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ANALYSIS OF THE INFLUENCE OF TECHNOLOGICAL PARAMETERS ON THE PROPERTIES OF DIAMOND-BEARING COMPOSITES USING 3D MODELING

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Abstract. *This paper presents a methodology for 3D simulation of the thermo-forced deflected mode in the sintering zone of diamond composite materials (DCM) and the grinding area, considering them as a unified system: "material to be machined – grain – metallphase – bond." The approach includes experimental studies of the 3D topography of interacting surfaces using laser scanning. A simulated 3D model of the system "diamond crystallites – metallphase – grain – bond" enables analysis of its behavior under various sintering and machining conditions, wheel performance parameters, grain anisotropy, and the presence or absence of cutting fluid. This methodology supports the development of an expert system for designing efficient, resource-saving combined processes for precision machining of superhard composite materials, with full consideration of their anisotropy.*

Keywords: *Diamond composite materials (DCM); single point diamond tools; simulation; expert systems.*

1. Introduction

Currently, in world practice, the methods of three-dimensional modeling are most often used, which is due to the need to increase the adequacy and information sufficiency of models. The prerequisite for such a transition is the development of the finite element method (FEM), hardware and software [1]. A review of the relevant publications shows that there is currently no complex three-dimensional methodology for studying the processes of processing diamond-abrasive tools, but there is a real prospect of its development. The creation of such a methodology will significantly reduce the volume of experimental studies to determine the best design data of diamond-abrasive tools, optimal conditions for their production and application.

The unique, potentially high properties of DCMs can only be fully realized if

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their type, grain, and concentration are used rationally, which is optimal for the given bond and the specified material to be processed (MM). To increase the efficiency of diamond grinding, it is necessary to solve the problems of the optimal combination of physical and mechanical properties of diamond grains, their granularity and concentration depending on the physical and mechanical properties of MM. These issues should be explored throughout the DCM lifecycle, including design, manufacturing, and application processes. Realization of the proposed methodology by experiment is very labour-intensive and expensive process.

The main stages of finite element analysis: 1. synthesis of system functional; 2. partitions of system on finite elements and selection of coordinate functions; 3. constructions of stiffness matrixes and reduction of load to vector of nodal loads; 4. synthesis of canonical equations; 5. solutions of a system of canonical equations and definition of values of degree of freedoms of a system; 6. definitions of DM of system under consideration [2].

2. Simulation of DCM sintering process

Operating efficiency of tools from diamond-composite materials is stimulated by a series of reasons, including structural defects connected with destruction of a portion of grains during tool manufacturing process. It was demonstrated at the Bakul Institute of Superhard Materials of National Academy of Sciences of Ukraine under the direction of academician N.V. Novikov, that up to 90% of diamond grains fail at sintering of composite diamond-containing materials such as "twesal" [2]. A similarity of sintering processes of diamond-containing composite materials such as "twesal" type and diamond-bearing layer of diamond wheels on metallic and ceramic bonds, and also measurement of grain size of diamond dust extracted from a fragment of diamond-bearing layer of a non-operated wheel, is evidence of breaking of diamond grains during the wheel manufacturing process [3]. Bond composition, mark of diamond grain, its graininess and concentration in cake, and also technological features of DCM manufacture are the factors which essentially influence the grain integrity.

The task, solved in the process of 3D simulation of DM of sintering zone of DCM is the determination of optimal combination of strength properties of bond and diamond grains, their graininess and concentration, at which integrity retention of diamond grains is provided during the DCM sintering process.

At simulation of the sintering process, the fragment of diamond-bearing layer of the wheel was presented as a cube of bond dimensioned 300x300x300 μm , in midpoint of which a diamond grain as an ellipsoid dimensioned 120x100 μm was placed, that corresponds to 100 % concentration of diamond wheel. The metallic

phase in diamond grain was simulated as an interlayer of 5–10 μm in thickness and of various form and length. The schematic diagram and the FEM model of DCM sintering process are shown in Fig. 1.

