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QUANTUM MECHANICAL APPROACH TO SPHERE BEDS IN THE CONTAINER-PACKING FRACTIONS AND RADIAL DISTRIBUTION FUNCTION

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A b s t r a c t. This paper is a continuation of the work on the new approach to the packing problems of randomly embedded granular material proposed by Góźdź and Pietrow. In previous paper a quantum mechanical approach (QMA) to packing was introduced and 2- and 3-dimensional packing experiments for circles (spheres) were generated on this basis. Packing fractions were calculated to test the ability to build 2- and 3-dimensional beds with correct properties. In this paper we continue testing the QMA model.

K e y w o r d s: granular material, quantum mechanical approach

INTRODUCTION

Applying the QMA approach, we are able to generate 2-dimensional and 3-dimensional packings of spherical and other shapes of grains. To check the properties of the packing we calculate packing fraction and the radial distribution function. We check the structures by analysing pictures of beds (sections of beds in a 3-dimensional case)and by analysing the density function in arbitrarily.

To determine characteristic functions, we generated packing of 20000 equal spheres for the 2- and 3-dimensional cases. Some of these functions are defined, in principle for infinite media. It requires removing the effect of the spheres that are on the edges of the bed. For example, for 20000 spheres in a 2-dimensional vessel with the baselength of $100R$ (R-radius of sphere) there are approximately 600 spheres in the four edges of the vessel, thus a deviation from the average value is about 3%.

CHARACTERISTICS OF THE STUDY MATERIAL

2-dimensional packing

Packing fraction

For 2-dimensional structures, the bonds of the packing fraction are not exactly determined. Especially the structure of random loose packing is not sufficiently known. From literature we know [2], that random packing occurs in the range of packing fraction from 0.82 to 0.89. In our research we obtained structures with packing fractions from 0.821 to 0.890, so we can generate a full range of 2-dimensional packings. The value of the packing fraction depends on the values of parameters in the computer programme describing the strength of the interaction potential [4] and the parameters in method for energy minimalisation.

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In Fig. 1 we can see the domain structure of the packing. The interior of the domain has an almost hexagonal structure. Within the domain, coordination number is about 6. Most of the packing consists of regions with a coordination number of about 4 (square packing) with numerous bridge structures. Locally these regions show low values of packing fraction and a decrease in the average packing fraction calculated of this bed. An average number of contacts for the whole bed is 4.4. For smaller vessels the average number of contacts is lower because the number of marginal-spheres is larger than the number of spheres forming a core in this case.

Functions of radial distribution

For the 2-dimensional packing two different types of radial distribution function were obtained. The first one, $Fr1$, is defined as an average density of the probability of finding a center of any sphere at the distance r from the center a fixed sphere. The maxima of this function indicate the distances from the n-th-class neighbours, where n is a number of maxima. For a regular crystalline packing the maxima of the $Fr1$ function are well defined. For example for a 2-dimensional close packing (hexagonal) the first maximum is observed at the distance $a = 2R$ (a is the lattice constant, R-radius of sphere) from any sphere. There are 6 neighbours at this distance. The second maximum is at $2R\sqrt{3} \approx 3.46R$ away from any sphere and the number of these 2nd-class neighbours is also equal to 6. For square lattices the number of 1st-class neighbours is 4 at a distance $2R$ and the number of 2nd-class neighbours is 4 at a distance of $2R\sqrt{2} \approx 2.83R$ from any sphere.

In random 2-dimensional beds we observed (Fig. 1) areas with different structures, especially hexagonal and square lattices. Therefore the $Fr1$ in random packing is only statistical function (Fig. 2).

