C \sim 0.83$), ordered zones appear. This can be compared with what occurs in equal disc assemblies in which a Random Close Packing limit exists for a packing fraction $C \sim 0.83$ above which some local order is present.

1. Introduction

The structure of bidimensional systems of equal discs have been extensively studied, mainly as dense packings [1]. Some interesting studies have also been devoted to the formation of these systems when they are densified. Experimentally, by contraction of a stretched rubber film on which discs were placed, Quickenden and Tan [2] have covered the range of packing fractions from $C = 0.1$ to the maximum value $C = 0.906$ obtained in the regular triangular packing. One of the main results of their study is the evidence, for the packing fraction $C = 0.830 \pm 0.015$, of a Random Close Packing (RCP) limit above which order appears in the packing. The same limit has been observed by Lemaitre et al. [3] in a packing built on an air cushion table. Using the radial distribution function, Berryman [4] has obtained the value $0.82 \pm 0.02$ for the RCP packing fraction, while, from topological arguments, Bideau et al. [1] have proposed the value $\pi^2/12 \sim 0.82$.

At the opposite of equal discs, polygonal grains, especially when they have an odd number of sides, do not arrange naturally to form regular packings. For example, the assemblies obtained by packing without care an ensemble of identical pentagons remain disordered. These disordered assemblies have been studied by Ammi et al. [5] who found that under a pseudocentral force, the packing fraction cannot be larger than 0.79. That study has also shown the importance of side-to-side contacts for the mechanical properties of the assembly.

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Fig. 1. — Periodic dense patterns (a) with pentagons (b) with heptagons.

However, we have recently shown both experimentally [6] and by numerical simulations [7] that it was possible to obtain crystalline assemblies of identical regular polygons. These assemblies are realized by parallel chains of translated polygons, alternatively oriented in one direction and the opposite (Fig. 1).

Though it does not seem intuitive, the construction of such bi-periodic lattices is always possible for convex grains [8]. In the case of pentagons, this disposition was found in the context of quasi crystal theory [9]. In our experiment, it corresponds to very compact assemblies (C \( \sim 0.92 \) for pentagons, \( C \sim 0.89 \) for heptagons) and it probably realizes the maximum possible packing fraction, though the question remains unsolved in the general case.

Then, the question arises as to the eventuality of a RCP limit, similar to that observed in assemblies of equal discs, when an assembly of regular polygons is densified. In order to answer that question, we have made numerical simulations. In Section 2, we present briefly the principles of the simulations. In Section 3 we give the results.

2. Principles of the Molecular Dynamics Simulations

Before bringing our simulation program into operation, we build a loose packing of identical polygons in the following way. We start from a packing of discs with a given low packing fraction (\( C = 0.1 \) to 0.4), that we position in a large circle using a RSA (Random Sequential Adsorption) algorithm [10, 11]. For each disc, we choose a direction randomly. A regular polygon with \( k \) sides is inscribed in the disc, with a vertex pointing in the chosen direction; so there is no correlation between the relative orientations of the polygons. This gives the initial configuration from which the program will operate. This program, which has been performed by Tillemans and Herrmann [12], handles the evolution of an assembly of convex polygons (the polygons must have more than 3 sides) using molecular dynamics. Molecular dynamics solves Newton’s equations for the translation and rotation of the particles:

\[
m_t \frac{d\mathbf{r}_i}{dt} = \sum_{j=1}^{N} \mathbf{F}_{ij} + \mathbf{F}_{ext}^{ext} \tag{1}
\]

\[
M_t \frac{d\Omega_i}{dt} = \sum_{j=1}^{N} \mathbf{L}_{ij}
\]
where \( m_i \) is the mass of particle \( i \), \( \mathbf{r}_i \) its position, \( M_i \) its momentum of inertia, \( \Omega_i \) its rotation velocity. \( \mathbf{F}_{ij} \) and \( \mathbf{L}_{ij} \) are the force and the torque imposed by particle \( j \) on particle \( i \) and \( \mathbf{F}_{i}^{\text{ext}} \) is an eventual external force acting on particle \( i \).

