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Detecting a Structure in Two Dimensions Combining the Voronoï Tessellation and a Shape Factor

Dijana Dujak[1)]
Aleksandar Karač[2)]
Zorica Jakšić[3)]
Darko Vasiljević[3)]
Slobodan Vrhovac[3)]

We present a methodology to quantify the structural changes in the internal structure of granular packing. To this end, we use the Voronoï tessellation and a specific shape factor which is a clear indicator of the presence of different domains in the granular packing. Distributions of the shape factor in a 2D granular system of metallic disks are experimentally investigated. The analysis of disk packings at a "microscopic" level requires a precise measurement of grain positions. For this reason, we develop an accurate image processing technique based on the Standard Hough Transform. It is found that the properties of the probability distribution of the shape factor of the Voronoï cells are in accordance with the fact that the packings of monodisperse hard disks spontaneously assemble into the regions of local crystalline order.

Key words: **granular materials, granular compaction, packings, shape factor, experimental results, military application.**

Introduction

PARTICLE technology spans over a range of product lines such as pigments, ceramics, drugs, cosmetics, coal and ores, minerals, herbicides, seeds, absorbents, explosives, etc. In the chemical industry alone, 60% of products are manufactured as particulates and a further 20% use powders as ingredients to impact specific end-use properties [1]. Problems with powder flowability, caking, compaction, physical and chemical stability, reactivity and efficacy, dispersability, and segregation are common for all industries. Clearly, particulate media pervade many other fields in addition to process and consumer industries, e.g. defence, occupational health, and the civil and environmental arenas.

We see the importance of fundamental research into granular matter. This was appreciated very early in mechanical and chemical engineering; physicists have joined in more recently [2 – 7]. Granular materials are large conglomerations of discrete macroscopic particles. If they are non-cohesive, the forces between them are strictly repulsive. The particles are usually surrounded by a fluid, most often air, which may play a role in the dynamics of the systems. At the root of the unique status of granular materials are two characteristics: ordinary temperature plays no role, and interactions between grains are dissipative because of the existence of static friction and the inelasticity of collisions. There are no long-range interactions between individual grains or between individual grains and the walls of a confining container. Granular matter refers to particle systems in which the size is larger than one micron. Below one micron, thermal agitation is important, and the Brownian motion can be seen. Above one micron, thermal agitation is negligible. Yet despite this seeming simplicity, a granular material behaves differently from any of other familiar forms of matter – solids, liquids, or gases – and should therefore be considered an additional state of matter in its own right.

An important element in the understanding of granular media is the description of the local arrangement of grains. The structure of granular materials is disordered but not random. Such an organisation is the consequence of several different mechanisms which are both physical (e.g. mechanical stability) and geometrical (e.g. close packing configurations). The one possible way of describing the neighbourhood and steric environment of a spherical grain is to build its Voronoï cell and study its size and shape, and the correlation to the sizes and shapes of its nearest neighbours. This method was initiated by Finney [8] to study non-crystalline molecular aggregates with a special attention to regular structures. The Voronoï tessellation has long been considered for applications in several research areas, such as astronomy [9], atomic physics [10], biology [11], metallurgy [12], materials science [13] and telecommunications.

Characterisation of microstructural properties of granular packings is a very demanding and complex problem. The main reason is an inability to obtain reliable data from experiments [14, 15]. On the other hand, data obtained from simulations describes mainly the ideal cases in which various external influences are neglected. Our analysis of

1) University of Zenica, Faculty of Metallurgy and Materials, Travnička cesta 1, 72000 Zenica, BOSNIA AND HERZEGOVINA
2) University of Zenica, Faculty of Mechanical Engineering, Fakultetska 1, 72000 Zenica, BOSNIA AND HERZEGOVINA
3) University of Belgrade, Institute of Phisics Belgrade, Prigrevice 118, 11080 Zemun, SERBIA

granular packings is based on the Voronoï tessellation, which allows us to unambiguously decompose any arbitrary arrangement of disks (spheres in 3D) into a space-filling set of cells. Our aim is to characterise the structure of disordered disk packings and to quantify the structural changes associated with different densities. The Voronoï diagrams are used to visualise the structural order in packing structures. Quantitative information on the type of order induced can be obtained by calculating the shape factor of the Voronoï cells. The shape factor and its distribution were introduced by Moučka and Nezbeda [16] for tracking the change in a structure where a liquid-like system approaches a disordered jammed state. The shape factor is a dimensionless measure of deviation of the Voronoï cells from circularity. This method enablesthe identification of the presence of different underlying substructures (domains) in the packing.

