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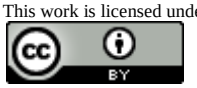

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MATHEMATICAL MODEL OF COORDINATION NUMBER OF SPHERICAL PACKING

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Abstract: The article considers a mathematical model of the coordination number, which allows obtaining an equation for multi component spherical packing in the entire range of its change. The resulting model can be used in both 2-d and 3-d spaces. The concept of the coordination index is introduced as a function of the inter-particle distance related to a single particle located near the central particle. The model provides unambiguous compliance between the simulated and calculated data on the coordination numbers of the spherical packing.

Keywords: spherical packing, coordination number, dimension space, coordination index, inter-particle distance.

I. INTRODUCTION

The theory of error correction codes has a number of natural analogs one of which is the theory of packing of spheres in Euclidean space. The study of spherical packing allows to consider the methods used in coding theory more deeply. Spherical packings like close-packed particle systems have been the subject of considerable attention for many decades mainly because of their role in understanding the nature of dispersed materials [1,2]. The structure of spherical packing is characterized by a number of physical parameters where the main ones are the packing density and coordination number. The coordination number is one of the most important parameters used for describing the spatial structure of random spherical packing [3]. The coordination number can be defined as the number of nearest neighbors in a close-packed system of particles located around the selected particle which allows estimating the degree of the proximity of particles to each other [4]. In the case of the definition of the coordination number concept it is necessary to consider the positional relationship relative to the central particle individually for each particle. Therefore it should be determined by analyzing the inter-particle distances.

In previous years considerable efforts were made to clarify the nature of the coordination number. This was mainly carried out through the use of three approaches: experimental methods [5, 6], methods of mathematical [7, 8] and computer simulation [9–11]. For the first time the problem of a theoretical estimate of a coordination number was considered in the work of F. Frank and J. Casper [12]. To determine the coordination number they used the

information on the number of planes formed on the Voronoi polyhedron. This approach assumed that all particles have the identical volume and all the planes in the polyhedron are equal. A few years later R. Hoppe [13] proposed another version such as lines connecting the selected particle with all its neighbors are drawn from the center of the polyhedron and secants of the plane are drawn at the points of the contact of the base particle. To find the contributions of all particles to the coordination number it is necessary to divide the area of all planes into the nearest (largest) plane.

A completely different approach belongs to J. Witing [14]. He accepted the contribution of an individual contacting particle to the coordination number equal to 1, at the double distance the contribution was already taken to be zero and in intermediate cases the linear interpolation was performed. In 1977, S. Batsanov and independently of him G. Brunner [15, 16] proposed to take into account the contribution of the surrounding particles to the coordination number in inverse proportion to the distances between the central particle and the neighboring particles. In 2008 to estimate the coordination number of a single-component spherical packing V. Bondarev and others [17] suggested using the empirical equation based on the exponential dependence of the coordination number on the inter-particle distance

$$Z = \sum_{i=1}^{m} \exp\{-\gamma[(r_i/\sigma)^6 - 1]\}, \qquad (1)$$

where γ is a constant; m is the total number of particles in the first and second coordination spheres; r_i is the interparticle distance between the central and i-th particle; σ is the particle diameter.

In 2015 it was revealed [18] that the coordination number is related to the density of regular spherical packing by the quadratic dependence

$$Z(n)=n_{max}\left[\left(\frac{2n}{\pi}\eta(n)\right)^2 - 1\right] + 2n,$$

where η is the packing density; n is the dimension of space; n_{max} is the maximum dimension of the physical space ($n_{max} = 6$).

The presented formula (2) of the dependence of the coordination number on the packing density and the dimension of space in regular spherical packing is deeply connected with the estimation of the degree of particles' proximity. In this article we are going to obtain the coordination number equation following the theoretical formalism which in its turn is based on the hypothesis of the location of the system particles in six-dimensional space. However the causality inherent in this equation shows that the dependent quantity here is the packing density which values can be determined on the data basis on the coordination number and the dimension of the space.

