Prevention of manufacturing defects of diamond composite materials by simulating the process at the micro level

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The efficiency of diamond abrasive tools is degraded for several reasons, one of the most significant being the destruction of most of the grains during the process of the manufacture of the tools. This paper presents a methodology for complex research into the destructive stresses in diamond composite tools during manufacture. Analysis of the stress-strain state of the diamond layer was carried out using the finite-element method in applications such as Ansys, CosmosWorks and LS-Dyna.

Keywords: coverings, destructive stress, finite element method, sintering

1. Introduction

International research on the simulation of processes has established an excellent tool for assessing and optimizing cutting and grinding.[1] Knowledge about the tool–workpiece interaction in grinding—depending on the chosen parameter combination—makes selective adaptation of the process strategy possible with regard to maximum workpiece quality or minimum machining time and high economic efficiency of the process.

The creation of a basic methodological foundation and a system of 3D-CAD simulations of diamond composite materials (DCM) at the stages of their manufacture and operation will

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Received 24 November 2012

allow the efficiency of their processing and application to be substantially raised. Modern trends in science-intensive products are characterized by extensive use of applied mathematics, frequently connected with the creation of computer aids.[2]

The performance of any abrasive product depends on the abrasive properties and grinding conditions (forces, chip thickness etc.) to which it is subjected. From the standpoint of testing conditions, the force per piece of grain and chip thickness are critical in determining which of the common wear/fracture mechanisms of a given abrasive becomes active.[3] The link between these two areas is important for predicting the most efficient grinding règimes to use with a given abrasive; one abrasive that is an excellent performer in high force per grit applications may be less than optimal in low force per grit applications.

Several methods are routinely used for the characterization of abrasive grains. These include the measurement of friability, hardness, toughness, and various abrasion and single-grit wear tests. None of these tests are application tests; hence, correlation to the actual behaviour of the grit in an abrasive product must be sought.[4]

Diamond compositions that make up the working layer of grinding wheels are a combination of heterogeneous components with a clear interface: diamond powder particles are evenly distributed and securely attached to a solid matrix (binder). It is known that the processing of superhard polycrystalline materials is accompanied by high values of the specific consumption of diamond grains.[5–7, 9] In production staged with the use of high temperatures there are about 10% of defect-free diamond grains in the finished diamond wheel.[5, 6]

The factors influencing the integrity of the diamond grains are, primarily, the technological features of making the tools as well as the structure of the sintered composition. Our research focuses on the study of the combination of the components of the diamond wheel (binder, diamond grain with metallic inclusions, and all possible types of coatings of diamond grains).

The binder has the greatest impact on the integrity of diamond wheel in general; particularly in the fixing reliability of the diamond grains in the wheel. The type of diamond grain determines its strength and is associated primarily with the content of metal inclusions, the shape of the grains, and internal and surface defects.

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The formation of microcracks in synthetic diamond during its manufacture may be due to the action of one or several mechanisms of thermal destruction.[5,6,8] This is due to the significant difference in the coefficients of thermal expansion (CTE) of diamond and metal inclusions. Heating to the sintering temperature leads to expansion of the metallic inclusions remaining in the diamond after the synthesis. It creates an internal pressure in the cavity of the grains that causes destruction of the structure. Thus, it is necessary to create a system for forecasting the future characteristics of diamond wheels before manufacture begins.

2. Principles underlying the work

Analysis of the stress–strain state of the diamond layer was carried out using the finite-element method with the help of applications such as Ansys, CosmosWorks, and LS-Dyna.

As a rule, finite-element models are divided into macro- and micromodels. In the majority of the macromodels, the grinding wheel is presented as a combination of heat source and given pressure. Now, micromodels are proving the most promising;[1] however, when developing them information about the behaviour of all elements under load conditions is needed.[4]

Through analysing current approaches in the study of grinding it is possible to identify the following directions:

- Fundamental analytical approaches, which aim to develop predictive models that are deductively derived from basic physical interrelationships. Based on knowledge of the process and the selection of appropriate physical quantities, physical models can be developed using mathematical formulations. For this, an understanding of the abrasive grain–workpiece interaction is essential.
- Kinematic models. Typical for these approaches is the three-dimensional view of the grinding process based on geometric interpenetration of the workpiece surface and the grinding wheel surface.
- Finite-element models. For the successful application of grinding processes knowledge and control of physical process data (e.g., forces, temperature and grinding energy) is essential.[15,16]

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Even if kinematic models can be used as a basis for further calculation of forces and grinding energy, the modelling of physical process data is certainly a domain of finite-element analysis (FEA).

