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THEORETICAL JUSTIFICATION OF RATIONAL CONDITIONS FOR PRODUCING DIAMOND WHEELS ON CERAMIC BONDS

Abstract. *The article describes the results of theoretical studies using 3D finite element modeling, which made it possible to determine the rational characteristics of diamond wheels on ceramic bonds. The influence of the parameters of the diamond-bearing layer on the change in its stress-strain state in the sintering zone of the diamond wheel has been studied. The results of finite element and microlevel 3D modeling of the sintering process of a ceramic-matrix diamond-containing composite are analyzed. The influence of the technological parameters of the process and the characteristics of the diamond wheel on the integrity of the grains during sintering was established, on the basis of which practical recommendations were given for the selection of diamond compositions with rational properties.*

Keywords: *Diamond grinding wheel; ceramic bond; diamond-bearing layer; diamond grain; grinding process; force and temperature factors; Finite element method; 3D model; diamond wheel sintering process; metal phase; equivalent stresses.*

1. Literature review

It is known that during the operation of diamond abrasive tools (DAT), the coefficient of effective use of diamond grains does not exceed 10%. The rest of the grains are destroyed even at the stage of tool manufacturing and fall out during grinding. The efficiency of diamond grinding depends largely on the characteristics of diamond wheels, and is also determined by the rational choice of the optimal technological parameters for their manufacture, which ensures the integrity of diamond grains at this stage. And this, in turn, contributes to the creation of prerequisites for their rational self-sharpening during the operation of the DAT [1, 2]. The information available in the literature on the mechanism of renewal of the cutting surfaces of grains during grinding and the conditions under which the rational self-sharpening of DAT is realized are contradictory and general, which does not contribute to the efficiency of their use. In the process of diamond abrasive processing, two cases most often take place: spontaneous uncontrolled self-sharpening of the wheel due to the tearing of grains from the bond, which leads to unjustified loss of diamonds, or its complete absence, leading to greasing of the working surface of the tool.

The choice of the composition of the diamond-bearing layer, depending on the purpose of the diamond wheel and the type of material being processed (PM), should be based on scientifically grounded recommendations for the optimal combination of concentration, grain size and strength of diamond grains, properties and structure of the bond, as well as coatings that protect diamond from destruction during composite sintering. [3]. This approach can ensure the integrity of diamond grains in the manufacture of tools, and will contribute to the creation of prerequisites for rational self-sharpening of grains during grinding.

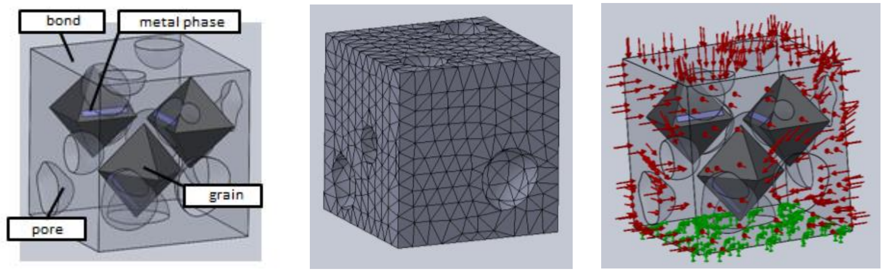
An equally important issue in the design of diamond wheels is the correct choice of technological parameters for the sintering of the diamond-bearing layer of the tool, taking into account the physical and chemical characteristics of the processes occurring in this case. Sintering of the diamond-bearing layer on typical ceramic bonds occurs at higher temperatures, sufficient for the graphitization of diamonds. Depending on the properties of diamond powders, their cost can differ hundreds of times. Therefore, the choice of the characteristics of the wheel, as well as the parameters of its manufacture, should not only provide the specified properties of the tool, depending on its purpose, but also take into account the production cost. To solve this problem, we used an approach based on the analysis of the results of three-dimensional modeling of the sintering process of the diamond-bearing layer, identifying the most significant factors that determine the stress level and the state of the grains during sintering of the diamond-bearing layer.

