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THE PACKING DENSITY AND THE COORDINATION NUMBER OF REGULAR SPHERICAL PACKING

Abstract. The article shows the receiving of density equation of regular spherical packing functioning as an effective coordination number and dimension of space on the basis of six-dimensional physical space determination. In addition, the article focuses on the improvement of the semi-empirical formula for determination of dependence of the coordination number from distance to the second coordination sphere of regular packing.

Keywords: modeling, regular spherical packing, packing density, coordination number, dimension of space.

As previously mentioned [1], the most important structural characteristics of their packing are the packing density and the coordination number in the theory of dense-packing particle systems. It is also pointed out that packing density characterizes the way of spatial placement of particles around some separately chosen particle and the coordination number determines the quantity of the particles located close to the chosen particle. A numerical data on the packing density of spheres η depending on the size of the coordination number Z in spaces of various dimensions was obtained by research.

As illustrated in table 1, regular packing of spheres has the greatest of possible packing density in one-dimensional space where packing density reaches its maximum value equal to one unit. The system of disks, located in two-dimensional space, has only two possible close-packed regular arrangements. They are a square packing with the coordination number equal to four and a hexagonal packing with the coordination number equal to six.

Table 1. Density of regular packing η spheres depending on the coordination number Z and dimension n of space.

Dimension, n	**Coordination number, Z**						
	2	**4**	**6**	**8_1**	**8_2**	**10**	**12**
1	1						
2		0,785	0,907				
3			0,524	0,605	0,68	0,698	0,74
R_2		$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{2/3}$	$\sqrt{6}/2$	$\sqrt{3}$

Note: 8_1 – Face-centered cubic packing (FCC); 8_2 – Body-centered cubic packing (BCC); R_2 – Distance to the second coordination sphere.

The biggest group of regular packings is presented by the systems of spheres located in three-dimensional space. There are several types of regular packing: a cubic primitive packing (Z=6), a body-centered cubic (BCC), a cubic hexagonal packing (Z=8), tetragonal packing (Z=10) and also two types of regular packing having identical coordination numbers Z=12: a face-centered cubic packing (FCC) and a hexagonal dense packing (HCP).

The packing, having identical values of coordination numbers, is of a particular interest. The prime examples of this type of packing are body-centered cubic packing and cubic hexagonal packing and also face-centered cubic and hexagonal dense packing. Moreover, face-centered cubic and hexagonal dense packing differ by topological character, but BCC and cubic hexagonal packing vary depending on the structural arrangement of spheres in the second coordination sphere. For determination of unambiguous distinction of previously mentioned spherical packing it was suggested to introduce the concept of effective coordination number [2]. A BCC-packing effective coordination number is defined as 8+(6) where number 6 defines quantity of the spheres placed in the second coordination sphere. It is accepted to present the value of the effective coordination number for tetragonal packing as 10+(4). However, such representation of coordination numbers does not give us the chance of the comparison of various packing. Besides, this concept does not allow us using them in mathematical calculations. To accomplish this task we illustrated the results of packing density of regular spherical packings depending on effective coordination number and dimension of considered space research.

The dependence of density of regular packing of particles from the coordination number in spaces of various dimensions was defined by building the mathematical model. Scientifically speaking, it is necessary to make several aprioristic assumptions. Firstly, we consider the space located in the static case in which the considered system of spherical particles can be defined as the six-dimensional space [3], which has rigid pair connection of own one-dimensional spaces and anti-spaces. The basis of such statement is a well-known expression for definition of the spatial interval s [4]

$$s=\pm\sqrt{\sum_{i=1}^{3}\Delta x_i^2}\,,\tag{1}$$

where $i=1,2,3$ is the number of the chosen one-dimensional subspaces.

Secondly, we introduce the concept of the generalized coordination number u, that represents the number of possible particle connectors concerning the subsequent space-like dimensions. Thirdly, we consider the change of values of the volumetric gain ΔW while changing the generalized coordination number at a size Δu in direct ratio to the volume W of six-dimensional space and in inverse proportion to the size of the generalized coordination number u. This assertion can be illustrated as the following:

$$dW=-A\frac{W}{u}du\,,\tag{2}$$

A is the constant of proportionality (at further consideration we accept this constant of proportionality equal to one unit).