- Molecular dynamic models. Molecular dynamics (MD) simulation using atomistic models appear to be attractive in order to gain a deeper understanding of microscopic material behaviour and structure and have been applied to study various material properties and phenomena covering gases, liquids and solids.[4, 17] The rather universal material representation in MD, considering microstructure, lattice constants and orientation, chemical elements and atomic interactions, allows the modeller to go beyond ideal, single crystalline structures or homogeneous material properties and to describe polycrystals, defect structures, premachined or otherwise constrained workpiece models and rough surfaces.[17]

Modelling of grinding requires knowledge of the grinding wheel topography to estimate the active grit concentration and distribution and how these may interact with the workpiece surface. Individual and combined interactions between the grit and the workpiece surface will influence the chip formation process and, hence, the grinding forces on and surface finish of the workpiece. More recently optical techniques[10] and replication procedures[11] have been used successfully. Models are required that consider the combined action of the grains, which are stochastically distributed on the grinding wheel surface. Tönshoff et al. have reviewed topography models and consider them in terms of the static or dynamic (i.e., involving those grains that actually take part in chip formation) grit concentrations.[12]

During the simulation of the stress–strain state of the elements of the sintering zone, the model is initialized with a static, uniformly distributed load in the form of pressure and temperature. This corresponds to the process parameters of sintering. The calculations were performed for a fragment of the diamond layer, which includes a single (several) diamond grain(s) surrounded by an array of binder. The model also simulated the effect of various types of coatings.

The work was based on the fundamental principles of the theory of cutting of materials: heat conduction theory and the mechanics of failure. Planning of the model experiments and processing of their results were performed on the basis of the theory of multifactorial experiments. This work is part of a comprehensive research project on the behaviour of diamond tools with high speed and self-sharpening processing. We assert that it is very important to consider the production and use of diamond tools in one system. This system provides for the exchange of data at each stage of the calculations and the ability to make adjustments in consequence.

3. Results and discussion

Our study dealt with the effect of binder type in grinding wheels, the type of metal phase, and the qualitative and quantitative composition of the diamond grains in the 3D system "workpiece–grain–metal phase–binder". In addition, the influences of thickness, composition, and geometric shape of the grains were determined. Diamond grains were simulated in octahedral form (dimension 140 micrometres); metallic inclusions were in the shape of plates, taking 5 to 10% of the volume of a grain.

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The technology of manufacturing diamond–metal composite tools by powder metallurgy makes significant changes to the properties of the final tool compared to the initial properties of the components used in its manufacture.[5–7] A few hypotheses for reducing the effect of destructive stress on the diamond grain have been verified by computational methods. Our first calculations were devoted to the simplest option, reducing the concentration of diamond grains in producing the tool. Concentration in this case is a weighted diamond content per unit of volume of diamond layer. With the concentration of 50% the weight of diamonds in the diamond layer will be 2.2 carat/cm^3, 75% 3.3 carat/cm^3 and 200% 8.8 carat/cm^3. Figure 1 shows diagrams of stress distribution in the investigated composite diamond layer.