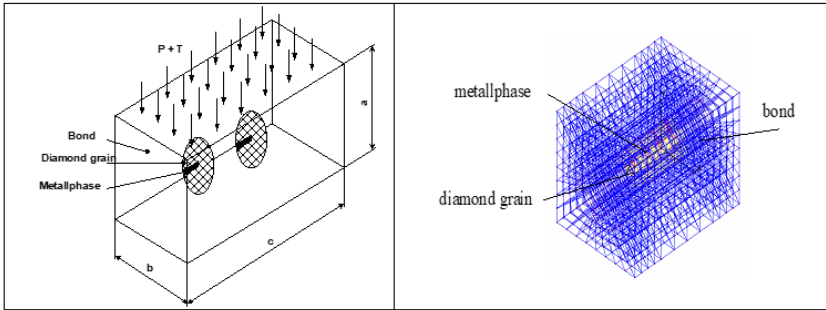


Fig. 1 (a) A schematic diagram and (b) the FEM model of "Bond - metallphase - grain" system

The calculations based on FEM in application package "Cosmos" and "Ansys" allow to obtain computerized quantitative assessment of principal and reduced stress, strain energy and density of strain energy in the elements to be sintered, depending on their sizes, physical-mechanical properties and conditions of sintering (temperature, pressure). The volumes of materials were considered as broken down, if reduced stress and/or density of strain energy in them exceeds the appropriate limiting values [2].

The sintering process of DCM of various concentrations on various metallic, ceramic and organic bonds with diamond grains of various strength from AC2 up to AC160T was modeled. The model was loaded by pressure and temperature conforming to an actual sintering process of DCM.

At the first stage the calculations were carried out for a fragment of diamond-bearing layer which includes a single diamond grain, surrounded by solid metal bond. Thus grain size, corresponding to the grain size of 50/40 up to 500/400, temperature and pressure of sintering, and also physical-mechanical properties of examined components of the cake were varied. At the second stage the fragment of diamond-bearing layer, which includes some diamond grains, integrated by means of bond, see Fig.1a, was considered. In this series the size ratio of the diamond grains and solid bond surrounding these grains was to varied that corresponded to various values of grain size and concentration (from 5 up to 200 %) of diamonds in the layer to be sintered. Grain and bond were considered as elastic solid bodies in the model.

Diamond grains were modeled as ellipsoids dimensioned from 50x30 up to 500x300 μm , depending on the grain size under consideration. Presence of metallic phase in diamond grains was modeled as interlayers oriented at random, the volumetric contents of which is 0,1–10 % depending on the marks of a grain [2,4]. The bond is considered as prismatic fragment dimensioned from 0,5x0,5x1,1 up to 3x3x6, depending on marks, size and grain concentration. The model is loaded by static monoaxial evenly distributed load by means of applied pressure and temperature. Theoretical research of sintering process of DCM on various bonds is carried out with the purpose to determine the conditions, under which the integrity of diamond grains in a material is ensured.

It is established that stresses exceeding the ultimate stress limit of diamond grains and placed along the metallphase interlayers results in the development in a grain. The stresses on the periphery of the grain being sintered are distributed in such a manner that can result in shearing grain submicroedges. As a result, the cutting edges are circularized, that can subsequently lead to the negative influence on cutting capacity of grains in diamond wheel. The outcomes of the 3D simulation of the DM of sintering zone of DCM are shown in Fig. 2.

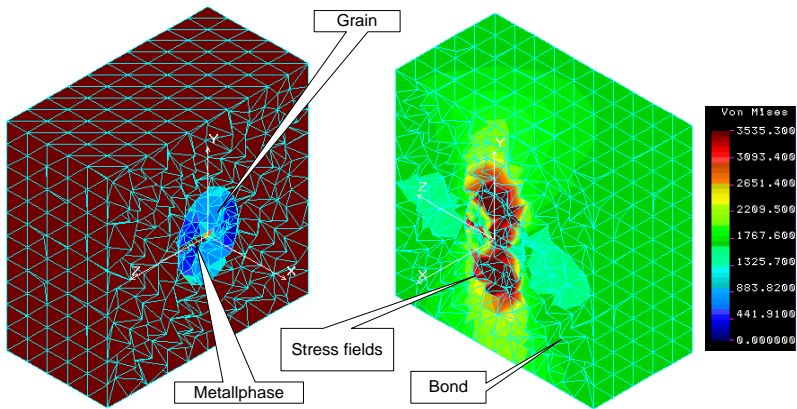


Fig. 2 (a) Section of 3D model "Grain – metallphase - bond" (b) and fields of reduced stress in the system at DCM sintering

By varying the combination of diamond grain strength and grain concentration in the wheel for various bonds, one can determine such combinations, at which retention of diamond grain integrity was provided. It is established, that not all of the commercial wheels with usable combination of brand of diamond grains and brand

of metal and ceramic bonds can be manufactured with standard concentration of diamond grains without failure of their integrity. So, for example, at sintering of wheel on bond M6-14 with diamond grains of brand AC6, the grain concentration in the wheel should not exceed 7 %, otherwise grains will be fracture as early as wheel sintering. It is shown, that for guaranteed retention of diamond grain integrity practically in all commercial wheels, their concentration should be much less than the applied one. Such tendency coordinates perform well with possibility and necessity of lowering the diamond grain concentration for the wheel up to the level of 10–15 % at grinding of superhard materials [2,5].