To reduce lengthy and labor-intensive experimental studies, theoretical modeling of the process of sintering the diamond-bearing layer of a grinding wheel was carried out by analyzing the stress-strain state (SSS) of the "bond-coating-diamond grain-metal phase" system using the finite element method. The *SolidWorks* software package was used to create models of a diamond-bearing layer fragment. To implement simulation experiments, the *ABAQUS* software package was used. The research task at this stage was to simulate the sintering process to determine the conditions for the formation of a diamond-bearing layer, ensuring the integrity of diamond grains in it. When carrying out model experiments, such a combination of its morphological characteristics was determined, which ensured the preservation of the integrity of diamond grains under the conditions of specified temperature and power loads.

2. Methods

To carry out simulation experiments, models of the grinding process have been developed (the system “bond - grain - metal phase - processed material”, Fig. 1).

In modeling, it was assumed that a fragment of a diamond-bearing layer in the form of a cube with a certain amount of diamond grains, bounded on all sides by a bond array [4, 5] can fully represent the diamond wheel as a whole.



a) b) c)

Figure 1 – 3D model (a), finite element mesh (b) and loading scheme (c) in the study of the sintering processes of the diamond-bearing layer

When creating the models, the shape, dimensions and properties of its elements were taken into account, which were considered elastic solid bodies. Since the most common form of diamond crystals is the octahedron [6, 7], the grain was designed with the geometry of an octahedron. The diamond grain sizes (grain size) were as follows: 50/40, 100/80, 125/100, 200/160. Local inclusions of the metal phase in the grains were created in the form of arbitrarily oriented parallelepipeds, the volumetric content of which was set depending on the grain grade (AS4 – 7.5%, AS6 – 6%, AS15 – 2.2% and AS32 – 0.6%) [8, 9, 10]. When modeling protective coatings on a diamond grain, a shell with a thickness of 100 mass% was created.

The bond was created in the form of prismatic fragments with sizes from 250 × 250 × 125 μm to 1000 × 1000 × 500 μm, depending on the size and concentration of grains in the diamond-bearing layer. In the volume of the bond, seating surfaces for grains were randomly placed, the amount of which varied depending on the concentration of diamonds (25% – 200%), which was set as the percentage of the volume of the binder and the total volume of grains. To reproduce the natural structure of the wheel in the body of the bond, pores of arbitrary shape with sizes from 80 to 100 μm were created. The relative pore volume in the model was varied in accordance with the selected porosity values of 10, 20, and 30%.

The element of the “processed material” system was modeled in the form of prismatic fragments with sizes from 250 × 250 × 125 μm to 1000 × 1000 × 500 μm. Examples of the main three-dimensional models developed for the finite element analysis of the stress-strain state of microvolumes of the diamond-bearing layer during grinding are shown in Fig. 1.

Finite element analysis was performed using eight-node *SOLID* elements. The *ANSYS* program was used to select the type of finite elements from the package library for each component of the system, build a finite element mesh and selectively refine it. When creating a mesh for metal phases, *Hex Dominant* and *Tetrahedron* elements were used. Thickening of the mesh was carried out in the areas where abrasive grains were embedded in the bond and in the inclusion of the metal phase, as well as on the contact surfaces of the system elements. This approach made it possible to more accurately simulate the deformation of the model fragments, taking into account the remoteness of the zones of edge effects.

Fixing the model (setting zero or other necessary displacements) was carried out using the attributes of the geometric model (points, lines, surfaces) [5]. The model was loaded with a static uniaxial uniformly distributed load in the form of the applied pressure and temperature values (Fig. 1). The choice of the boundary loading parameters was carried out taking into account the temperature and force loads accompanying the sintering of the diamond-bearing layer. So, when simulating the conditions of hot pressing or free firing of the diamond-bearing layer of the wheels, the model was subjected to a uniform temperature load from 500 to 800°C, which corresponds to the conditions for the production of DAT using ceramic (550÷800°C) bonds [11, 12, 13, 14]. The force load was varied in the range of 30–50 MPa, corresponding to the pressing pressure in the manufacture of diamond wheels [15, 16]. The analysis of the influence of the loading parameters of the models was carried out in three versions: only taking into account the effect of pressure; only taking into account the heating temperature and with the simultaneous application of pressure and temperature.