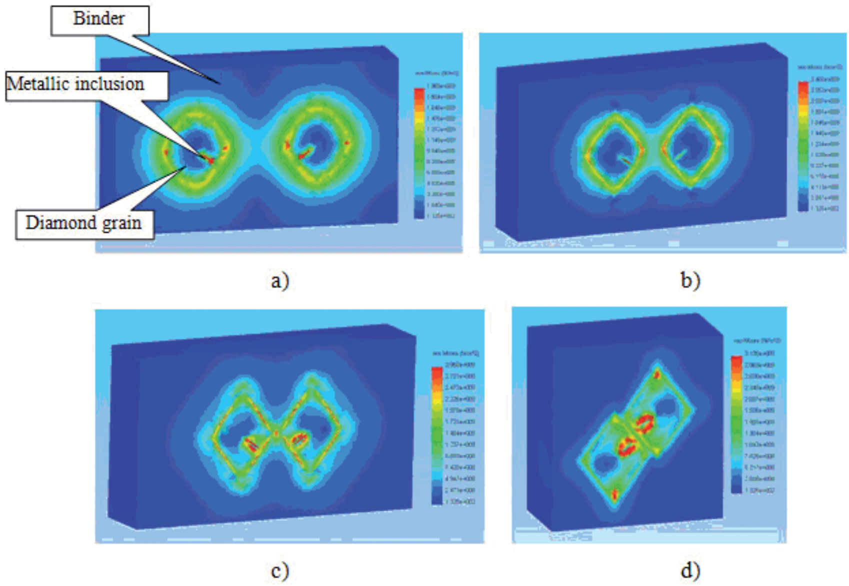

Figure 1. Stress distribution in the investigated composite diamond tool (σ_{max} = 3.32 GPa, metallic binder, sintering temperature 600 °C. a) probable location of grains with 50% concentration; b) probable location of grains with 75% concentration; c) probable location of grains with 150% concentration; d) probable location of grains with 200% concentration.

The high stress values in the system can be increased by compression of the diamond layer during its sintering due to increased concentration of the diamond grains. The higher the number of inelastic diamond grains in the composite the lower the ability to compress it, which means more stress is caused by the same pressure on the system. Each type of diamond grain and binder has its own recommended concentrations. Moreover, with high concentration values the importance of the orientation of the diamond grains with respect to each other increases.

As already mentioned, there is a significant difference between the coefficients of thermal expansion of diamond and of their metal inclusions. There was thus a need for research into the influence of the quantitative and qualitative composition of the metallic inclusions of the diamond grains on the stress–strain state during sintering, and to determine the optimal combination of metallic inclusions with the material of the binder. Figure 2 shows the simulation of the manufacturing process of diamond composite material in the case of 5 and 10% metallic inclusions in each diamond grain.

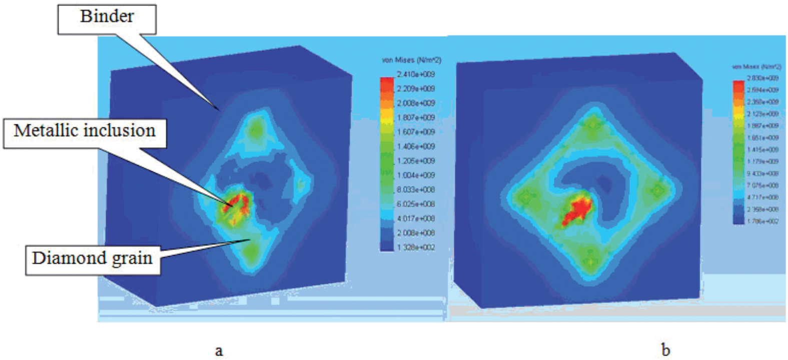

Figure 2. Influence of diamond grain properties and process conditions of sintering on the integrity of the diamond tool. a, 5% (by volume) metallic inclusions; b, 10% metallic inclusions; $\sigma_{max} = 2.42$ GPa.

For all types of considered diamond grains the greatest stress values correspond to zones near the metallic inclusions. Obviously, this is due to the significant difference in the reduced modulus of elasticity and coefficient of thermal expansion (CTE), which, under the influence of the sintering temperature, leads to expansion of the metallic inclusions by 15–20%. Analysing the results of the calculations, we can conclude that the optimum combination of metallic inclusions and binder occurs when the metallic inclusions have a low CTE and a low modulus of elasticity, and the binder in turn is sufficiently strong.

Because synthetic diamond has anisotropic properties, a series of experiments was conducted to confirm the adequacy of the previously obtained result. The existing literature gives the results of multiple tests to identify the properties of diamond in different orientations.[5,6] We will take into account the option in which the modulus of elasticity exposed at one of three shear planes ({110} / {111} / {101}) was respectively 900/750/700 MPa (Figure 3).