Having integrated this equation in limits for volume from the maximum value W_{max} to some value W and for the generalized coordination number from the value u to minimum u_{min} we receive

$$W=\frac{W_{\max}u_{\min}}{u}.\tag{3}$$

According to [5] the volume of area W occupied by particles in six-dimensional space can be calculated with a square of volume V of the three-dimensional space $(W=V^2)$ that allows us to show the following expression: (3)

$$V=V_{\max}\sqrt{\frac{u_{\min}}{u}}\,.\tag{4}$$

The packing density of particles η by definition criteria can be presented as

$$\eta=\frac{V_p}{V},\tag{5}$$

where V_p is the volume of the solid phase of spherical packing.

If to accept the volume of the firm phase V_p as a constant, substituting in the formula (5) expression (4) for the packing density, we derive the following equation:

$$\eta=\eta_{\min}\sqrt{\frac{u}{u_{\min}}}\,.\tag{6}$$

The generalized coordination number u is the function of the effective coordination number z and dimension of space n. In addition, we consider that the coordination number and dimension of space are independent parameters. Therefore, this statement allows us to deduce the expression for the generalized coordination number u in the integrated form

$$u(z,n)=\int_0^z dz+\int_{2n}^{6} dn\,,\tag{7}$$

where the lower limit in integrated expression for dimension of space includes the above-mentioned assumption about tough pair connection of one-dimensional subspaces. After deriving the integration of the equation (7) for the generalized coordination number u we will receive the following expression

$$u(z,n) = z + 2(3-n). \tag{8}$$

Taking into account expression (8) and the equation (6) for the packing density we receive

$$\eta = \eta_{\min}\sqrt{\frac{z+2(3-n)}{z_{\min}+2(3-n)}}. \tag{9}$$

The minimum packing density η_{min} can also be expressed through the dimension of space

$$\eta_{\min} = (\pi/2n)^{\delta(n)}, \tag{10}$$

where $\delta(n)$ is a discrete function that is presented as:

$$\delta(n) = \begin{cases} 0, & n=1; \\ 1, & n=2,3. \end{cases} \tag{11}$$

Taking into consideration that the minimum coordination number $z_{\min}$ in three-dimensional space for dense spherical packing matters equal to six, we will finally receive

$$\eta = (\pi/2n)^{\delta(n)}\sqrt{(z+6-2n)/6}. \tag{12}$$

The derived equation (12) allows us to count density of regular spherical packing at any values of coordination numbers and the considered spaces of dimensions. At the same time, real values of packing density for BCC and tetragonal packing will be implemented at other values of coordination numbers that is regarded as the effective coordination numbers.

Therefore, the effective coordination number according to the formula (12) for BCC-packing equal z=10,125, and for tetragonal packing: z = 10,6665. Let us also pay attention to the fact that for all other spherical packings the effective coordination number completely coincides with value of the most coordination number (contact number).

In order to check the accuracy of the offered approach, we will examine the formula of the effective coordination number through its dependence on distances between the chosen particle and its neighbors in the second coordination sphere. For this purpose we will use already known semi-empirical expression for the determination of the dependence mentioned earlier [6]

$$z = \sum_{i=1}^{m}\exp\{\alpha[1-(r_i/\sigma)^6]\}, \tag{13}$$

where r_i is a distance between the particle and its i neighbor; σ is the diameter of the particle; m is the number of the particles belonging to the areas of the first and second coordination spheres; and α is the constant.

We will determine the value of constant α drawing on the values of coordination number of a particle in case of the body-centered cubic packing. Having integrated the value of the effective coordination number for this packing (z=10,125) and also the value of distance r for particles of the second coordination sphere from table 1 into equation (13), we can precisely calculate the size of this constant. Its value will be $\alpha = 0,75744$ in this case. Taking into account the outcome of this formula (13) and the acquired constant for tetragonal packing, we will determine the size of the effective coordination number: $z = 10,6665$ that coincides with the design value up to the 4th sign after the comma.

To sum up, we have considered the problem of definition of the equation of packing density of regular spherical packings depending on the effective coordination number and dimension of space and so we can draw a set of conclusions.

1. Realizing the concept of the six-regularity of physical space allows to derive the equation of density of regular packing of spheres as function of the effective coordination number and the dimension of space.

2. The semi-empirical formula for determination of dependence of the coordination number from the distances to the second coordination sphere of regular packing can be also used in three-dimensional case.

3. The received numerical values of effective coordination numbers for body-centered cubic and tetragonal packing enabled to change the high-quality consideration of structural characteristics into their quantitative implementation.

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