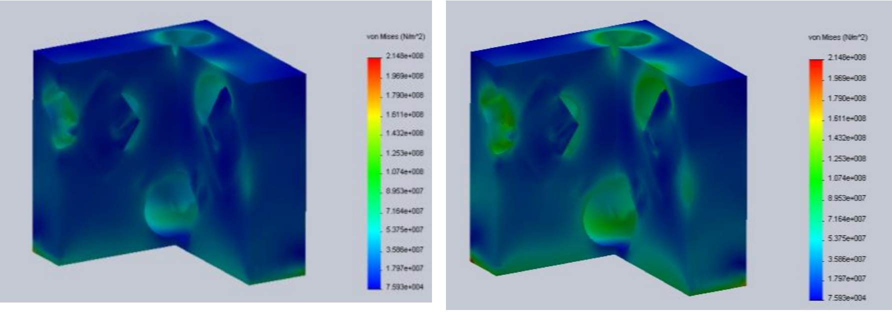
The calculation model included the following characteristics of the system elements: elastic modulus (E), bulk compression modulus (G), thermal coefficient of linear expansion (TCLE, α), Poisson's ratio (μ), yield stress (σ_0), thermal conductivity coefficient (λ). The setting of the properties of grains was carried out according to the reference data [17, 18], taking into account the information on the temperature dependences of the properties of synthetic diamond.

3. Results

The main difference between ceramic-bonded diamond wheels is the high sintering temperature of the diamond-bearing layer (700-800°C). In a number of cases (especially when using fine-grained diamond powders), this causes destruction and graphitization of grains [19–21].

Theoretical calculations made it possible to quantify the stresses in the elements of microlevel models of the "metal phase - diamond grain - bond - pore" system depending on the sintering conditions, as well as the concentration of diamonds, their size, composition and properties of the metal phase and the bond. In this case, we investigated the behavior of grains of grades AS2, AS4, characterized by an increased content of the metal phase and minimum strength properties.

Modeling the sintering process of a diamond-bearing layer on a ceramic bond made it possible to evaluate the role of temperature and force effects, both separately and during joint manifestations. In figures 2 and 3 are shown examples of stress distribution diagrams and the results of calculating the maximum equivalent stresses σ_{eq} arising in the system under conditions of power and temperature-power loads. Characteristics of the 3D model (Fig. 1, a): diamond grains AS6 125/100 (σ_{st} = 0.2 GPa); metal phase: 6% $Fe_{95}Si_5$; bond K1-01, porosity 15%.



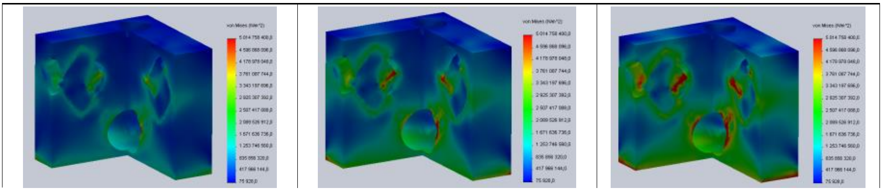
a) – σ_{eq}=3,11MPa

b) – σ_{eq}=3,82MPa

Figure 2 – Stress distribution in the "metal phase - diamond grain - bond - pore" system at power loads P=30 MPa (a) and P=50 MPa (b)

Calculations have shown that loading the specified system (Fig. 1, a) only by pressure in the range of values typical for the technology of sintering wheels on ceramic bonds insignificantly affects the level of arising stresses and does not lead to a violation of the integrity of diamond grains of these grades (Fig. 3, table). This fact made it possible to conclude that the pressure (in the range of 30 – 50 MPa) from the point of view of grain integrity is an insignificant factor and practically does not cause destructive stresses.

The stresses arising during the sintering of diamond wheels under the influence of temperature are distinguished by much higher values and a characteristic distribution pattern: their increase is especially observed in the places of inclusions of the metal phase in the grain along the contour of the sphere inscribed in the octahedron. With an increase in temperature, the stresses in the system under study increase, which is explained by a significant difference in the values of the TCLE of the metal phase and diamond, as well as the structural heterogeneity of the latter.



a) – T=400 ºC b) – T=600 ºC c) – T=800 ºC

Figure 3 – Distribution of stresses in the system "metal phase - diamond grain - bond - pore" at temperature and power loads

Table – Influence of temperature and power loads on equivalent stresses

Pressure	T= 400 ºC	T= 600 ºC	T= 800 ºC
P = 0 MPa	σ_{eq}=63,85 MPa	σ_{eq}=590,92 MPa	σ_{eq}=748,76 MPa
P =30MPa	σ_{eq}=64,06 MPa	σ_{eq}= 591,23 MPa	σ_{eq}=749,03 MPa
P =50MPa	σ_{eq}=64,74 MPa	σ_{eq}=591,86 MPa	σ_{eq}=749,81 MPa