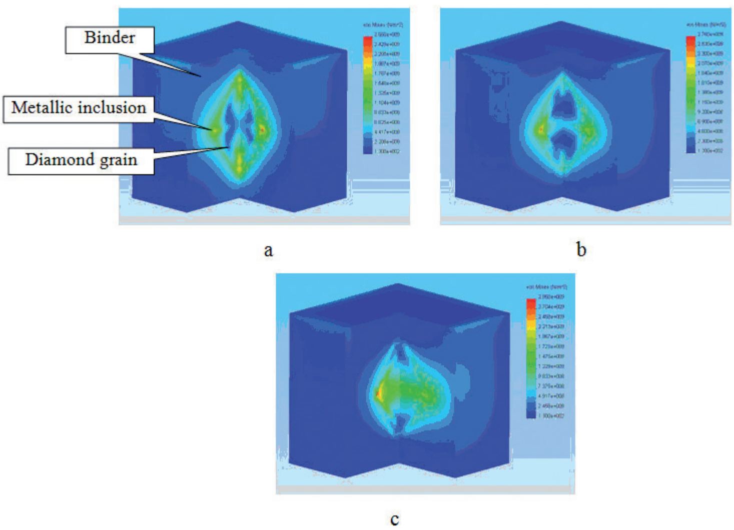

Figure 3. Stress distribution in the 3D model "grain–metallic inclusion–binder" taking the anisotropy of diamond into account. Orientation of the frontal plane as the plane of the crystal: a, {110}; b, {111}; c, {101}. $\sigma_{max} = 2.61$ GPa.

Analysing the results of equivalent stress, it may be concluded that the pattern of the stress–strain state of the diamond layer is different for different orientations of the diamond grain. However, calculations showed that the tension changes by only 10%, so the results of the previous calculations without the anisotropy can be considered adequate.

Another way to improve the characteristics of the diamond tool is to coat the diamond grains. In order to examine this statement, computational experiments to study the stress–strain state of the sintered diamond composite material have been conducted. On the basis of these simulations, multifactorial dependencies were obtained and a mathematical description of the sintering process of the diamond composite layer was obtained. A wide range of factors and series of experiments were included in a huge number of calculations. This was done in order to encompass the full range of materials used in the manufacture of diamond wheels.

Figure 4 shows an example of the calculation of stress–strain state (worst case) in the 3D model with a ceramic binder, nickel inclusions in the diamond grains and a sodium borosilicate glass covering (coating).

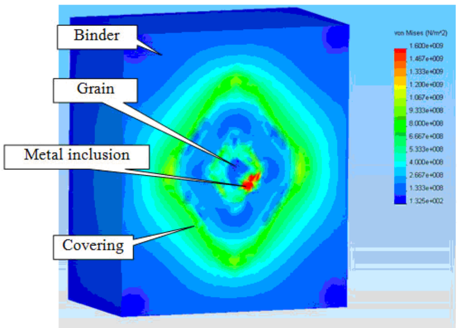

Figure 4. Example of calculation of the stress field using sodium borosilicate glass covering and ceramic binder. $\sigma_{max} = 1.63$ GPa.

The base model, with different coatings (thickness of 15 micrometres), was loaded at temperatures from 100 to 800 °C. Stresses in the investigated system are shown in Figure 5. By analysing the values of the equivalent stress it can be concluded that the use of a sodium borosilicate glass coating increases the value of breaking stress in the grains by about 40%, compared with coatings having inclusions of copper or molybdenum.

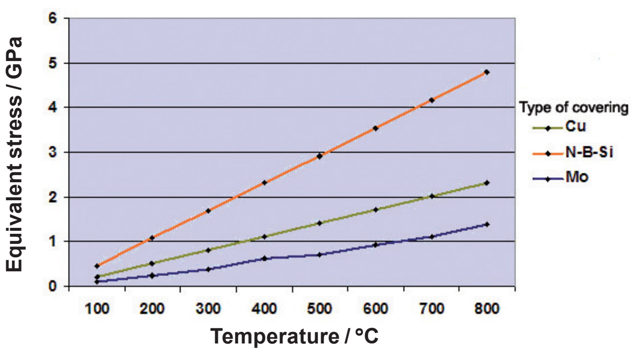

Figure 5. Dynamics of stress increase in the system "grain–coating–metallic inclusion–binder" with a coating thickness of 15 micrometres.