When two polygons \( i \) and \( j \) approach each other, they slightly overlap (Fig. 2). The force \( \mathbf{F}_{ij} \) acting on polygon \( i \) at the point of contact (the point of contact is defined as the middle of the contact line built by taking the two points \( a \) and \( b \) of intersection of the sides of the overlapping polygons, see Fig. 2) can be written as the sum of a normal and a tangential component:

\[
\mathbf{F}_{ij} = \mathbf{F}_{ij}^{\text{n}} \mathbf{n} + \mathbf{F}_{ij}^{\text{t}} \mathbf{t}
\]

where \( \mathbf{n} \) and \( \mathbf{t} \) are the unitary vectors respectively normal and tangential to the contact line. The normal force is decomposed into two parts, an elastic part proportional to the overlap area, and a dissipative part:

\[
\mathbf{F}_{ij}^{\text{n}} = \frac{EA}{L_c} - m_{ij} \gamma_n \mathbf{V}_{ij}^{\text{n}}
\]

while for the tangential force we take:

\[
\mathbf{F}_{ij}^{\text{t}} = -\min(m_{ij} \gamma_t |\mathbf{V}_{ij}^{\text{t}}|, \mu |\mathbf{F}_{ij}^{\text{n}}|).
\]

In these expressions, \( E \) is the Young modulus, \( A \) the overlap area, \( L_c \) the diameter of a disc that would have the same area as the polygons and \( m_{ij} = m_i m_j / (m_i + m_j) \) is the effective mass of the couple of polygons \((i, j)\). \( \mathbf{V}_{ij} = \mathbf{V}_i - \mathbf{V}_j \) is the relative velocity, \( \gamma_n \) and \( \gamma_t \) are the dissipation parameters in the normal and tangent directions and \( \mu \) is the friction coefficient. The torque imposed by particle \( j \) on particle \( i \) is

\[
\mathbf{L}_{ij} = \mathbf{F}_{ij} \times \mathbf{K}
\]

where \( \mathbf{K} \) is the vector linking the center of the contact line to the center of mass of the polygon \( i \) (Fig. 2). When a polygon, say \( j \), rotates, its rotation modifies the overlapping areas of the polygons with which it is in contact, and then the values of \( \mathbf{F}_{ij} \), \( \mathbf{L}_{ij} \) and \( \mathbf{K} \); the modification of \( \mathbf{F}_{ij} \) and \( \mathbf{L}_{ij} \) due to the rotation of \( j \) affects the motion (translation and rotation) of polygon \( i \) through relation (1).

At the motion of polygon \( i \) resulting from its interactions with its neighbours, we surimpose, at each time step \( \tau \) of the simulation, a displacement of each polygon \( i \) towards the center of mass of the packing according to the equation

\[
\mathbf{r}_i(t + \tau) = \mathbf{R}_m + \alpha (\mathbf{r}_i(t) - \mathbf{R}_m)
\]

Fig. 2. — Illustration of a collision between two polygons.
Fig. 3. — Evolution in a semi logarithmic scale of the packing fraction of an assembly of pentagons with time (the time unit corresponds to 500 iterations).

where $\mathbf{r}_i(t)$ is the position of the polygon $i$ at time $t$, $\mathbf{R}_m$ the position of the center of mass of the packing and $\alpha$ a real number between 0 and 1. In that way, we realize an isotropic contraction of the packing, close to that used by Quickenden and Tan [2] to simulate the compression of a dilute monolayer on a liquid surface. The trajectories of the particles are computed using a fifth order predictor corrector method [13].

3. Numerical Results

We will present in detail the results we have obtained for assemblies of regular pentagons, as to the evolution of the packing fraction, of the coordination numbers and of the void space structure during the densification process. At the end of this paragraph, we will summarize briefly the main results for heptagon assemblies.

3.1. Packing Fraction. — We use the following method to calculate the packing fraction. In order to avoid the edge effects, we consider only the “internal” polygons that have their center in the central zone of the packing, zone limited by a circle of radius 80% of the radius of the circle circumscribing the packing. We determine a mosaics by drawing the Voronoi tessellation of the centers of the internal polygons. The ratio of the total area of those polygons to the total area of the mosaics gives us a good approximation of the packing fraction. That method gives exact results for packings of circular grains. It introduces some error for polygons because a polygon is not necessarily completely inside its Voronoi cell. However, for a large enough packing, the error is weak because there is some compensation between the area of the part of the “internal” polygons which is outside the mosaics and the area of the part of the “external” polygons which falls inside the mosaics.