Voronoï tessellation

The Voronoï diagram is a special kind of decomposition of a metric space determined by distances from the specified family of objects (subsets) in the space. It is also referred to as the Voronoï tessellation, the Voronoï decomposition, or the Dirichlet tessellation [17]. The Voronoï tessellation is one of the simplest mathematical models of a cellular structure. Given a set $\mathcal{A}$ of discrete points in the plane π, for almost any point $x \in \pi$ in the plane π, there is one specific point ai $\in \mathcal{A}$ which is closest to x. The set of all points of the plane which are closer to a given point ai $\in$ A than to any other point aj $\neq$ ai, aj $\in \mathcal{A}$, is the interior of a convex polygon usually called the Voronoï cell of ai. The set of the polygons {Pi}, each corresponding to (and containing) one point ai $\in \mathcal{A}$, is the Voronoï tessellation corresponding to $\mathcal{A}$, and provides a partitioning of the plane π. The Voronoï cells are convex and their edges join at trivalent vertices (i.e. each vertex is equidistant to three neighbouring disks.). The Voronoï tessellation can be defined for general N-dimensional Euclidean spaces.

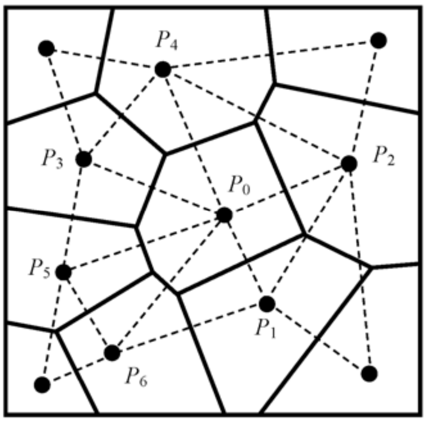

Figure 1. The "perpendicular bisector method" for constructing the Voronoï diagrams in 2D

Given a set of centres, there is a relatively easy way to generate the corresponding Voronoï diagram. In the perpendicular bisectors method, used in this research, one starts from a given centre (P_0) and detects the nearest (P_1) centre to it (see Fig.1). A part of the perpendicular bisector on the $\overline{P_0P_1}$ line will form the first edge of the Voronoï polygon corresponding to (P_0). Then the second nearest centre (P_2) is detected and the perpendicular bisector on $\overline{P_0P_2}$ is constructed. This algorithm is continued with the third (P_3), fourth (P_4), ... , n-th (P_n) nearest centre, until the perpendicular bisectors on $\overline{P_0P_3}$, $\overline{P_0P_4}$,..., close a stable polygon which does not change after considering any more distant points. Repeating the above algorithm for all centres, the Voronoï tessellation of the whole space (Fig.1.) can be obtained. For regularly packed disks in 2D, these polygons are hexagons, as illustrated in Fig.2. Any deviation from the regular hexagonal structure leads to a "deformation" of the Voronoï hexagons.

Shape factor

The study of how space is repartitioned around the disks is essential for understanding the local arrangement of disks and their local organisation. For this purpose we use the Voronoï partition and a novel concept of the shape factor (parameter of non-sphericity) to measure the topology of the Voronoï cells.

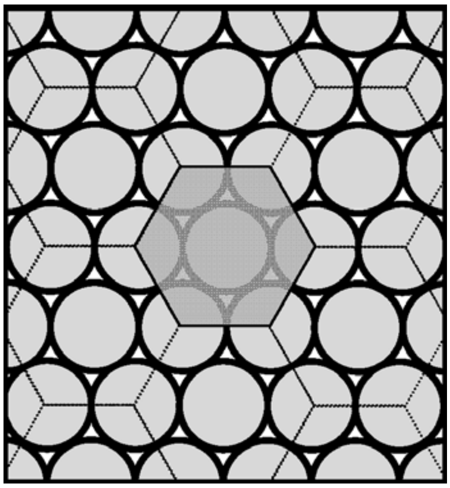

Figure 2. Two-dimensional hexagonal package of equal disks. Disk centres are vertices of regular hexagons

The shape factor ζ of the Voronoï cell is defined as

$$\zeta = \frac{C^2}{4\pi S} \tag{1}$$

where C is the circumference of a Voronoï cell and S is its surface area [16, 18]. Thus a circular structure has a shape factor of $\zeta = 1$, while for a convex polygon, the more anisotropic the polygon, the higher $\zeta > 1$; e.g. for a square $\zeta = 4/7 \approx 1.273$, for a regular pentagon $\zeta = \pi/5\tan(\pi/5) \approx 1.156$, and for a regular hexagon $\zeta = 6/\sqrt{3\pi^2} \approx 1.103$. Generally, for a regular N-sided polygon we have $\zeta = (N/\pi)\tan(\pi/N)$, which sets a lower bound for other N-sided polygons. Using the shape factor, we are able to identify the occurrence of different domains in numerically or experimentally obtained packings of particles. Every domain is made up of the grains whose Voronoï polygons have similar values of the shape factor. The shape factor is calculated for each Voronoï cell, except for the opened cells located at the boundaries which have infinite volumes.