This leads to a significant expansion of the inclusions of the metal phase with an increase in the sintering temperature and, as a consequence, to the appearance of internal stresses in the diamond grain, which can lead to the cracks formation in its volume and its subsequent destruction. By the nature of the distribution of the limiting values of the stress arising in the system at thermal power stresses, they are similar to the picture of thermal stresses, while their value at the same power load increases significantly. With an increase in the sintering temperature to 600°C and higher, stresses arise in the grain, localized in the region of inclusions of the metal phase, which can destroy the grain itself.

Each brand of diamond powder has characteristic performance properties, determined by the shape and morphology of grains, as well as microstructural features of their structure. It also represents the arithmetic mean of the compressive strength of all grain sizes of a given grade, expressed in newtons [22]. According to [23–24], with an increase in the strength of diamond powders, the number of metal phase inclusions in them decreases (for example, in diamonds of grades AS4, AS6, AS15, AS32, the content of the solvent alloy reaches 7.5; 6.0; 2.2 and 0, 6 wt%, respectively). The presence of inclusions of the metal phase reduces the thermal resistance of diamonds and the value of their breaking load.

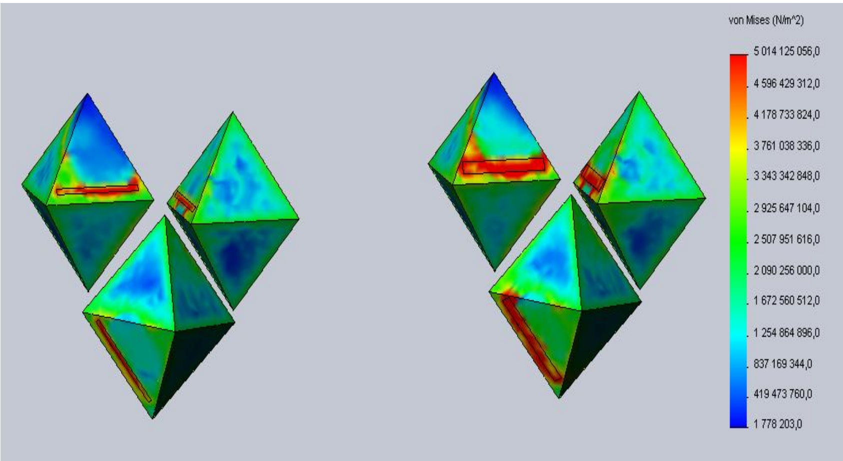
Within the framework of theoretical studies, we determined the influence of the quantitative and qualitative characteristics of the metal phase (depending on the grade of diamonds and the composition of the metal catalyst) on the level of stresses arising in the grains under loads corresponding to the sintering conditions of the ceramic matrix diamond-containing layer of the tool. Since the ultimate tensile strength of diamond is lower than that of compression, the calculated values of the maximum tensile stresses were taken as a fracture criterion, which were compared with their ultimate strengths for diamonds of various grades and grain sizes [25–28]. As shown in [29, 30], stresses exceeding the ultimate strength of diamond and located at the boundaries of the metal phase inclusions cause the development of internal cracks in the grain. However, this is not a sufficient condition for grain damage, the destruction of which begins if the breaking stresses propagate in a significant volume of the grain (more than 10%).

As the reaction of the model to loading, we considered the equivalent stress at the mesh nodes belonging to the elements of the system under study (grain and metal phase). Using the *ABAQUS* software, the limiting stress value in the studied area of the system was set, in accordance with which the gradation of the equivalent stress was built on the epure and scale. According to the calculation results, the grain volume (V_{cr}) was determined, in which the stresses exceeded the ultimate tensile strength of diamonds for a given grade and grain size. Fig. 4 shows examples of epure, obtained for the case of using diamonds AS6 [$\sigma_{st} = 0.2$GPa] and AS15 [$\sigma_{st} = 0.53$GPa] with the $Fe_{95}Si_5$ metal phase and its percentage in them 4% and 2.2%, respectively.