Optimum combinations of properties of bond and diamond grains with maximum allowable concentration of them in DCM, which ensure retention of their integrity during the manufacturing process, are established due to the carried out calculations. The optimum ratio of strength of bond, diamond grains and their concentration in diamond-abrasive tool, obtained at the first stage, are only limiting parameters and should be determine more exactly for the process of diamond grinding depending on the strength properties of material to be machined [6].

3. Simulation of process of diamond-abrasive machining of DCM

The reduced modulus of elasticity of the eutectic, see Table 1, and its thermal-expansion coefficient differ essentially, about 4 times, i.e. the diamond $\alpha_1=3.7 \times 10^{-6}$ and the metallphase $\alpha_1=3.7 \times 10^{-6}$, from the corresponding properties of diamond, at heating (up to the temperature of the inclusion), this eutectic extends, creating, therefore, an internal pressure which may result to uncontrolled macrodestruction of the diamond grains, to the occurrence of grids of microcracks and the migration of the metallphase on a surface. The level of the pressure on a plane can be estimated from the ratio [2,7],

$$q = \bar{K}_2(\alpha_2 - \alpha_1)(T_1 - T_0) \quad (1)$$

where K_2, α_2 , – are the reduced compression modulus and thermal-expansion coefficient of the metallphase nickel-manganese, respectively, being in an equal proportion $K_2=150.77$ GPa, $\alpha_2=14.1 \times 10^{-6}$; T_1 is the temperature at which there is an output of the metallphase drops on the surface of the diamond accompanied with formation of cracks. According to Ref. [8], this temperature corresponds to 973 K.

The thermal-expansion coefficient of diamond is in the range up to 750 K, $\alpha_1=3.7 \times 10^{-6}$ K. The value of the thermal pressure in a cavity with metallphase according to equations (1) will be equal to $q=144.5$ MPa. However, the given analytical

sequence does not take into account the influence of the force factor on the stress level in diamond grains and is solved in conditions of 2D simulation.

In our case three possible variants of orientation of a grain relative to polycrystal in 3D modeling are considered: the contact of a grain to a polycrystal on the tip of a grain (point contact); an edge (linear contact) and a face (flat contact – imitation of wear platform on a grain). Various combinations of these variants were considered when studying the combined action of the grains.

The loading of the models was associated by: specifying (α) the displacement U_y of the top plane of a bond (kinematic influence – imitation of cross-feed S_{tran}) and (b) the imposition of the pressure of the top plane of a bond (force impact of normal and tangential components of cutting force – imitation of the elastic grinding pattern). The advantage of such an approach is the possibility to study the 3D DM, both at the elastic grinding pattern and on the rigid one, allowing for the comparison of results of these investigations.

The characteristic model parameters may be listed: the displacement of the average node of the top surface of a bond (value of cross-feed), U_y^{CB} ; the displacement of the top node of a grain (embedding of grains in a bond), U_y^3 ; the displacement of node of contact of a grain with a polycrystal (elastic embedding of grains in work-piece material), U_y^{PK} ; the reduced stresses (according to Mises criterion) in the top node of the contact of a grain with a bond, σ_{CB} ; the reduced stresses in node of contact of a grain with a polycrystal, σ_{PK} .

At temperature as early as 700–1000°C thermal stresses, which valued as commensurable ones with the bending strength and the tensile strength of diamond grains, can occur in microzones of several crystallites. Given technique allows to estimate the "contribution" of the force and temperature factors to the DM of system.

From the analysis of the results presented in Table 1, it may be concluded that the higher the temperature of grinding the more essential is the role of thermostress.

