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Determining the Thickness Coating of Grinding Powders of Synthetic Diamond Based on a Specific-Surface Approach and using an Extrapolation-Affine 3D Model of Grain

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Abstract: Methodological features of indirect determining of thickness coating of grains grinding powders of synthetic diamond are analyzed. A newly revised classification of known methods for determining the thickness of the coating is proposed. The prospects of the methods based on the application of an external specific surface are noted. A positive feature is the proposal to determine the thickness of the coating separately for each grain of the sample, followed by the generalization of the results by calculating the arithmetic mean. This calculation scheme allows you to get more reliable information about the thickness of the coating. The expediency of using an extrapolation-affine 3D grain model in such a calculation scheme is substantiated. Using the extrapolation-affinine 3D grain model allows for determining the thickness of the coating of diamond powder grains without the traditional assumption about the spherical shape of their grains and with less error. For an example of grinding powder AC125 400/315, the advantage of such a 3D model compared to a 3D model in the form of a sphere is proved. The method proposed on the basis of such methodical innovation can be used for powders of other abrasive materials.

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1. INTRODUCTION

The coating is one of the effective methods of grain surface modification of synthetic diamond (SD) powders, cubic boron nitride, and powders of other superhard materials (SHM) [1-4]. The main purpose of such a technological operation is to increase the efficiency of the abrasive tool (AT) manufactured using thus modified powders. The coating is also acting (effective) means of influencing the operational and technological properties of products intended for use in mechanical engineering, chemical, and other industries. Among the main tasks of such influence is the protection of work surfaces from the action of aggressive outer environments, mainly from corrosion [5-7] and increasing the working life of machine parts [8, 9].

An important characteristic of the coating is its thickness. It significantly affects the strength of maintenance of the grains of grinding powders in the cutting layer of AT, and hence the specific consumption of abrasive powder. That is why, the specific consumption, as a characteristic of the processing process, and is one of the main criteria for the effectiveness of AT [1]. The thickness of the coating also affects the microhardness and crack resistance of the obtained modified surfaces and their structure [7, 10, 11]. In this case, the greatest positive effect of such modification is often achieved only with the optimal thickness of the coating [12–14]. For example, tests modified diamond grinding powder SD (modern mark AC32) with a grain size of 125/100 by coating showed that increasing the thickness of the nickel coating above the optimum was not accompanied by an increase in the stability of the tool [15]. Therefore, it is important to have information about the thickness of the coating and hence the methods of determining it.

A rather detailed analysis of the state of affairs in determining the thickness of the coating in relation to SD powders and powders of other SHMs was performed in [16]. It was noted that this issue was not given due attention for a long time. The main focus was on the technological aspects of coating [2-4, 15]. And this is reflected in the availability of publications on this topic. A small number of publications consider obtaining new analytical dependences for the indirect determining of the thickness of the coating of SHM grinding powders. Among the latest publications in this area, it is worth noting the publication [17]. It obtains and presents analytical dependences of indirect coating thickness determination for new 3D grain models. In particular, such as

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cuboctahedron, truncated octahedron, and ellipsoid. The error of determining the thickness of the coating, which is introduced by the proposed new and known 3D models and the corresponding analytical dependences, was also investigated. The directions for further development of such research are formulated. Among such areas, the most important is the involvement of new 3D models of grain and obtaining on their basis analytical dependences for practical calculations of the thickness of the coating of powder SHM. Therefore, the development of new methods for determining the thickness of the coating of SD powders remains an urgent scientific and applied task.

All known and applied in practice methods for determining the thickness of the coating of SD grinding powders are inherently indirect. They are based on the relationship between the thickness of the coating with the individual physical properties of the object of the coating as a solid and certain physical phenomenon. Physical properties are used, for example, by the fundamental pycnometric ratio between the density, mass, and volume of a solid and the additive property of the volume of such a body. X-rays, X-ray microtomography, and laser interferometry are used as physical phenomena. Each of the above two methodological approaches has found its application [2, 18].