In order to clearly distinguish the domains made up of different Voronoï polygons, we classify the polygons according to their values into eight groups $G_1 - G_8$ as given in Table 1. The group G_1 comprises near-regular hexagons, while other groups include less regular figures. To differentiate polygons belonging to different groups G_1 - G_8, we use the colour coding in accordance with the definitions given in Table 1. This allows us to easily distinguish the local arrangements of grains for the used packings [19, 20].

Table 1. Classification of the Voronoï polygons into eight groups G_1 – G_8 according to the values of the shape factor ζ (Eq.(1))

Group	Range	Colour
G_1	$\zeta < 1.108$	yellow
G_2	$1.108 < \zeta < 1.125$	magenta
G_3	$1.125 < \zeta < 1.130$	cyan
G_4	$1.130 < \zeta < 1.135$	red
G_5	$1.135 < \zeta < 1.140$	green
G_6	$1.140 < \zeta < 1.160$	blue
G_7	$1.160 < \zeta < 1.250$	white
G_8	$1.250 < \zeta$	black

Applied method: description and verification

A commonly faced problem in computer vision is to determine the location, number or orientation of a particular object in an image. For example, in the automated inspection of electronic assemblies, interest lies in analyzing images of the products with the objective of determining the presence or absence of specific anomalies, such as missing components or broken connection paths. A good example of military application is the use of infrared imaging to detect objects with strong heat signatures, such as equipment and troops in motion. One problem could, for example, be to determine the straight roads on an aerial photo. This problem can be solved using the Hough transform for lines. Often the objects of interest have other shapes than lines, it could be parables, circles or ellipses or any other arbitrary shape. The general Hough transform can be used on any kind of shape, although the complexity of the transformation increase with the number of parameters needed for describing the shape. In the subsequent text, we will look at the Circular Hough Transform (CHT).

The experimental study of granular packings requires a precise measurement of grain positions. For this reason, the development of an accurate image processing technique has been a central aspect of the design of the experimental setup. The images of various 2D packings are systematically acquired in high resolution (at least 600×600 dpi) and 256 gray levels. First, image intensity values are adjusted in order to increase the contrast of the output image. Both the centre and the diameter of each grain are accurately determined using the image processing program based on the Standard Hough Transform (SHT) [21].

The Hough transform can be described as a transformation of a point in the x, y-plane to the parameter space. The parameter space is defined according to the shape of the object of interest. Since objects in this research are circles, the Circular Hough Transform (CHT) has been used [22], with the parametric representation of the circle given by

$$
\begin{aligned}
x &= a + r\cos q \\
y &= b + r\sin q
\end{aligned} \tag{2}
$$

where a and b are the centre of the circle in the x and y direction respectively and r is the radius. Thus the parameter space for a circle belong to R^3.

The process of finding circles in an image using the CHT is as follows. First we find all edges in the image by using an edge detection technique; one can choose between Canny, Sobel or Morphological operations. At each edge point, we draw a circle with its centre in the point with the desired radius. At the coordinates which belong to the perimeter of the drawn circle, we increment the value in our accumulator matrix which essentially has the same size as the parameter space. In this way, we sweep over every edge point in the input image drawing circles with the desired radii and incrementing the values in our accumulator. The accumulator now contains numbers corresponding to the number of circles passing through the individual coordinates. Thus the highest numbers (selected in an intelligent way, in relation to the radius) correspond to the centre of the circles in the image. The accumulator array, being three dimensional if the radius is not held constant, can grow large quite fast. Its size depends on the number of different radii and especially the image size. The computational cost of calculating all circles for each edge points increases with the number of edge points which is usually a function of the image size. The overall computation time of the CHT can therefore quickly reach an infeasible amount of time for large images with many edge points.