Table 1 – Dependence of intercrystallite thermal and thermo-forced stresses on temperature

Value, MPa	Temperature, °C							
	500	600	700	800	900	1000	1100	1200
Maximal	24,04	28,85	33,65	38,46	43,27	48,08	52,88	57,69
	28,2	29,56	34,12	40,17	44,27	51,11	53,34	60,45

Minimal	9,55	11,46	13,37	15,28	17,19	19,10	21,01	22,92
	10,11	13,34	15,21	17,54	19,98	21,56	23,57	25,12

Numerator – reduced thermostresses without taking into account force factor.

Denominator – the reduced thermo-forced stresses.

Note that, at temperatures of the order 700–800°C tensile stresses, exceeding the corresponding ultimate stress limit of diamond, occur in diamond matrix due to the anisotropy of thermal expansion of diamond and the difference in coefficients of thermal expansion of the diamond and the metals-catalysts.

If these stresses can initiate intercrystallite destructions in the areas adjacent to non-oriented metal inclusions, then intracrystallite brittle fracture will be initiated in the field of diamond, covering the oriented metal inclusions. Note, also, that, due to these stresses the sites of flat compression of diamond appear where a crystal is subjected by local destruction, if the stresses reach critical values and a grid of microcracks appear on the surface of diamond grains. Thus, thermally activated processes can intensity microdestruction (self-sharpening) of diamond grains at grinding.

Finite element modeling using the FEM package "COSMOS" was carried out for the validation of the proposed hypothesis. The FE model and results of computation of the deflected mode of system "bond – grain – metallphase – workpiece material" are presented in Fig. 3 (a) and (b), respectively.

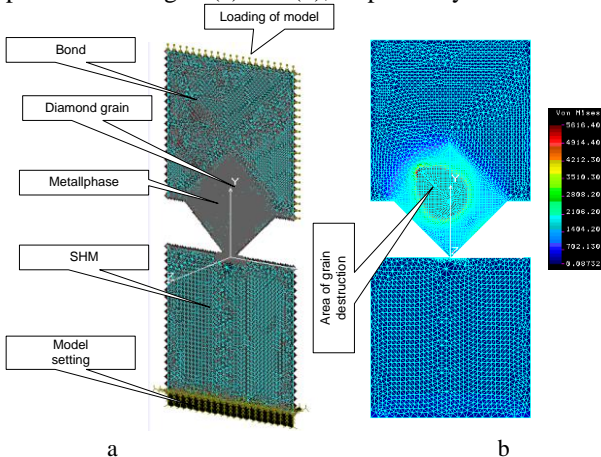


Fig. 3 (a) FEM model of system "bond – grain – metallphase – workpiece material" and (b) results of computation of deflected

Since in the real process of diamond grinding the considered technical system is loaded not only by force impacts, but also temperature ones, it is necessary to determine the values of principal and reduced stresses and also the values of deformations, strain energy and density of strain energy in each element of the system "workpiece material – grain – bond" caused by force, temperature and total (thermo-forced) loading. For this purpose the values of the contact temperature and the temperature of lubricant-cooling agent input in the grinding area were specified, too, in addition to the value of normal pressure or cross-feed.

The temperature in the grinding area predetermines the process of self-sharpening of diamond grains in many respects. The FE simulation results reveal that the value of the thermo-forced stresses in diamond grains and, consequently, the probability of their macrodestruction are reduced considerably, due to the presence of lubricant-cooling agent in the grinding area, see Fig. 3.

Subsequently, affects the temperature factor essentially the efficiency of the process of self-sharpening of diamond wheels. Both force (reduced stress exceeds the tensile strength of the workpiece material) and power (strain energy in an element exceeds the limiting value) criteria of destruction were used to determine the amount of damage workpiece material and diamond grains. The package allows to calculating the values of strain energy and density of strain energy in each element of the system. Thus, it is possible to determine the amount of elements with supercritical values of reduced stress or supercritical strain energy. In order to obtain the most reliable computing results of amount of destroyed workpiece materials and diamond grains, the FEM grid of elements of the system "workpiece material – grain – metallphase – bond" was thickened when approaching the contact area (to damage zone) up to the sizes of element volume not exceeding $10^{-4}\mu\text{m}^3$, i.e. much less than the really damage amount obtained once by a diamond grain during grinding.

Using the 3D simulation of DM of system "workpiece material – grain – metallphase – bond" and the specially developed program for computing the amount of destroyed and dropped out (loss) grains and the amount of damage workpiece materials, it is possible to theoretically estimate the major parameters of the self-sharpening process at diamond grinding of superhard materials, namely the specific consumption and the specific wear of diamond grains. Numerical results regarding the amount of destroyed grains, V_d and dropped out from a bondgrains, V_{loss} , depending on the working height of grains and the critical size of their embedding, h_{cr} .