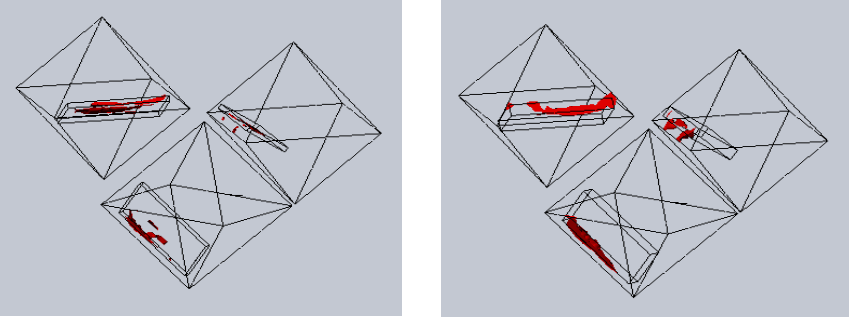
As can be seen from the data obtained, the maximum level of equivalent stresses recorded in the areas of the metal phase in the grain differs insignificantly for diamonds of different grades (the difference is ~ 4%). At the same time, the volumes of grains in which stresses exceeding the limiting level for diamonds of the indicated grades are noted differ significantly (for diamonds of the AS6 grade this indicator is 2.5 times higher).

To obtain more complete information on the influence of the qualitative characteristics of the metal phase on the integrity of diamond grains during sintering, cases with different compositions of the metal phase containing cobalt, nickel, and iron are considered. The results of model experiments on the effect of the composition of the metal phase (content 6%) on the value of σ_{eq} in the grain are shown in Fig. 5.

Since at this stage of research, the most interesting is the analysis of the influence of the metal phase on the stresses arising in the diamond grain during sintering, the image of the bond in this illustration is hidden. Analysis of the distribution epures of stresses arising during the thermal-force loading of the model shows that the maximum values of the equivalent stresses are fixed in the region of inclusions of the metal phase, whereas in the absence of the metal phase in the diamond grain, the maximum stresses are localized at the boundary of the contact between the diamond and the bond.



AS15, σ_{eq}= 722,37 MPa AS6, σ_{eq}= 780,23 MPa

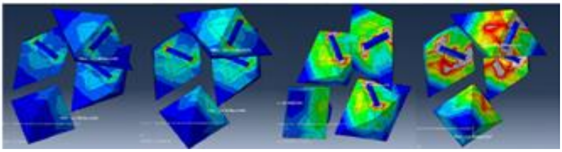


V_{cr}=4,73 % V_{cr}=9,56 %

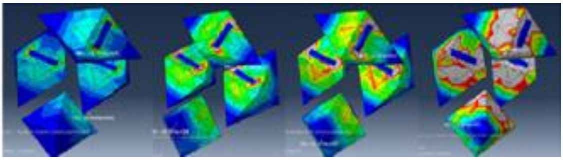
Figure 4 – Characteristics of the stress-strain state of the system "metal phase - diamond grain - bond - pore" during sintering of the K1–01 bond (sintering parameters P = 30 MPa; T = 700°C)

Stresses exceeding the ultimate strength of diamond grains are located along the boundary of inclusions of the metal phase, which suggests the appearance of an internal crack in the grain. At the same time, the stresses at the grain periphery are distributed in such a way that they will facilitate the separation of the protruding sections from the grain. This can cause rounding of the cutting edges of the diamond grains, which can adversely affect the cutting ability of the diamond wheel.

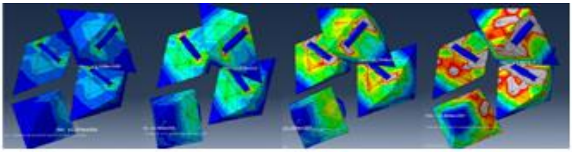
The calculation results indicate (Fig. 6) that, with an increase in temperature loads from 500 to 800°C (at a constant pressure of 30 MPa) in grains of grade AS6 125/100, an increase in maximum stresses from $\sigma_{600°C}$ = 703.22 MPa is observed up to $\sigma_{800°C}$ = 1721.5 MPa (for the metal phase of composition $Ni_{39.6}Mn_{59.6}(Cr_3C_2)_{0.8}$) and from $\sigma_{600°C}$ = 526.06 MPa to $\sigma_{800°C}$ = 999.65 MPa (for the metal phase of composition $Fe_{44}Co_{44}(Cr_3C_2)_{12}$).