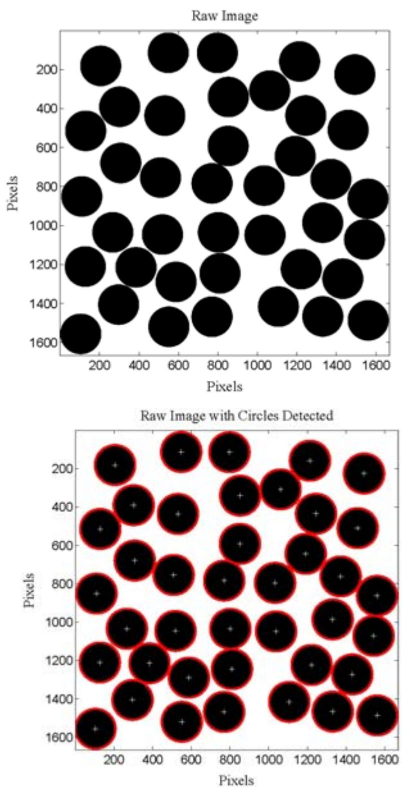

Figure 3. Two-dimensional system of disks from numerical simulation (left); detection of the disks' circumferences and associated centres (right).

It is desirable to be able to find circles from the accumulator data. One approach is to find the highest peaks for each a, b plane corresponding to a particular radius, in the accumulator data. If the height of the peak is equal to the number of edge pixels for a circle with the particular radius, the coordinates of the peak do probably correspond to the centre of such a circle. But the centre of a circle can also be represented by a peak with a height less than the number of edge pixels, if, for example, the circle is not complete or is of elliptical shape. If it is difficult to locate exact peaks, the accumulator data can be smoothed.

In order to verify the method, the known positions of disks in an image are compared to those obtained using the image processing technique based on the CHT. The image is produced using the method of random sequential adsorption (RSA) of disks [23–25]. As a result of the simulation, an image of the 2D packing in the postscript format is produced, where positions and diameters of all disks are known (see Fig.3(a)). The image is then converted into a bitmap grayscale image and analysed as described above. As a result, a raw image with circles (red line) and their centres (white crosses) is produced for further comparison with the simulation data (see Fig.3(b)). Excellent results have been obtained, the error being less than 0.1%. It is also found that the accuracy of the circle detection depends greatly on the parameters controlling the CHT algorithm.

Results and discussion

The experimental setup used in this research (see Fig.4) was already described in details elsewhere [19, 20] and only a brief description is given here. The two-dimensional granular packing consists of metallic cylinders contained in a rectangular box made of two parallel glass plates, with an inner gap of thickness 3.4 mm, slightly larger than the height of the cylinders, $h = 3.00 \pm 0.01$ mm. The lateral walls of the box delimit a rectangular frame of a height of $H = 340$ mm and a width of $L = 300$ mm. The box is secured on a heavy plane that can be inclined so one could set an arbitrary inclination angle $\theta \in [0, 90]^{\circ}$ from the horizontal plane. The cylinders of diameters $d = 4.00, 5.00$ 0, and 6.00 ± 0.05 mm were used to prepare the monodisperse packings.

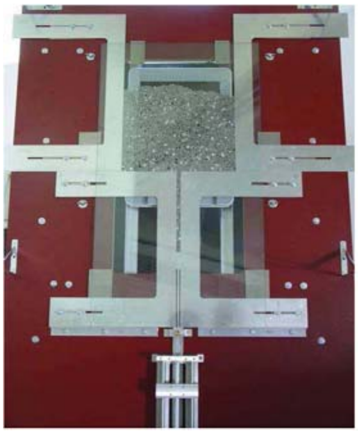

Figure 4. Photograph of the experimental setup

The experimental procedure consists of the following steps. The cylinders are randomly deposited onto the initially horizontal glass plate without contact between them. The box is turned into the vertical position, allowing the cylinders to glide on the glass plate to the bottom of the box forming a package. The measured packing fractions of these disordered packings are $\rho = 0.78 - 0.86 \pm 0.01$ with densities being far from the close packing limit $\rho_{cp} = \pi / 2\sqrt{3} \approx 0.91$. The bitmap images of packings are systematically acquired by means of an HP ScanJet 3800 fixed below the bottom glass plate of the rectangular container. In the output bitmap image as shown in Fig.5, the diameters of grains are $d_1 \approx 94$, 118, and 142 pixels.