As it can be seen from the above mentioned, the structural characteristics of spherical packing are currently well studied but so far there is no theoretical basis for calculating the parameters of spherical packing. Especially there are few works devoted to the coordination number due to the complexity and uncertainty of the results of experimental measurements of this characteristic. For this reason, due to the necessity of eliminating such a gap the purpose of the presented research became the definition of the mathematical model for estimating the coordination number of spherical packing.

II. EXPERIMENTAL SIMULATION OF COORDINATION NUMBER

2.1 Formulation of the problem

To build a mathematical model of the coordination number of the spherical packing we will at first consider the geometric side of this problem and for this purpose we will impose a number of restrictions.

First, we assume that the dimension of the space in which the spherical packing is located is defined as a six-dimensional static space [3].

Secondly, we will put that the considered spherical packing is close-packed particle systems. In other words, in the area occupied by this packing there are no emptiness same or more than a size, as the size of particles of the smallest component of system.

Thirdly, let us assume that it is possible to consider the coordination number as the sum of the contributions of all the particle neighbors and each of these contributions is evaluated independently from each other [17].

(1) Based on these limitations we will carry out the formulation of the problem. Suppose we have a multi-component spherical packing in which all particles are spherical and have different sizes. Let us choose some particle inside the packing which we will hereafter call the central particle. Also let m neighboring particles be placed near the central particle at unique (not equal) distances.

Let us single out inside the spherical packing a separate cluster consisting of four particles contacting with each other (Fig. 1a). We will consider the particle with number 1 as a central one, the particle with number 2 as coordinated (connected) with the central particle and the particles 3 and 4 will be as particles-neighbors. In this case it is necessary to choose the assessment of the degree of participation of the coordinated particle in determining the coordination number of the central particle as the main goal of this work.

It is necessary to consider the process of changing the distance between the central and coordinated particles to achieve this goal. If we change the distance between the centers of the considering particles, this will lead to a change in the region occupied by the cluster. At the same time there will also be a displacement of neighboring particles which in accordance with the requirement of having a close-packed system must contact necessarily with the central and coordinated particles. When the distance between the centers of the central and coordinated particles is changed, the void area for each of the particles-neighbors of the central particle will be also changed.

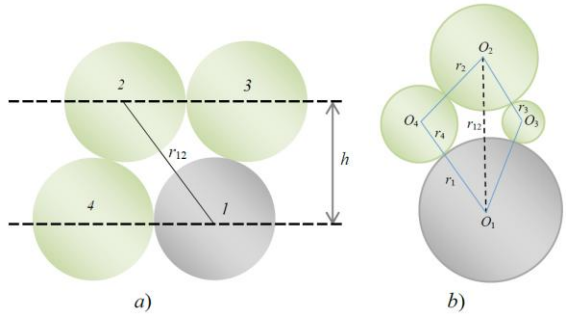

Figure 1: Image of a 2-D cluster of spherical packing:

a) a single-component system; b) a multi-component system

Basing on the presented assumptions the problem can be formulated as follows. It is necessary to find an expression for estimating the coordination number based on such parameters as the inter-particle distance and void area of the selected cluster taking into account the contributions of each particles-neighbors of the central particle in the spherical packing. Now when the problem is defined unambiguously, we proceed to simulating the coordination number of spherical packing based on a formalized approach which can lead to a deeper understanding of the physical nature of the coordination number.

2.2 Coordination index

To build a mathematical model of the coordination number we will introduce additionally a new function that allows us to estimate the contribution of each individual particle to the coordination number of the central particle. We assign this function the name coordination index f_c. This index will be a criterion of pair-wise coordination for assessing the location of the spherical packing particles relative to each other. The maximum value of the coordination index is taken equal to unity in the case of direct contact of the particle-neighbor and the central particle. The lower limit is considered to be consistent with the minimum zero value which is practically achieved at an inter-particle distance greater than $2\sqrt{2}r_1$ (r_1 is the radius of the central particle).Therefore, the limits of the change in the coordination index can be represented as non-equality:$0 \le f_c \le 1$.In this case the coordination number Z can be determined by summing the coordination indexes of all the particles-neighbors located near the central particle

$$Z = \sum_{i=1}^{m} f_{ci} ,$$

where m is the number of neighboring particles in the first and second coordination spheres. We summed up the indexes in equation (3) supposing that the coordination indexes of individual particles-neighbors of the central particle are independent of each other.