Figure 3 gives the evolution of the packing fraction of an assembly of 500 pentagons from an initial value $C = 0.06$. First the packing fraction increases exponentially with the time. Very few contacts are created. Some clusters of all sizes and shapes appear. The number of clusters then decreases while their size increases. We end with one big cluster involving all the particles. Small local reorganizations occur in this big cluster, and a quasi stationary state is reached in which the structure of the packing is still disroted (it can be noticed that, in contrast to the densification under a central force that we used in [7] to obtain crystalline assemblies, here there is no nucleation).
When we stopped the simulation, the packing fraction was practically constant: it was close to 0.85. This value is well below the value 0.92, we obtained for the crystalline packing we have described in [6,7]. Conversely, it is much larger than the value, 0.79, obtained experimentally by Ammi et al. [5] for disordered packings: the reduced possibility of local reorganization in that latter case probably explains that difference. Figures 4 to 6 show the evolution of the structure of the packing during the last steps of densification (the overlaps between the polygons are not visible because they are very small). In the densest packing (Fig. 6), one can see a few crystalline zones, not very extended, with the same structure as the ones we have previously obtained experimentally [6] and studied theoretically [7].
3.2. THE COORDINATION NUMBERS. — The contacts between polygons are generically of 2 kinds: side-to-side and side-to-vertex (Fig. 7). Actually, some other kinds of contacts may occur but they may be considered as limit cases of the preceding ones: vertex-to-vertex, or side-to-side with the 2 sides in contact on their whole length. With regular polygons having a number of sides less than or equal to 6, another kind of configuration can take place as 3 grains may be in contact at the same point but this is exceptional. All those limit cases will not be considered here. Let \( z_{ss} \) and \( z_{sv} \) be the average numbers of side-to-side and side-to-vertex contacts per polygon and let \( z = z_{ss} + z_{sv} \) be the total average coordination number.

Figure 8 gives the evolution with time of the distribution of the coordination numbers of the packing (only the numbers 3, 4, 5 and 6 are shown, without distinction between the two types of contacts). In the first part of the process, only few contacts are created and this does not affect very much the proportions of the presented numbers. Then, one observes a fast increase, corresponding to the growth of small clusters and their union in a central cluster. From a time \( t \sim 25 \), the grains in that cluster rearrange (note that \( t \sim 25 \) corresponds also to the time from which the packing fraction begins to vary much more slowly (Fig. 3)); this leads to an increase.
of the largest (> 4) values of coordination at the expense of the smaller ones (≤ 4). Finally a quasi-stationary state is reached. However, there are still some fluctuations of the coordination numbers, and one can notice strong correlations between the different values (particularly the values 4 and 5). The evolution of the average coordination number \( z \) with the packing fraction is much more regular (Fig. 9).

The side-to-side coordination number is difficult to be measured because the objects are in motion and they can slightly overlap. We have chosen to consider that two pentagons are in side-to-side contact if the angle between the sides is less than one degree: the values obtained in that way are very close to but slightly smaller than those we obtain by eye looking with care at a large scale drawing of the assembly (about 2 cm for the side length of a grain). Figure 10 shows the corresponding evolution of the side-to-side coordination number: a net increase can be seen for a packing fraction around \( C = 0.8 \).

3.3. THE VOID SPACE. — The distribution of the number \( n \) of sides of the polygons of the void space has been measured by eye on pictures of assemblies with packing fraction close to 0.8. The values we give in Table I must be considered only as approximate. The distribution

Fig. 8. — Distribution of the coordination numbers (only the values 3, 4, 5 and 6 are shown) as a function of time.

Fig. 9. — Evolution of the mean coordination number \( z \) with the packing fraction \( C \).
Fig. 10. — Evolution of the side-to-side coordination number with the packing fraction $C$.