Considering the above generalized scientific and methodological basis for the development of methods for determining the thickness of the coating of grinding powders SD, we can present a new scheme of their classification compared to that proposed in [16]. Its essence is as follows. All methods are divided into two groups. The first includes methods based on the use of a pycnometric relationship between the density, mass, and volume of a solid and the additive property of its volume. Such methods, on the one hand, are indirect.

On the other hand, they additionally require knowledge (information) about the 3D shape of the coating object and provide the possibility of analytical representation of its volume with subsequent analytical transformations in order to obtain the appropriate calculation dependence. According to the classification [16], this approach was proposed to be called pycnometric-additive. However, given the above arguments, it would be more appropriate to call the methods of this group indirect-analytical. This group includes the methods described in [19-21].

It is appropriate to combine the methods based on the use of the above-mentioned physical phenomena into a separate second group. It is proposed to briefly call the methods of this group direct methods for determining the thickness of the coating of SD grinding powders, although, in essence, they are also indirect. However, unlike indirect-analytical methods, the practical implementation of these methods does not necessarily involve a 3D model of the object of the coating, i.e., the grain of grinding powder. The methods of this group can be applied to abrasive powders with both a thin layer (film) and a non-thin layer coating applied to their grains. They can also be applied to objects of a different nature than abrasive powders with a coating applied to their surface [18].

2. SPECIFIC SURFACE METHOD FOR DETERMINING THE THICKNESS OF THE COATING OF SD GRINDING POWDERS BASED ON EXTRAPOLATION-AFFINE 3D MODEL OF GRAIN

One of the directions of the modern development of indirect-analytical methods for determining the thickness of the grain coating of abrasive powders is the use of the external specific surface for this purpose. Based on this method, according to the classification [16] were allocated to a separate subgroup of specific surface methods. Here, the outer specific surface interpretation is accepted according to the definition and classification are given in the known classical work [22]. The positive advantage of these methods is that the structure of the corresponding calculated dependences does not include the geometric parameter of grain size. Another positive feature is that the thickness of the grain coating, in this case, can be calculated based on the outer specific surface of the grinding powder. In turn, the outer specific surface can be determined either experimentally by one of the methods described in [23] or calculated analytically based on a 3D model of the grain. The above advantages of specific-surface methods allow the use in this methodological scheme and 3D models of grain, different from the classical spatial bodies, such as a cube, sphere, ellipsoid, and others. The general calculation formula for determining the thickness of the grain coating on the basis of the specific-surface approach is as follows.

$$h = \frac{\mu}{\rho_M F_{oss}} \tag{1}$$

where ρ_M is the density of the coating material; $\mu = m_M/m_a$ - degree of coating; m_a is the mass of material spent on the coating of diamond powder with mass m_a; F_{oss} - the outer specific surface of the powder. Dependence (1) can be converted to another type, more convenient for the case when the outer specific surface of the powder allows analytical representation, i.e., it can be calculated indirectly by the analytical method. By definition $F_{oss} = S/m_a$, where S is the surface area of the abrasive powder to be coated. The mass m_a,, using the pycnometric ratio, can be represented as $m_a = \rho_a V$, where V is the volume of abrasive powder to be applied to the coating, ρ_a is the density of the abrasive powder material. As a result, we get

$$h = \frac{\mu \rho_a V}{\rho_M S} \tag{2}$$

In [22], formula (1) is concretized for SD grinding powders in the case of a 3D model of grain in the form of a sphere

$$h = \frac{\mu d \varphi}{6} \frac{\rho_a}{\rho_m} \tag{3}$$

where ρ_a is the density of the diamond, d is the average grain size of the diamond before coating; φ is an empirical coefficient that depends on the geometry of the grains and characterizes the deviation of its volume from the volume of a sphere with a diameter equal to the average grain size. For SD grinding powders, the authors propose to take it equal to 0.7. In this regard, it should be noted that such an assumption about the 3D shape of the grain introduces a significant error in determining the outer specific surface of diamond powders, and with it as a result of determining the thickness of their coating.