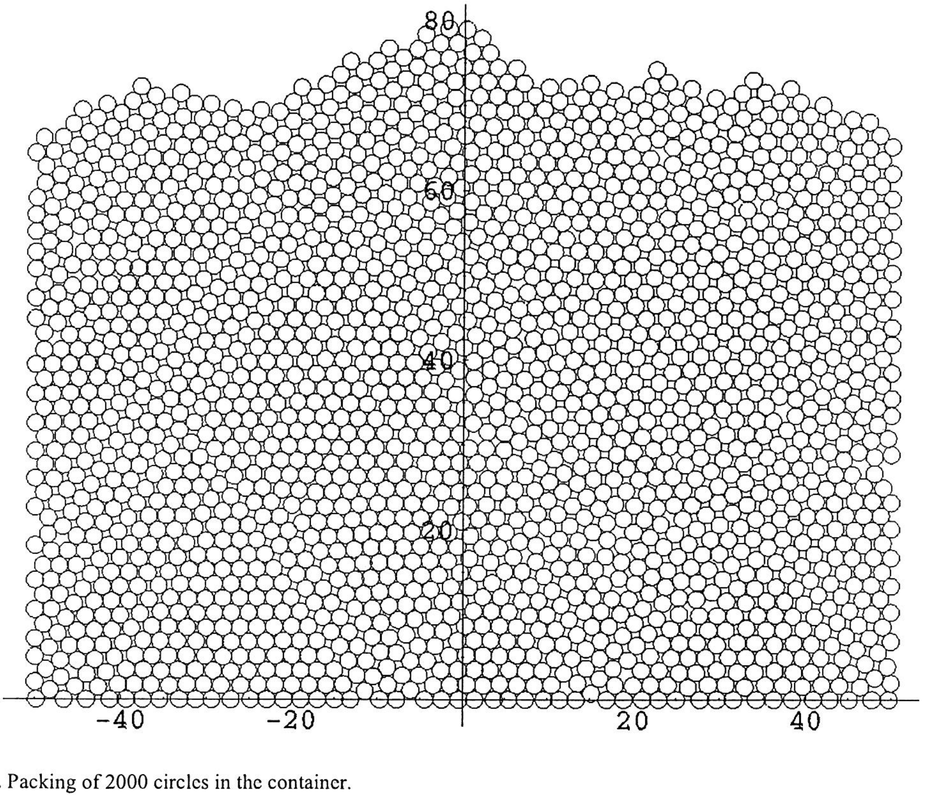

Fig. 1. Packing of 2000 circles in the container.

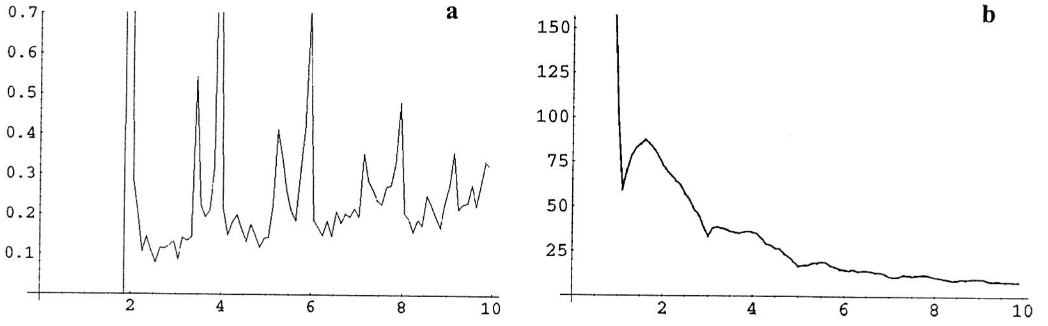

Fig. 2. Radial distribution function *Fr*1 (a) and *Fr*2 (b) in the 2-dimensional case.

To draw this function, we need to divide the probability on any portion of distance by its average r due according to the formula (a2) to obtain the probability density. Therefore the function does not increase with an increasing radius.

One may calculate another type of radial distribution function (*Fr*2). It is defined as the average probability density of finding a point belonging to any sphere at a distance r from any sphere. The *Fr*2 function is shown in Fig. 2.

Force values and force directions at contact areas

Our method of description of granular materials allows us easily to assign forces to contacts areas. This is an important characteristic needed for further considerations of mechanical properties. In Fig. 3 one can see the forces in the state without stress. The lengths of arrows are due to the forces values.

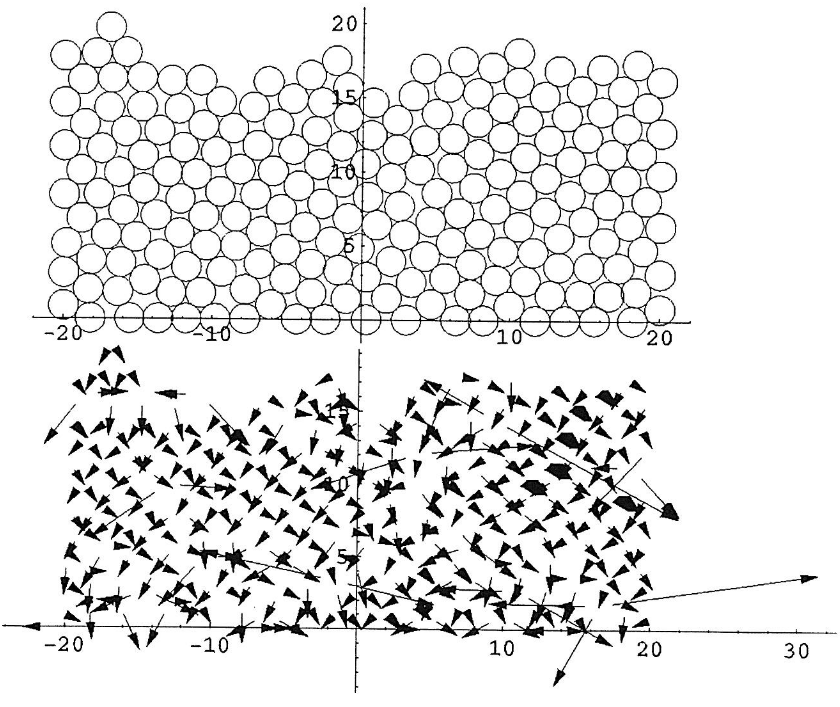

Fig. 3. Contact forces.