Table I. — Distribution % of the number $n$ of sides of the polygons of the pore space. $\langle n \rangle$ is the average number of sides and $\mu_2(n)$ the variance.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$C = 0.78$</th>
<th>$C = 0.81$</th>
<th>$C = 0.84$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>20.9</td>
<td>23.6</td>
<td>38.5</td>
</tr>
<tr>
<td>4</td>
<td>23.4</td>
<td>26.1</td>
<td>24.2</td>
</tr>
<tr>
<td>5</td>
<td>1.6</td>
<td>3.0</td>
<td>1.7</td>
</tr>
<tr>
<td>6</td>
<td>13.6</td>
<td>13.7</td>
<td>15.6</td>
</tr>
<tr>
<td>7</td>
<td>10.1</td>
<td>10.2</td>
<td>7.2</td>
</tr>
<tr>
<td>8</td>
<td>3.8</td>
<td>4.4</td>
<td>4.8</td>
</tr>
<tr>
<td>9</td>
<td>8.9</td>
<td>7.7</td>
<td>4.2</td>
</tr>
<tr>
<td>10</td>
<td>3.8</td>
<td>3.3</td>
<td>1.9</td>
</tr>
<tr>
<td>11</td>
<td>4.7</td>
<td>2.5</td>
<td>0.4</td>
</tr>
<tr>
<td>$&gt;11$</td>
<td>9.2</td>
<td>5.5</td>
<td>1.5</td>
</tr>
<tr>
<td>$\langle n \rangle$</td>
<td>6.62</td>
<td>5.92</td>
<td>4.86</td>
</tr>
<tr>
<td>$\mu_2(n)$</td>
<td>15.16</td>
<td>8.06</td>
<td>5.38</td>
</tr>
</tbody>
</table>

presents the following characteristics:
1) when the packing fraction increases, it shrinks towards the small values of $n$ (above $n = 11$, the number of sides becomes difficult to determine),
2) the most numerous polygons are triangles, quadrilaterals and hexagons,
3) there are very few polygons with 5 sides. This is because these polygons lead to extreme situations: the case $n = 5$ can be realized only with four angles with measure of $2\pi/5$ or three angles with a sum $\pi/5$, which is very unlikely.

3.4. RCP LIMIT. — In the experiment on discs by Quickenden and Tan [2], the packing fraction first increased steeply to $C = 0.83$ and then changed slowly from this value to $C = 0.906$ corresponding to the ordered triangular packing. The packing fraction $C = 0.83$ then appears as that of the RCP.
In our simulations on pentagons, we have a similar variation of $C$ (Fig. 3). However, when we stop the densification after several hours of simulation, we are still far from the crystalline state ($C = 0.92$), in a state of much lower packing fraction ($C \sim 0.85$). All the variations we have presented show that the packing is still slowly evolving. A careful examination of the pictures of Figures 5 and 6 shows that there are no ordered zones when $C = 0.81$ but that such small zones exist for $C = 0.84$. For pentagons, the RCP limit could then correspond to a packing fraction $C$ around 0.83, very close to that of the RCP of discs. Moreover, let us notice that $C = 0.83$ is also the value of the packing fraction at the intersection of the two straight lines fitting the variations of the packing fraction respectively at low and large times (Fig. 3).

We have obtained similar results in all simulations we have performed. We have never obtained either the crystalline packing or large ordered zones: the different quantities we have studied saturate for a packing fraction close to 0.85 and the ordered zones remain small; it is probable that, in the dense state, some decompaction would be necessary to allow a better rearrangement.

3.5. **HEPTAGON ASSEMBLIES.** — The same study has been performed on assemblies of regular heptagons. It shows qualitatively the same behaviour as assemblies of pentagons. Using the same arguments as for pentagons, the RCP limit is obtained for $C \sim 0.84$.

4. **Conclusion**

Our numerical study of the densification of assemblies of regular polygons show that ordered zones appear at high packing fraction. This behaviour can be compared to that found in disc assemblies in which a Random Close Packing structure is known to exist. The maximum packing fraction is nearly the same for discs and polygons, $C \sim 0.83-0.84$.

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**References**