More precisely, the thickness of the coating of diamond powders, the spatial and geometric shape of the grains, which is a priori different from the ball (which is typical for grinding powders SD and other SHM), can be calculated from the extrapolation-affine 3D model of grain. The method of calculating the volume and surface area of the grain, and through them, the outer specific surface of the powder to be coated, is described in [24]. The required initial data can be obtained by diagnosing on the device DiaInspect.OSM [18] morphometric characteristics of the initial powder. Such a methodological scheme involves the calculation (determination) of the external specific surface area using an extrapolation-affinity 3D model of the grain, followed by substituting its value in formula (1) or in formula (2). This innovation significantly expands the scope of the practical application of formulas (1) and (2). This is achieved due to the fact that the extrapolation-affine 3D model of abrasive powder grain inherits from the real grain 5 of its parameters: maximum (F_{max}) and minimum (F_{min}) diameters, Feret of projection of grain, its height (H_z), perimeter (L) and area (A_t) projection. All these geometric parameters are provided by the device DiaInspect.OSM. According to this number of inherited parameters of the actual grain, the extrapolation-affine 3D model significantly outperforms the known 3D models. In addition, the need to use the empirical coefficient φ, which appears in formula (3), is eliminated. This increases the accuracy of the estimated determination of the volume and surface area of the grain and its outer specific surface area.

3. INVESTIGATION OF RELATIVE ERROR OF DETERMINATION OF COATING THICKNESS USING EXTRAPOLATION-AFFINE AND OTHER 3D GRAIN MODELS

This study was conducted by testing. A parallelepiped was adopted as a test 3D grain shape, and a sphere, cube, cuboctahedron, ellipsoid, and extrapolation-affine 3D model served as 3D grain models. Note that the choice of a parallelepiped, in this case, is in no way related to a particular abrasive powder and is more methodical than applied. Such a binding is not significant given the achievement of the declared goal of the study, which is a quantitative analysis of the error in determining the thickness of the coating by different methods and using different 3D models of grain. This use is due only to the fact that the parallelepiped is a three-parameter body, and it facilitates the process of matching its defining geometric parameters with the defining geometric parameters of the adopted 3D grain models.

Regarding 3D models of grain, the sphere and the cube were most often used in the known indirect-analytical (according to the new classification) methods for determining the thickness of the coating of SHM grinding powders. Kuboktahedron is a characteristic 3D shape of a grain of high-strength SD grinding powders. The ellipsoid before the extrapolation-affine 3D grain model was considered [26] the closest analog of the actual grain shape of grinding powders of SD regardless of their static strength. Subsequently, this was substantiated and analytically [27].

The defining geometric parameters of the test grain were the edges of the parallelepiped, for which the notation $A \geq B \geq C$ is introduced, and $A = B$ is taken. The surface area of a parallelepiped as a test grain is expressed by the dependence $S_{prl} = 2(AB+AC+BC) = 2A(A+2C)$. With regard to the 3D models considered here, their defining geometric parameters will be the edge of the cube (a_{cb}) and cuboctahedron (a_{cbo}), the diameter of the sphere (D), and the half-axis of the ellipsoid ($a \geq b \geq c$). Regarding the defining geometrical parameters of the extrapolation-affine 3D model, it is legitimate to accept the above-mentioned morphometric characteristics of the grain projection as such: F_{max}, F_{minx}, H_z, L, and A_t. The relationship between the defining geometric parameters of the test grain and the accepted 3D models in the form of a cube, sphere, and cubic octahedron is given by the following dependencies

$$a_{cb} = \sqrt{\frac{S_{\text{prl}}}{3}}, \quad D = \sqrt{\frac{S_{\text{prl}}}{\pi}}, \quad a_{cbo} = \sqrt{\frac{S_{\text{prl}}}{3+\sqrt{3}}} \tag{4}$$

in accordance. These dependencies are obtained by equating the surface areas of the parallelepiped and the surface areas of the corresponding 3D grain models and then solving the obtained equations with respect to a_{cb}, D, and a_{cbo}, respectively. The obtained values of these defining parameters are given in Table **1** (column 2).