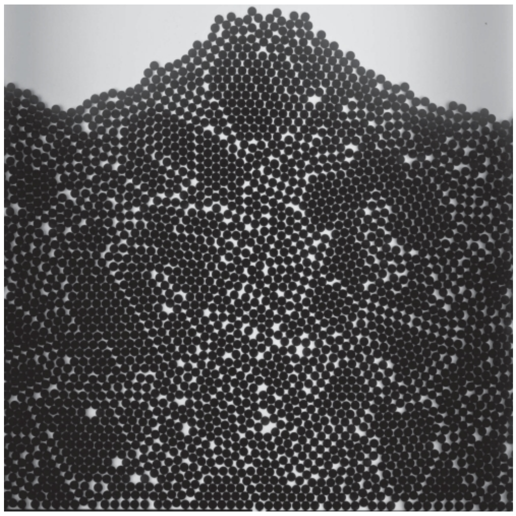

Figure 5. Typical snapshot of the experimentally obtained packing.

The images are then analysed using the procedure explained in Sec. III. The analysis can be performed on the whole system or on the region of interest and it allows us to detect both the centres and the diameters of cylinders with a high resolution of 0.04 mm. Fig.6 presents snapshots of the CHT analysis for the experimentally obtained layer at density ρ=0.79. The centres of almost all grains detected by the image processing are marked with red cross hairs in Figures 6(a) and (b), and with red dots in Fig.6(c) with circles designated with blue lines.

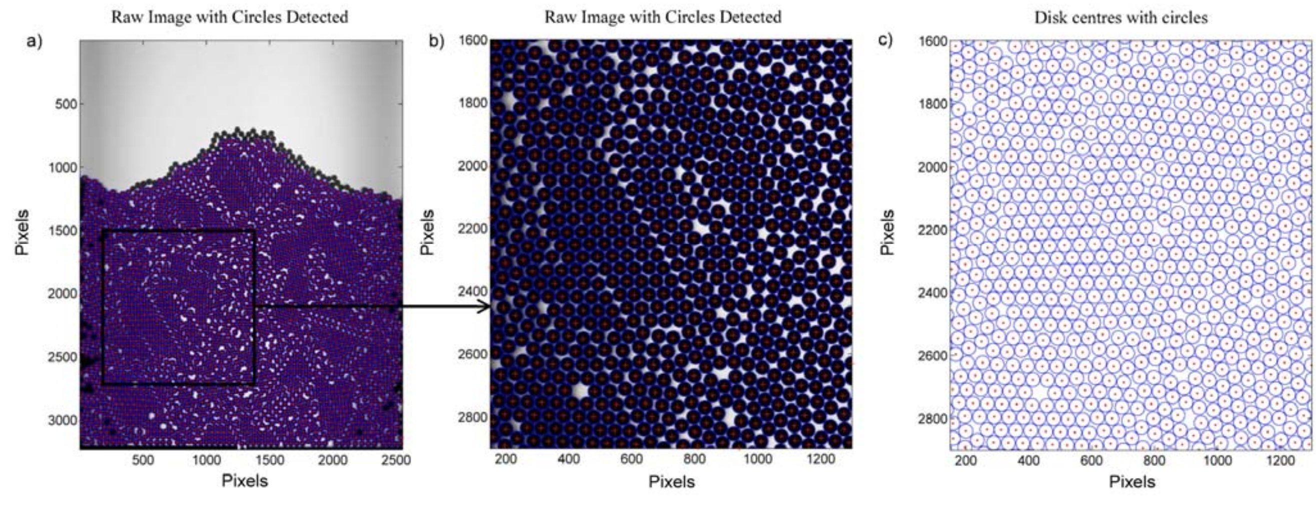

Figure 6. CHT analysis of the packing at density ρ=0.79: (a) The whole domain; (b) A part of the same snapshot with the centres. (c) Extracted disk centres and circles

Now we need to determine the Voronoï tessellation for a discrete set of points (centres of disks) in the plane. As already explained, for a given two-dimensional set of monodispersed disks, the Voronoï tessellation is a uniquely defined set of space-filling, non-overlapping and convex cells, each of which encloses one and only one of these disks. Fig.7 illustrates the resulting cell distribution for the tessellation of experimentally obtained packing of disks (ρ=0.79).

Let us now analyse the microstructural properties of the packing configurations by exploring local neighbourhoods using the Voronoï tessellation. It has to be noted that for this purpose a frequently investigated parameter in the literature on granular packings is the coordination number, i.e. the average number of disks in contact with a given disk [14, 26]. This is a very simple topological quantity which gives important information about the local configurations and the packing stability and determines the cohesion of the material when liquid capillary bridges between particles are present. Its value depends on the definition of ''contact", i.e. the minimal or cut-off distance dc between two disks below which they are regarded to be in contact. The coordination number is very sensitive to the changes of cut-off distance dc. Although simple in its definition, such a number is unavoidably an ill-defined quantity for granular systems. Indeed, the information about the positions of all grains is not sufficient to determine such a number: two grains can be arbitrarily close, but not touching.