To calculate the forces we used a known formula:

$$\vec{F} = -\nabla V,$$

where ∇ is the gradient operator and V is an interaction energy function proportional to the value of spherical overlap [4].

Isotropy of density

One of the methods of analysing the structure of material is a determining its density along any line or plane. This allows to establish the domain structure of a 2-dimensional material and its lack in the 3-dimensional case [8]. The method allows us to observe planes or lines distinguished by the method of pouring, e.g., for the cone pouring we are able to distinguish a line at the maximum angle of pouring. In this direction local density is more homogeneous than in any other directions. An example of the density function for suitable material packing is shown in the Fig. 4.

3-dimensional packing

Packing fraction

The value of the packing fraction for random loose packing in a 3-dimensional case is 0.58. For the close packing the fraction is 0.63 [2] up 0.67 [1]. Our simulations provided us with beds with packing fractions covering the whole range. It was observed, that packing fraction depends strongly on the ratio of lengths of container edges to the spheres radius. Some results relevant to this problem were obtained by Scott [6]. In our case we found, that the length of container edges equal to $70R$ is still too small to obtain a stable structure, i.e., a small increase or decrease in the lengths of these edges changes the packing fraction significantly. This problem requires further investigations and more computation.

Function of radial distribution

Similarly, we determined a $Fr1$ function for the 3-dimensional packing (Fig. 5).

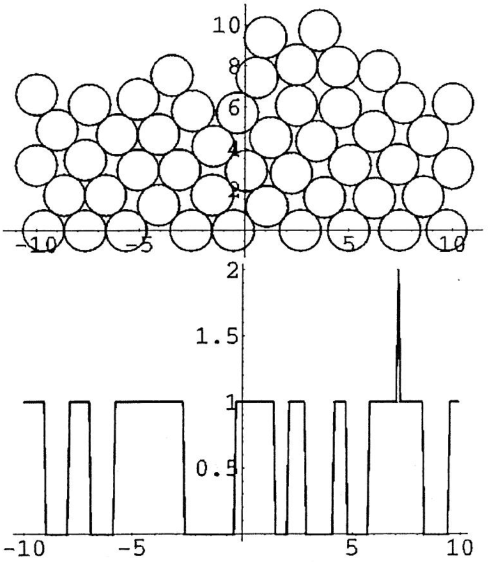

Fig. 4. Packing of 50 circles and local denisty along the line $z = 7$.

Its maxima for regular close packing *fcc* are: 1st for $\frac{a}{\sqrt{2}} = R$ for 12 neighbours, 2nd for $\frac{4R}{\sqrt{2}} \approx 2.83R$ (6 neighbours). For the *bcc* structure the first maximum is at a distance of $\frac{a\sqrt{3}}{2} = 2R$ and the second is at $\frac{4R}{\sqrt{3}} \approx 2.31R$ for 8 and 6 neighbours, respectively. Finally, for the *sc* packing, the first maximum at a distance of $2R$ is for 6 neighbours and the second (12 neighbours) is at $2\sqrt{2R} \approx 2.83R$. For granular materials we have 3.3-3.5R in the case of the second maximum [1].

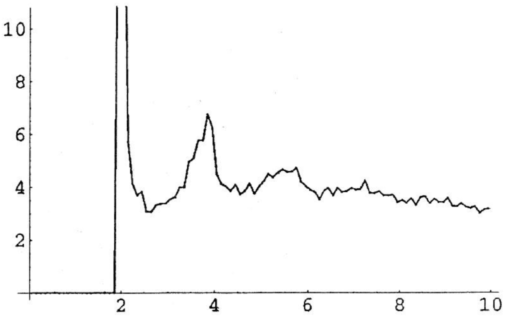

Fig. 5. Radial distribution function $Fr1$ in the 3-dimesnional case.

CONCLUSIONS

From the characteristics shown above we conclude, that the QMA packing model seems to be a good and quite general method to obtain packings with desired parameters. In future we plan to determine other useful characteristics such as contact distribution functions which will enable us to determine mechanical properties of the material. Flexibility of both the theoretical and numerical methods within this approach allows us to consider more realistic problems than it is possible with other methods

APPENDIX

For a 2-dimensional case an average density over any area S in polar coordinates is:

$$< \rho > (r) = \frac{\int \rho \mathrm{d}S}{S} = \frac{\int_{r_1}^{r_2} \int_{\alpha_1}^{\alpha_2} \rho(r,\alpha)\, r\, \mathrm{d}\alpha\, \mathrm{d}r}{S} \tag{a1}$$

where S is an area of circle with the radius r, ρ (r, α) a local density. In the discrete form, which is helpful for the numerical calculations we arrive at:

$$\frac{\sum_r r \sum_\alpha \rho \Delta\alpha \Delta r}{\pi r^2} = \sum_r \frac{\sum_\alpha \rho \Delta\alpha}{\pi r} \Delta r. \tag{a2}$$

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