To obtain the defining geometric parameters in the case of an ellipsoid, we will proceed from the equality of the surface areas of the parallelepiped and the ellipsoid. In this case, use the known approximate Knud Thomsen formula [28] to determine the area of the ellipsoid

$$S \approx 4\pi\left[(a^p b^p + a^p c^p + b^p c^p)/3\right]^{1/p} \tag{5}$$

where p≈1.6075. Equating the surface areas of the parallelepiped and the ellipsoid, assuming $a = A/2$, $b = a$, and solving the obtained equation with respect to c, we obtain

$$c = \left\{\left[3\left(\frac{S_{\pi P \pi}}{4\pi}\right)^p - a^{2p}\right]^p \frac{1}{2a^p}\right\}^{1/p}$$

Table 1: Surface area and volume of 3D grain models, results, and relative error (δ,%) of determining the thickness of the coating (*t*, μm) of grains by indirect-analytical (I) and specific-surface (II) methods using different 3D models grain (actual 3D grain shape - parallelepiped; *A* = 200 μm, *B* = *A*, *C* = 100 μm, actual coating thickness - 5 μm, degree of coating - 0,27276, ρ_a/ρ_M = 0,78)

3D grain models	Defining parameters of actual grain and accepted 3D of his models, μm	S, μm^2	V, μm^3	Methods of determining coating thickness				δ_{II}/δ_I
				I		II		
				t	δ_I, %	*t*	δ_{II}, %	
Parallelepiped	*A*, *B*, *C*	160000	4000000	5.01	0.11	5.32	6.38	56.8
Cube	a_{cb} = 163.30	160000	4354649	5.42	8.45	5.79	15.81	1.87
Sphere	*D* =225.68	160000	6018022	7.49	49.87	8.00	60.04	1.2
Cuboctahedron	a_{cbo}=130.02	160000	5181132	4.32	13.65	6.89	37.79	2.77
Ellipsoid	*A*=*B*=200, *C*=139.71	160000	5852034	7.35	47.00	7.78	55.63	1.18
Extrapolation-affinine	F_{max}=223.61, F_{min}=200, *L*=800, A_t=40000 μm^2	124784	2666622	—	—	4.55	9.0	—

During testing, it was assumed that the test diamond grain (ρ_M =3.51 g/cm^3) size *A*=200 μm, *B*=*A*, *C*=100 μm, was applied titanium (ρ_M =4.5 g/cm^3) coating, thickness *h*=5 μm. Calculated according to the method [29] with such data, the degree of the coating was μ=0.27276.

When matching the defining geometric parameters of the test grain in the 3D shape of a parallelepiped and extrapolation-affine 3D model, it was assumed that the actual shape of the projection of the test grain, in this case, will be a square with side lengths *A*. Given this, and based on the geometric essence of the maximum diameter, Feret took: $F_{\max} = A\sqrt{2}$, and other defining parameters were as follows: F_{min}=*A*, *L*=4*A*, and A_t=A^2. As for the grain height, H_z, it was assumed to be equal to *C*, i.e., H_z =100 μm was assumed. Analytical representation of the surface area and volume, which are factors of the specific surface area of the adopted 3D models of grain, and the results of the test determining grain thickness by indirect-analytical (I) and specific-surface (II) methods are given in the Table **1**.