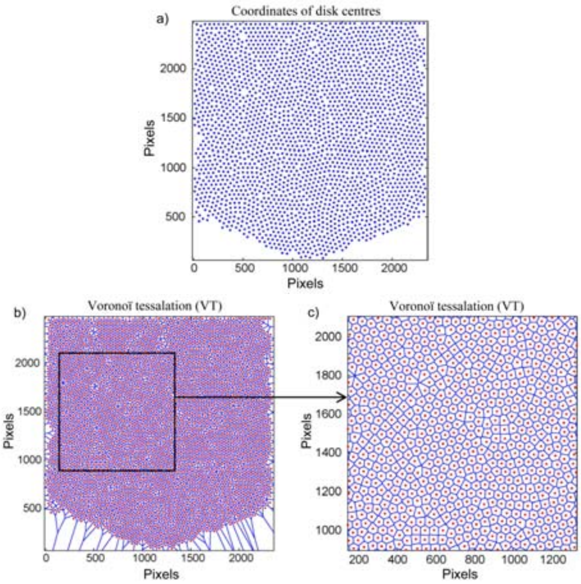

Figure 7. Voronoï tessellation of a set of point particles (centres of disks). Diagrams correspond to the experimentally obtained packing at density $\mathscr{A}$ =0.79: (a) Centres of disks; (b) Voronoï diagram; (c) The part of the same diagram. The centres of grains are marked with dots

On the other hand,the Voronoï cell method has an advantage in that there are no arbitrary choices for the neighbouring criteria. Two disks sharing a common cell edge are neighbours. Nevertheless, this is also the weakness of the Voronoï method because neighbours which are rather far from the central disk (sphere in 3D) contribute to the shape of the cell. We measured the occurrences of cells with $n_c \geq 3$ edges. The resulting distribution of Voronoï neighbours for packing at density $\rho = 0.79$ is shown in Fig.8. We can observe that the granular layer consists almost entirely of disks whose Voronoï cells are distorted pentagons, hexagons and heptagons. We thus get a narrow probability distribution of Voronoï neighbours centred at $n_c = 6$ (hexagons).

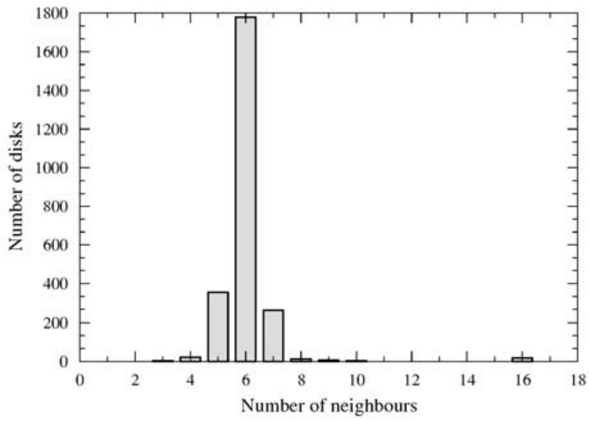

Figure 8. Distribution of Voronoï neighbours for packing shown in Fig.7. The number of opened cells located on the boundaries are also indicated as number of cells with n_c = 16 edges.

Fig.9 allows us to easily distinguish local arrangements of grains for used packings. Here we show the Voronoï tessellation for the same disks configuration as in Fig.7. To differentiate polygons belonging to different groups $G_1 - G_8$ we use colour coding in accordance with the definitions given in Table 1. The values of the shape factor for all Voronoï polygons are shown in Fig.9(b). In Fig.9 we can see a mixture of various Voronoï polygons. It is obvious that the polygons belonging to the G_7 and G_6 classes dominate, where G_7 and G_6 polygons are mostly distorted pentagons and heptagons. It means that the disks are distributed randomly. Furthermore, large islands of near-regular hexagons belonging to G_1 and G_2 classes are found. Optical imaging brings evidence that disks spontaneously tend to form ordered hexagonal patterns. In addition, small domains made up of $G_3 - G_5$ polygons, respectively, can also be detected. One feature of Fig.9 is the fact that disks tend to organise themselves locally into close packing configurations. Such a local organisation is limited to short distances yielding an overall disordered packing.