a) – metal phase $Fe_{44}Co_{44}(Cr_3C_2)_{12}$, σ_{eq} = 612,55 MPa



b) – metal phase $Fe_{95}Si_5$, σ_{eq} = 725,16 MPa

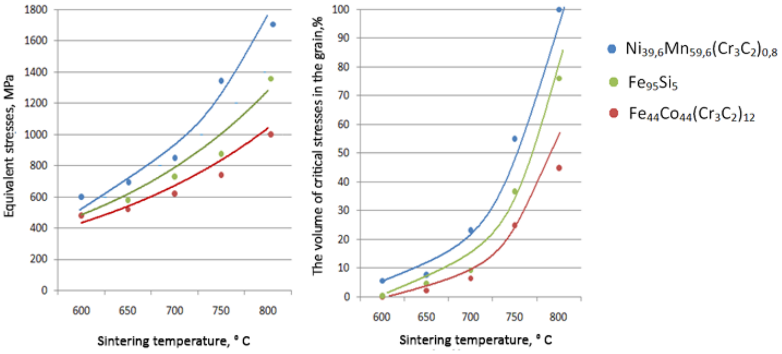


c) – metal phase $Ni_{39,6}Mn_{59,6}(Cr_3C_2)_{0,8}$, σ_{eq} = 835,63 MPa

Figure 5 – Epures of stress distribution in grain during sintering
(sintering parameters: K1-01 bond with 15% porosity; P = 30 MPa; T = 700°C)

The different level of the arising stresses is due to the significant difference (more than 2 times) in the TCLE of the indicated metal phases containing different amounts of cobalt, nickel and iron. At the sintering temperature of diamond wheels on a ceramic bond K1-01 (~ 750°C), stresses arise in the grains of AS6 125/100 powder that exceed the ultimate tensile strength of diamonds (0.2 GPa). It follows from this that when using diamonds of low strength grades (contaminated with metal inclusions), the sintering temperature should not exceed 550 ° C.

For diamond grains AS15 125/00 in the absence of nickel in the composition of the metal phase, the maximum sintering temperature can reach 650°C. Otherwise, the sintering temperature must be reduced to 600°C. Compliance with these conditions will ensure the integrity of the grains at the stage of manufacturing diamond wheels when using synthetic diamonds of low grades.



a) b)

Figure 6 – Temperature dependences of equivalent stresses (a) and volumes of critical stresses in a grain (b) for AS6 125/100 diamonds containing a metal phase of different composition

In the case of using synthetic diamonds, the choice of catalyst metals should be based on the observance of two conditions: low thermal conductivity and minimum TCLE while maintaining a high elastic modulus. This conclusion is explained by the fact that a decrease in thermal conductivity will lead to a slowdown in the heating of metal inclusions, and, as a consequence, a decrease in their thermal expansion, which, in turn, will contribute to a decrease in stresses in the system. An increase in the elastic modulus of the metal phase increases its tensile strength; however, the nature of the temperature dependence of the elastic modulus for various catalyst metals (as well as the features of the temperature dependences of thermal conductivity and TCLE) significantly reduce this effect.

Based on the foregoing, it is advisable to use iron-based solvent alloys as catalysts in the synthesis of diamonds, for example, $Fe_{44}Co_{44}(Cr_3C_2)_{12}$ or $Fe_{95}Si_5$, the first of which is characterized by minimal thermal conductivity and TCLE, and the second has an optimal combination of thermal conductivity and elastic modulus, which will be help to minimize the equivalent stresses in the diamond grain.

4. Summary

Adherence to the general recommendations for all diamond wheels regarding the design principles of DAT leads to grain damage already at the stage of tool manufacturing, which can be the reason for the low efficiency of diamond abrasive processing. An analysis of modern research aimed at increasing the efficiency of DAT manufacturing and the results of our own experiments indicates the efficiency of using an approach based on microlevel 3D modeling of the behavior of a diamond-bearing layer at the stage of tool manufacturing in the design of DAT on a ceramic bond. The studies carried out at this stage have led to the following conclusions:

The integrity of diamond grains at the stage of manufacturing DAT on ceramic bonds is mainly determined by the temperature factor. The force factor (pressure during workpiece molding) within the studied limits (up to 50 MPa) practically does not affect the stress distribution in the sintered diamond-bearing layer and does not cause the appearance of destructive stresses in the grain.