Calculations were performed at μ= 0.27276, ρ_a/ρ_M = 0.78. The thickness of the coating by the specific surface method was calculated depending on (2). The procedure for determining the thickness of the coating involved three stages. In this case, each of these three stages was performed autonomously, i.e., separately from the others. In the first stage, the morphometric characteristics of the initial (uncoated) powder were diagnosed using the DiaInspect.OSM devise. As a result of the diagnosis, an Excel file with morphometric characteristics for each grain of their control sample (sample) was obtained. The list of these characteristics included the following F_{max}, F_{min}, H_z, *P*, and A_t. In the second stage, the degree of coverage μ, included in the formula (2), was determined. According to formula (2), the coating thickness was calculated in the third stage for each grain of the control sample (sample) of grinding powder. After completing this procedure, the generalization of the results obtained for individual grains was performed by calculating their arithmetic mean. The effectiveness of such a calculation scheme was confirmed by studies conducted in [24] on the example of the outer specific surface of diamond powders. In the case of coating diamond powder grains, such a calculation scheme allows for receiving more reliable information. We should also add that the above-cited publication [24] provides a detailed description of the mathematical apparatus for constructing an extrapolation-affine 3D model of grain and algorithms for calculating its volume and surface area. In parallel, the coating thickness was also determined by the indirect-analytical method for each of the studied 3D grain models. The general calculation formula of such a method for 3D models of grain in the form of regular one-parameter bodies (in our case, such are a cube, a sphere, and a cuboctahedron) was obtained in [16] in the form

$$h = \frac{d}{2}\left[\sqrt[3]{\mu\frac{\rho_a}{\rho_M}+1}-1\right] \tag{6}$$

where $d=a_{cb}$ for a cube, *d*=*D* for a sphere, and $d=a_{cbo}$ for a cuboctahedron. For these one-parameter bodies, formula (6) gives the exact result. However, its practical application to SHM powders is very limited (or even impossible) because the actual 3D grain shape of such abrasive powders is far from one-parameter spatial bodies of the correct shape. However, in our case, the values of the thickness of the coating obtained by this method will allow us to estimate the error caused by the application of the specific-surface method in combination with the studied 3D models of grain. Note that the calculation formulas of indirect-analytical determining of the thickness of the coating for three-parameter spatial bodies in the form of a parallelepiped and an ellipsoid are of the same type and have the following form

$$h = A\frac{S_1}{4S_2}\left\{\sqrt{1+\frac{4S_2\tilde{B}\tilde{C}\mu}{S_1^2}\frac{\rho_a}{\rho_\pi}}-1\right\} \tag{7}$$

where $A \geq B \geq C$ is the axis of the ellipsoid or the edge of the parallelepiped. The general methodical scheme of obtaining formula (7) is given in the above-cited work [16].

4. RESULTS AND DISCUSSION

The available information allows to analyze the influence of the adopted (from the list studied in this work) 3D model of grain on the thickness of the coating and to quantify the relative error of its calculation by indirect-analytical and specific-surface methods in the case when the actual 3D grain shape is a parallelepiped. Comparative analysis of the information presented in the Table **1** shows that in the conditions of the study, the smallest error (9%) in determining the thickness of the coating by the specific surface method gives the use of an extrapolation-affine 3D model of grain. The second in this indicator is the 3D model of the grain in the form of a cube (relative error δ_{II} = 15.81%). This is expected because a parallelepiped and a cube are close spatial bodies. The much greater relative error is provided by using a 3D model of grain in the form of a cuboctahedron (37.79%), a very large - 3D model in the form of the ellipsoid (55.63%), and the sphere (60.04%).