We investigate a contribution to coordination number of the central particle of a particle, separate; coordinate with her, who is her close neighbor. Let's carry out modeling of an index of coordination of particles assuming that two more other next particles at the same time are in continuous contact both with central, and with a coordinate particle (Fig. 1*b*).

Based on the previously considered conditions, as the initial parameters responsible for the change in the coordination index we take W_0 as the initial volume occupied by the cluster in 6-D space and the values of the radii of spherical particles (i=1, …, 4).

For estimating the change in the void area we shift the center of the coordinated particle by the quantity Δr relative to the center of the central particle. Then the volume of the 6-D space for the considering cluster will be changed by the quantityΔW. At the same time the void area formed within this cluster which at this stage we consider as a two-dimensional object will be also changed. In this case the input data are Was the volume of 6-D space; $S_v$as the void area related to the central and coordinated particles and r_{12}as the inter-particle distance between them. We will also assume that the coordination index depends on the size of the initial void area S_0 and the dimension n of the considering space. Therefore, the coordination index can be represented as a function:

$$f_c = F(W, S_v, W_0, S_0, n, r_{12})$$

We give the derivation of the coordination index equation below which ideology coincides with the course of determining the equation for packing density in [11]. The limits of the change in the coordination index here can be given from a value being equal to one (contacting particles) to some arbitrary value f_c and for a volume of 6-D space from the initial W_0 which is achieved with contacting particles to a volume W where the coordination index is f_c. The remaining parameters in the equation we consider to be independent of the volume of 6-D space.

To write the differential equation we assume that the infinitesimal changes in the absolute values of the coordination index Δf_c and the relative volume increments ΔW of the six-dimensional space are directly proportional. We also assume that small changes in the absolute values of the coordination index Δf_c are proportional to the coordination index f_c itself and to the relative void area S_v. This statement can be written as a differential equation:

$$df_c = -A\frac{f_c S_v \omega(n)}{S_0 W_0} dW .$$

Where A is a coefficient of proportionality; $\omega(n)$ is a function that takes into account the effect of dimension n of the considered space on coordination index f_c. We integrate this equation within the following frames: for the volume from the minimum value of W_0 to some current value of W and for the coordination index from the maximum value $f_{c\,max} = 1$ to the current value f_c. In this case the solution of the differential equation (4) can be represented as

$$f_c = \exp[-A\frac{S_v \omega(n)}{S_0 W_0}(W - W_0)], \qquad (5)$$

According to [1] the size of the area W occupied by particles in six-dimensional space can be expressed in terms of the square of the volume V of the three-dimensional space $W = V^2$ that allows writing $W = \frac{\pi^2}{4} r_{12}^6$. Entering the expression for W_0 in a similar way through the radii of the central r_1 and coordinated r_2 particles, equation (5) can be converted to the following form

$$f_c = \exp[-A\frac{S_v \omega(n)}{S_0}\left((r_{12}/(r_1+r_2))^6 - 1\right)] \quad (6)$$

2.3 The area of the voids and the dimension of the space

We calculate the void area S_v on the basis of the expression for the area of the quadrangle $O_1O_4O_2O_3$ (Fig. 1*b*) excluding the area of the sectors included into the considered space

$$S_v = \frac{k}{2}\left(r_{12}r_{34} - \frac{\pi}{180°}\sum_{i=1}^{4} \angle O_i r_i^2\right) \quad (7)$$

where $\angle O_i$ is the internal angles of the polygon bounding the void region of the cluster. The constant k in the formula (7) determines how much of the area of the cluster voids refers only to the central and coordinated particles.

$$k = \sum_{i=1}^{2} r_i^2 \Big/ \sum_{i=1}^{4} r_i^2 \quad (8)$$

To obtain more accurate values equation (6) for the coordination index must be supplemented with a semi-empirical expression that takes into account the dependence of the coordination index on the dimension of the space obtained with the help of regression analysis methods

$$\omega(n) = \alpha - \beta(n_{max} - 2n) \quad (9)$$

The approaches used in considering 3-D packings also allow us to consider the dependence on the dimension of space that gives the following values of coefficients for a linear equation on the basis of known values of coordination numbers:α=1.01and$\beta = 0.025$.