The role of the qualitative and quantitative characteristics of the metal phase present in synthetic diamonds in the process of their destruction during sintering of the diamond-bearing layer has been determined and their relationship with the technological parameters of the process has been revealed. It has been substantiated by calculation that the main reason for the premature destruction of grains during sintering of the diamond-bearing layer is the stresses in the grain, caused by a significant difference in the TCLE of diamond and metal phase (3.5÷8 times for different solvent alloys). With a decrease in the content of the metal phase, the thermal resistance of diamonds increases. When using diamonds of grades AS32 and higher, the sintering temperature of the diamond-bearing layer, at which the appearance of stresses destroying the grain is excluded, can be increased to the softening temperature of known ceramic bonds. When making DAT using cheaper diamonds of grades AS2 - AS15, the sintering temperature of the diamond layer should be reduced to 550÷650 ºC in order to avoid the destruction of grains. A comparative analysis of the effect of the properties of some solvent alloys on the level of stresses arising in the grain is carried out. The choice of the $Fe_{44}Co_{44}(Cr_3C_2)_{12}$ solvent-alloy is substantiated, which makes it possible to reduce the level of stresses arising in the grain during sintering of the diamond-bearing layer.

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ТЕОРЕТИЧНЕ ОБГРУНТУВАННЯ РАЦІОНАЛЬНИХ УМОВ ВИГОТОВЛЕННЯ АЛМАЗНИХ КРУГІВ НА КЕРАМІЧНИХ ЗВ'ЯЗКАХ

Анотація. *Аналізуються результати проведених теоретичних досліджень із застосуванням 3D моделювання методом кінцевих елементів, що дозволило визначити раціональні характеристики алмазних кругів на керамічних зв'язках. Вивчено вплив параметрів алмазоносного шару на зміну його напружено-деформованого стану в зоні спікання алмазного круга. Встановлено вплив технологічних параметрів процесу та характеристик алмазного круга на цілісність зерен при спіканні, на підставі чого надано практичні рекомендації щодо вибору алмазних композицій з раціональними властивостями. Аналіз сучасних досліджень, спрямованих на підвищення ефективності виготовлення ААІ та результатів власних експериментів, свідчить про ефективність використання при проектуванні ААІ на керамічних зв'язках підходу, заснованого на мікрорівневому 3D моделюванні поведінки алмазоносного шару на етапі виготовлення інструменту. Проведені на цьому етапі дослідження дозволили зробити висновки, що цілісність алмазних зерен на етапі виготовлення ААІ на керамічних зв'язках визначається переважно температурним фактором. Силовий фактор (тиск при формуванні заготівки) в досліджуваних межах (до 50 МПа) практично не впливає на розподіл напружень в алмазоносному шарі, що спікається, і не викликає появу руйнівних напружень у зерні. Визначено роль якісних та кількісних характеристик металофази, що присутня у синтетичних алмазах, у процесі їх руйнування при спіканні алмазоносного шару та виявлено їх взаємозв'язок з технологічними параметрами процесу. Розрахунковим шляхом обґрунтовано, що головною причиною передчасного руйнування зерен при спіканні алмазоносного шару є напруження в зерні, зумовлені суттєвою різницею КЛТР алмазу та металофази (у 3,5÷8 разів для різних сплавів-розчинників). Зі зменшенням вмісту металофази термостійкість алмазів підвищується. При використанні алмазів марок АС 32 і вище температура спікання алмазоносного шару, при якій виключена поява напружень, що руйнують зерно, може бути збільшена до температури розм'якшення відомих керамічних зв'язок. При виготовленні ААІ з використанням більш дешевих алмазів марок АС2 – АС15 температура спікання алмазоносного шару повинна бути знижена до 550÷650 °С, щоб уникнути руйнування зерен. Проведено порівняльний аналіз впливу властивостей деяких сплавів-розчинників на рівень напружень, що виникають у зерні. Обґрунтовано вибір сплаву-розчинника* $Fe_{44}Co_{44}(Cr_3C_2)_{12}$, *що дозволяє знизити рівень напруження, що виникає в зерні при спіканні алмазоносного шару.*

Ключові слова: *алмазний шліфувальний круг; керамічна зв'язка; алмазоносний шар; алмазне зерно; процес шліфування; силовий та температурний фактори; метод кінцевих елементів; 3D-модель; процес спікання алмазного круга; металева фаза; еквівалентне напруження.*