Interesting in the information-methodical sense is the relative comparison of the relative error of the indirect-analytical determining the thickness of the cover by dependences (6) and (7). The following two factors are of interest in this comparison. The first of them is the influence of the presence or absence of simplifications adopted in the construction (derivation) of dependencies (6, 7). Such dependencies are obtained by the analytical solution of the basic equation of indirectly determining the thickness of the coating. In turn, this basic equation is obtained based on the balance of grain volumes of abrasive powder, the volume of the coating material to be applied to the grain, and the volume of grain with a coating applied to its surface. Since the grain as a spatial body has three geometric dimensional parameters, the resulting expression is an equation of the third degree with respect to *h*, i.e., cubic. The algorithm for solving such equations is quite complex and involves a number of cumbersome transformations. However, for thin-layer coatings, i.e., when $h/L \ll 1$ (*L* is a characteristic parameter of grain size), the member containing h^3 can be neglected. Thus, the cubic equation is reduced to a quadratic equation, solving which we obtain the dependence (7) to determine *h*, which is valid for three-parameter models in the form of an ellipsoid and a parallelepiped. As can be seen in the example of a parallelepiped, the relative error due to such neglect is small and is only 0.11% (Table **1**). Note also that in the case of single-parameter 3D grain models, the need for the above simplification is eliminated. For such 3D grain models, the cubic equation allows for an exact solution, i.e., an exact calculation formula in the form (6).

Regarding the criterion of accordance with the defining geometric parameters of the 3D model of grain and its actual geometric parameters as a factor influencing the relative error of indirectly finding the thickness of the coating, the results obtained in our study are not enough for a full comparative analysis. In our work, only one such criterion was used - the condition of equality of the surface area of the test grain and its 3D model. However, even in such circumstances, it can be concluded that this factor has a significant impact on the error in determining the thickness of the coating. Depending on the 3D model, as shown by the analysis given in the Table **1** information, it can range from 8% to 50%. Therefore, expanding the range of such criteria is one of the ways to continue further research on this topic.

The general data analysis Table **1** shows that the specific-surface method gives 1.18–56.8 times greater relative error in comparison with the indirect-analytical method. This ratio of the relative errors of these methods is consistent with its theoretical justification, which was performed in [16]. If we analyze only the specific surface method, as shown by the analysis given in Table **1** information, the relative error is from 9% to 60%, again depending on the adopted 3D grain model. At the same time, the extrapolation-affine 3D model of grain delivers the minimum error.

This ratio confirms the high adequacy of the extrapolation-affine 3D model of grain, which was also proved by the example of determining the number of grains of synthetic diamond powders in one of their carats [30]. This advantage allows us to reasonably recommend an extrapolation-affine 3D model of grain for use in the methodical scheme for determining the thickness of the coating of abrasive powders by the specific surface method.

5. CONCLUSIONS

A newly updated classification of known methods for determining the thickness coating of grain grinding powders synthetic diamond has been performed. Studies have confirmed the viability and feasibility of using methods based on the use of the outer specific surface. The use of an extrapolation-affine 3D grain model in such a calculation scheme is substantiated. It was found that the specific surface method based on the extrapolation-affine 3D grain model delivers 1.7–6.7 times less relative error in determining the thickness of the coating compared to other possible, including characteristics of diamond powders 3D grain models. It is established that the specific-surface method based on the extrapolation-affine 3D model of grain delivers 1.7–6.7 times less relative error in determining the thickness of the coating compared to other possible and including characteristics of diamond powders 3D models of grains.

The use of extrapolation-affine 3D grain model allows for determining the thickness of coating grain of grinding powders synthetic diamond without the traditional assumption about the spherical shape of their grains and with less error. The method proposed on the basis of such methodical innovation can be used for powders of other abrasive materials.

For the first time, an algorithm was used to determine the thickness of the coating separately for each grain of the sample, followed by a generalization of results by calculating arithmetic mean. The effectiveness of such a calculation scheme was confirmed by studies conducted in [24] on the example of the outer specific surface of diamond powders. In the case of applying the coating on the grains of these powders, such a calculation scheme allows for obtaining more reliable information about its thickness.

Further research on the subject of this publication should be continued to identify the most optimal criteria for matching the parameters of different 3D models of grain with morphometric characteristics of abrasive powders, which are diagnosed by modern automated technical means.

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