III. RESULTS AND DISCUSSION

The obtained theoretical results were then compared with known calculation data for regular spherical packings. We would like to note that the coordination numbers for regular 2-D packing were determined by displacing the layers taking into account the division of their height into several parts. Here we also took into account the fact that having determined the packing densities, it is possible then to calculate their coordination numbers by the formula (1).

To estimate the coordination number we define a number of additional calculation data for the two-dimensional case on the density of regular packing and the distance between the central and coordinated particles (Fig. 1a).In addition to the known data on the square packing: η = 0.7854; Z = 4; $R = 2\sqrt{2}r_1$ (R is the radius of the second coordination sphere); $h = 2r_1$ as well as hexagonal packing: η = 0.9069; Z = 6; $R = 2\sqrt{3}r_1$; $h = \sqrt{3}r_1$ it is necessary to have data for three more additional regular packings. Therefore similar data were calculated for various values of coordination numbers: Z = 4.5; 5.0; 5.5 using the formula (2). The coefficient of proportionality A was accepted equal 0.7575. Also, in case of consideration of mono-systems of particles to which regular packings belong small changes of the void area when calculating was not considered. The results of the calculations are presented in Table 1.

Table 1: – The results of the calculation of the coordination number (CN) of regular spherical packings

Packing density	Newton's number	Second coordination area		Theoretical CN	Calculated CN	Ratio error, %
		Number of particles	Sphere radius, *R*			
Space dimension*n*=2						
0.785	4	4	2.828	4.0	4.025	0.62
0.818	4	2	2.404	4.5	4.461	0.88
0.848	4	2	2.231	5.0	5.020	0.41
0.878	4	2	2.103	5.5	5.549	0.89
0.907	6	6	3.464	6.0	6.0	0.0
Space dimension*n*=3						
0.524	6	12	2.828	6.0	6.057	0.94
0.605	8	6	2.828	8.0	8.028	0.35
0.680	8	6	2.309	10.125	10.103	0.22
0.698	10	4	2.449	10.667	10.65	0.16
0.741	12	12	3.464	12.0	12.0	0.0

As we can see in Table 1, the ratio error in the calculation of the coordination number is the order value of tenths of a percent. Thus, the considered model of coordination number reproduces well the data on the determination of the coordination number. The coordination number equation for multi-component spherical packing can be used for describing the state of the particles and the numerical estimate of the coordination number now reduces only to finding the inter-particle distances.

IV. CONCLUSION

Our research allowed us to carry out a theoretical study of the coordination number of the spherical packing. In the process of research we found the model approximations in 2-D and 3-D spaces for the coordination number of spherical packing. Our theoretical results are in excellent agreement with the calculation data for regular structures and they can also be used in considering multi-component random spherical packings.

The introduced concept of the coordination index makes it possible to calculate analytically the coordination number based on the consideration of the pair-wise coordination of particles. In our research we showed that the coordination index is a function that depends uniquely on the area of the cluster voids, the dimension of the considered space and the quantity of the inter-particle distance. The reliability of this

equation is confirmed by the results of computer simulation and known experimental data.

In conclusion we should emphasize that a complete understanding of the coordination number requires further theoretical studies. The concept of the coordination number in its basic sense also constitutes the basis for estimating the local densities of any systems of particles. Using this concept, everyone can not only determine the structural features of close-packed systems but also linear densities, for example, the number of branches on a tree trunk and also use the concept of coordination number to estimate local densities of celestial bodies such as planets, constellations, etc.

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