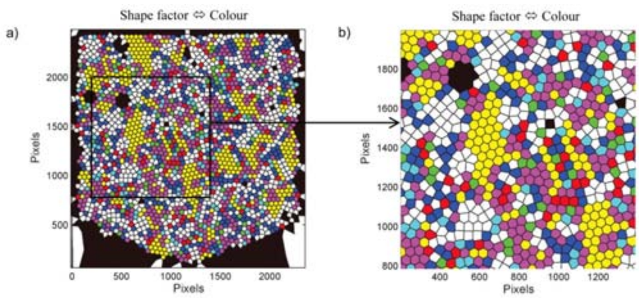

Figure 9. Voronoï diagram obtained from the positions of disks, for the same disks configurations as in Fig.7. (a) Voronoï cells are coloured according to their shape factor ζ (Eq. (1)). Colour coding of Voronoï polygons is defined in Table 1. (b) Also, a part of the same diagram is shown

To further quantify the structural properties of the packings, we consider the probability distribution $P(\zeta)$ of the shape factor ζ. The distribution function $P(\zeta)$ is related to the probability of finding a Voronoï cell with the shape factor ζ (see Fig.10). It is normalised to unity, i.e. $\int_0^\infty d\zeta P(\zeta) = 1$. The experimental results for the distribution $P(\zeta)$ of the shape factor ζ are given in Fig.11 for the packings of disks of diameters $d = 4$ and 6 mm at density $\rho = 0.83 \pm 0.01$. The packing fractions and distribution functions $P(\zeta)$ have been calculated from an average over 10 initial preparations of packing. From these results we observe that the distribution $P(\zeta)$ does not depend on the diameter of the grains. The curves of distribution $P(\zeta)$ are asymmetric with a long tail on the right-hand side, which progressively reduces while the packing structure gets more compact (the Voronoï cells become more circular at higher values of the packing fraction). This narrowing of the probability distribution $P(\zeta)$ corresponds to the decrease of the fraction of Voronoï polygons belonging to $G_5 - G_7$ classes. In other words, as the density increases, the distribution becomes more localised around the lowest values of the shape factor (for a regular hexagon, $\zeta = 6/\sqrt{3\pi^2} \approx 1:103$).

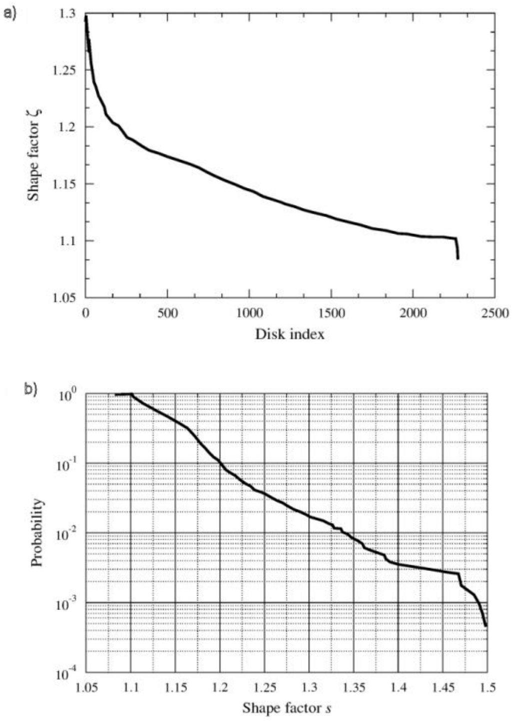

Figure 10. (a) Values of the shape factor for all Voronoï polygons, for the same disks configurations as in Fig.7; (b) The probability that the value of the shape factor ζ is greater than *s*

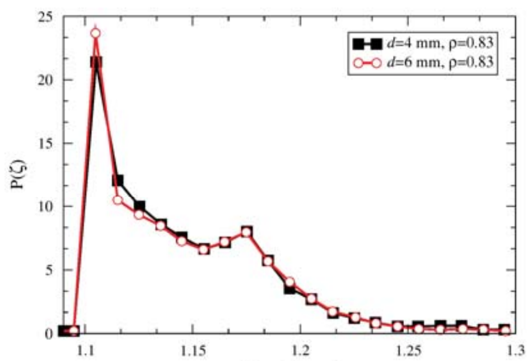

Figure 11. Experimental results for the probability distribution $P(\zeta)$ of the shape factor ζ. The experimental results correspond to the packings of disks of diameter d =4(□) and 6 (○) mm at density ρ=0.83.