The specific wear is defined as

$$\alpha_w = \frac{V_d}{V_{\text{FEM}}}$$

and the specific consumption

$$q = \frac{V_G + V_{GS}}{V_{SHM}}$$

where V_{SHM} is the volume of the damaged workpiece material. Calculation, of these values, depending on the physical-mechanical properties of the workpiece material, grains, modulus of elasticity of bond, cross-feed, grinding speed and normal pressure.

It is possible to re-distribute the energy input in grinding area between the system elements owing to control of the contact parameters (value of relative actual area) and dynamics of interaction of the elements of the system "workpiece material – grain – bond" (speed, feed, normal pressure, introduction of energy of ultrasonic vibrations in the area).

The technique of 3D simulation of DM of system "workpiece material – grain – metallphase – bond" allows to determine the conditions under which the maximal part of energy input in grinding area will be directed to microdestruction of the workpiece material, minimizing microdestruction – self-sharpening of diamond grains, eliminating their loss from a bond.

Investigations of the effect of the wheel working surface (WWS) topography parameters on 3D DM of the system have shown, that if the diamond grain even insignificantly projects from a bond ($h_p \neq 0$), i.e. the bond does not contact to workpiece material, so the stress occurs in the diamond grain, which is sufficient for the process of self-sharpening (microdestruction). If the grain is completely embedded in a bond ($h_p = 0$), it is not self-sharpened due to the volumetric "crimping" by a bond and the absence of free boundaries. In this connection productive process of workpiece material grinding should be put into practice only under condition of realization of interaction of the first type in system "WWS – workpiece material" i.e. without a contact of bond to workpiece material.

The time history of changing parameters of the topography of wheel working surface (WWS) during self-sharpening was experimentally verified employing the technique of laser scanning and electronic data processing the changes of 3D parameters of the WWS, sub-microrelief of separate diamond grains, were investigated in order to estimate the relative reference area of the surface topography, t_{ps} [2,8]. Thus, it is possible to determine the value t_{ps} both at macrolevel (WWS), and at microlevel, i.e. a microrelief of separate diamond grains. The value of sub-microrelief of separate diamond grains is the important parameter at definition of the actual contact area in the system "DCM-grain", which is difficult to obtain by other ways, since the sub-microrelief of diamond grains determines the efficiency of self-sharpening of diamond grains.

The experimental result reveal that, when grinding superhard materials by wheels on an organic bond under theoretically determined conditions of wheel self-

sharpening parameters, its relief remains practically constant for a long time, see Fig. 4.

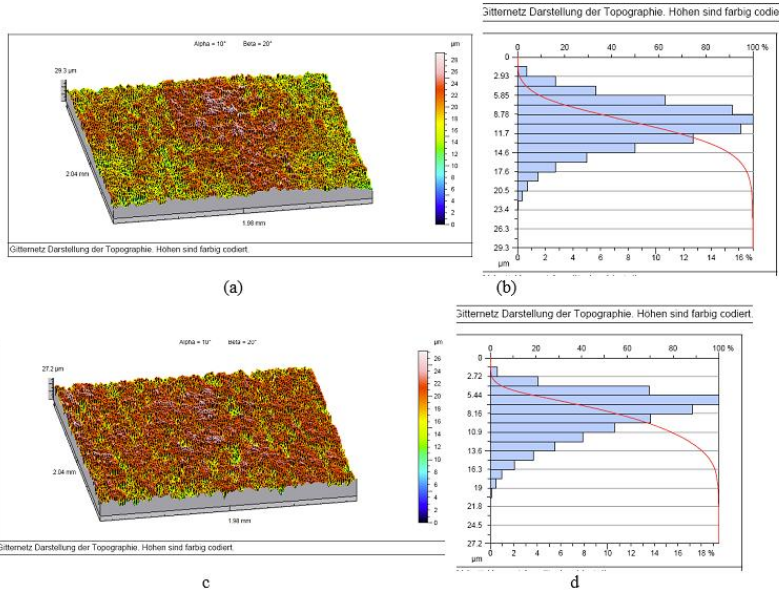


Fig. 4 (a, c) 3D topography of WWS and (b,d) relative distribution function of relative reference area of WWS; a,b – after 30 s of grinding c,d – after 5 min of grinding