Conclusions

The organisation of grains at a local level has been studied by analysing the geometrical characteristics of the local volumes associated with a natural way of subdividing the volume into local parts - the Voronoï partition. The shape factor ζ has been a quantifier of the circularity of the Voronoï cells associated with the individual particles. It gives a clear physical picture of the competition between less and more ordered domains of grains. We found that disks tend to organise themselves locally into ordered hexagonal patterns. The probability distribution $P(\zeta)$ of the shape factor ζ is very sensitive to small structural changes of the packing. The narrowing of the distribution $P(\zeta)$ corresponds to the increase in the fraction of the near-regular Voronoï cells. In particular, unlike in three-dimensional cases, these distributions have two peaks which clearly indicate the existence of local configurations with hexagonal and quadratic symmetry. Recent experiments have indicated that the same type of structural organisation may occur in a quasi-two-dimensional driven system of hard spheres [27] where regions of crystalline order are interspersed by relatively disordered grain-boundary regions.

The results presented here provide the starting point for further investigations. Further experiments are needed to understand various factors that influence the microstructural properties of packing such as particle anisotropy, particle shape and frictional properties of grains. The promising direction of research concerns the 3D extension of this investigation. It is known that the tendency towards a crystalline order is much less spontaneous in three dimensions than in the two-dimensional case [14]. Furthermore, the dimensionality of the packing determines the nature of the tail of the probability density of contact forces inside the packing [28], which is also relevant to the process of granular compaction.

Acknowledgments

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Detekcija strukture u dve dimenzije kombinacijom Voronojieve teselacije i faktora oblika

Prezentirana je metodologija za kvantifikovanje strukturalnih promena granularnog pakovanja. U tu svrhu koristimo Voronojievu teselaciju i faktor oblika koji predstavlja indikator prisustva različitih domena u granularnom pakovanju. Eksperimentalno su izučavane distribucije faktora oblika u dvodimenzionalnom granularnom sistemu metalnih diskova. Analiza pakovanja diskova na "mikroskopskom" nivou zahteva precizno merenje položaja granula. Zato smo razvili preciznu tehniku analize slika koja je bazirana na standardnoj Hough−ovoj transformaciji. Nađeno je da su svojstva distribucije verovatnoće faktora oblika Voronojievih poligona u saglasnosti sa činjenicom da se pakovanja jednakih diskova spontano organizuju u regione kristalne uređenosti.

Ključne reči: **granulisani materijali, granularna kompaktifikacija, pakovanja, faktor oblika, eksperimentalni rezultati, vojna primena.**

Обнаружение структуры в двух измерениях, сочетающих тесселяции Вороноия и форм -факторов

Мы представляем методологию количественной оценки структурных изменений в гранулированной упаковке. Для этой цели мы пользовались тесселяцией Вороноия и форм-фактором который образует показатель присутствия различных областей в гранулированной упаковке. Экспериментально мы изучали распределение форм-факторов в двумерной зернистой системе металлических дисков. Анализ упаковки дисков на "микроскопическом" уровне требует точного измерения положения гранул. Таким образом мы разработали методику точного анализа изображения, основанного на стандартной Хьюо-трансформации. Было установлено, что свойства распределения вероятностей форм-факторов полигонов Вороноия находятся в соответствии с фактом, что упаковки из равных дисков спонтанно организуются в области кристаллических заказов.

Ключевые слова: **гранулированный материалы, гранулированная компактность, упаковки, форм-факторы, экспериментальные результаты, военные применения.**

Détection de la structure à deux dimensions en combinant la tessellation de Voronoï et le facteur de la forme

La méthodologie pour la quantification des changements structuraux chez les emballages granulés est présentée dans ce papier. On utilise dans ce but la tessellation de Voronoï et le facteur de la forme qui est l'indicateur de la présence de différents domaines dans l'emballage granulé. On a examiné expérimentalement la distribution du facteur de la forme dans le système granulé des disques en métal à deux dimensions. L'analyse de l'emballage de ces disques exige le mesurage précis de la position des granulés au niveau „microscopiques". Pour ce faire on a développé une technique précise de l'analyse d'image. Cette technique est basée sur la transformation ordinaire de Hough. On a constaté que les propriétés de la distribution de probabilité du facteur de la formes des polygones de Voronoï étaient en bon accord avec le fait que les emballages des disques identiques étaient organisés spontanément en régions des ordres cristallines.

Mots clés: **matériaux granulés, compactage granulé, emballage, facteur de la forme, résultats expérimentaux, application militaire.**