4. Conclusions:

Summarizing the main features of the numerical and experimental results reported pertaining to 3D simulation of diamond composite materials, the following conclusions may be drawn:

1. The methodology of 3D simulation of processes of manufacturing, machining and exploiting of DCM is developed and found as a result of use of CIT.
2. The methodology of 3D simulation of thermo-forced deflected mode of the sintering zone of DCM and grinding area as the unified system "material to be machined - grain - metallphase - bond", which includes experimental study of 3D topography of interacting surfaces by laser scanning is proposed. Simulated 3D model of the deflected mode of the system "diamond crystallites – metallphase - grain - bond", which allows to analyze its behaviour depending on modes and conditions of

sintering and machining, wheel performances taking into account anisotropy of grains, and availability or absence of cutting fluid is developed on this basis.

3. For the first time the rational compositions of type, graininess and concentration of diamond grains with marks of metallic, ceramic and organic bond, which ensure the integrity of grains in DCM are defined on the basis of 3D simulation of deflected mode of DCM, originating in the sintering process of its components. It is established that, decrease of diamonds concentration in the wheel up to 5–40 % allows to ensure minimum defectiveness of wheel grains at optimum selection of their marks, graininess and bond type. Recommendations on optimum diamond-metallic and ceramic compositions for the manufacture of grinding wheels are provides.

4. Based on the worked out methodology it is possible to create the expert system for development of effective technological resource-saving combined processes of precision machining of superhard composite materials, taking into account their anisotropy. The proposed methodology allows to elaborating high-effective technological processes of preliminary and precision machining of various DCM, that permits an increase of productivity about 1,5–2 times, a reduce of the expenditure of expensive diamond grains on 30–40 % and increasing reliability of single-point tool from superhard materials by 20–40 %, that is very important in CAM. The developed expert system for prediction and optimization of processes of manufacturing and exploiting of diamond-abrasive tool will essentially promote tool production.

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АНАЛІЗ ВПЛИВУ ТЕХНОЛОГІЧНИХ ПАРАМЕТРІВ НА ВЛАСТИВОСТІ АЛМАЗОВМІСНИХ КОМПОЗИТІВ ЗА ДОПОМОГОЮ 3D-МОДЕЛЮВАННЯ

Анотація. У цій роботі запропоновано методологію 3D-моделювання термовимушеного деформованого режиму зони спікання АКМ та зони шліфування як єдиної системи "матеріал, що оброблюється - зерно - металофаза - пов'язок", яка включає експериментальне дослідження 3D-топографії взаємодіючих поверхонь за допомогою лазерного сканування. На цій основі розроблено імітаційну 3D-модель деформованого режиму системи "алмазні кристали - металофаза - зерно - пов'язок", яка дозволяє аналізувати її поведінку залежно від режимів та умов спікання та обробки, характеристик круга з урахуванням анізотропії зерен, а також наявності або відсутності рідини для різання. Вперше раціональні склади типу, зернистості та концентрації алмазних зерен із ознаками металевого, керамічного та органічного пов'язку, які забезпечують цілісність зерен у АКМ, визначені на основі 3D-моделювання відхиленого режиму АКМ, що виникає в процесі запікання його компонентів. Встановлено, що зниження концентрації алмазних зерен у крузі до 5-40 % дозволяє забезпечити мінімальну дефектність зерен круга при оптимальному виборі їхніх позначок, зернистості та типу пов'язку. Надаються рекомендації щодо оптимального алмазно-металевого та керамічного складу для виготовлення шліфувальних кругів. На основі розробленої методології можливо створити експертну систему для розробки ефективних технологічних ресурсозберігаючих комбінованих процесів прецизійної обробки надтвердих композитних матеріалів з урахуванням їх анізотропії. Запропонована методологія дозволяє розробити високоефективні технологічні процеси попередньої та точної обробки різних АКМ, що дозволяє збільшити продуктивність приблизно в 1,5-2 рази, зменшити витрати на дорогі алмазні зерна на 30-40 % і підвищити надійність однокочового інструмента з надтвердих матеріалів на 20-40 %, що є дуже важливим у АКМ. Розроблена експертна система для прогнозування та оптимізації процесів виробництва та експлуатації алмазно-абразивного інструменту фактично сприятиме виробництву інструментів.

Ключові слова: алмазні композитні матеріали (АКМ); однокочові алмазні інструменти; моделювання; експертні системи.