For the mathematical description of the process and to achieve a reduction in the number of experiments, we used the theory of multivariate experiment planning. The mathematical model used to describe the process has the form giving stress as:

$$Y = b_0 + \sum b_i X_i + \sum b_{i,j} X_i X_j + \sum b_{ii} X_i^2 + \ldots \tag{1}$$

The following mathematical model was used to describe the process of sintering:

$$\begin{aligned} Y = {} & 31.09 - 0.39X_1 - 0.17X_2 - 2.29X_3 + 3.60X_4 + 0.85X_1X_2 + 0.85X_1X_3 + 0.85X_1X_4 + \\ & 0.61X_2X_3 + 1.60X_2X_4 + 0.38X_3X_4 - 12.89X_1^2 - 8.60X_2^2 + 14.50X_3^2 - 10.03X_4^2 . \end{aligned} \tag{2}$$

The chosen factors were: the sintering temperature (X_4 from 400 to 800 °C); the coefficient of thermal expansion of metallic inclusions in the grains (X_1 from 1×10^{-6} to 1.7×10^{-5} 1/K); the elastic modulus of the binder (X_2 from 1.9×10^{11} to 6.9×10^{11} N/m^2); the elastic modulus of the coating (X_3 from 1.1×10^{11} to 9×10^{11} N/m^2). Figure 6 shows an example of the stress dependence of the coefficient of thermal expansion of metallic inclusions on the sintering temperature while using different coverings. *We have thereby established a combination of coating and binder that significantly reduces the damaging effects of temperature on the diamond grains during the sintering process.*

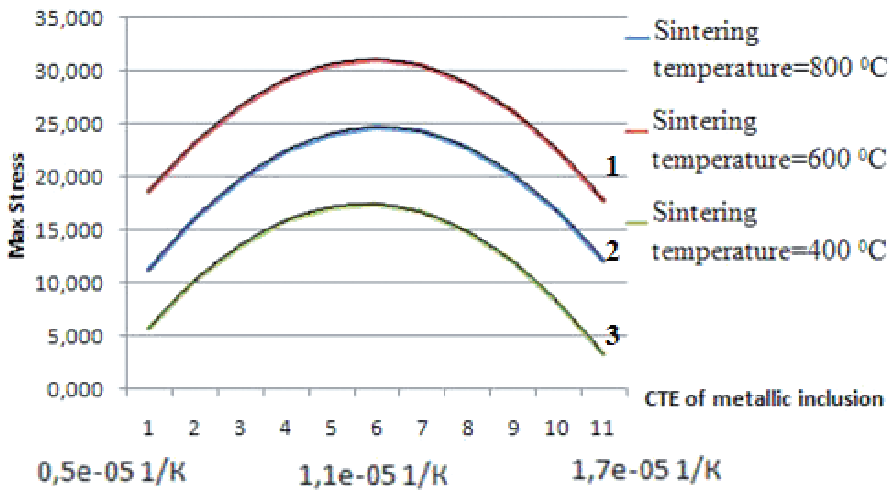

Figure 6. Dependence of stress on the coefficient of thermal expansion of metallic inclusions, for different sintering temperatures using different coverings: 1, $y = -0.515x2 + 6.110x + 12.99$; 2, $y = -0.515 \times 2 + 6.279x + 5.549$; 3, $y = -0.515 \times 2 + 5.940x + 0.375$.

As mentioned earlier, the link between processes of production and operation of diamond tools also must be considered. This is due to the extreme temperature loads. Dynamic calculations were based on the finite-element method using the Johnson–Holmquist failure criterion for ceramic and other brittle materials.[13]

Although experimental testing is always necessary, there is considerable motivation for the development and validation of numerical models in this area. With respect to ballistic impacts on ceramics, the response of the ceramic is dependent on the size of the ballistic piece, its velocity, construction and material, the material supporting the ceramic (backing) and, of course, the mechanical properties of the ceramic.[13] It will be appreciated that to understand these dependencies through experimental testing, given the considerable degree of scatter in this type of data, can be very costly and time-consuming.

While several constitutive models exist to describe the response of ceramics to various types of loading, the Johnson–Holmquist (JH-2) model[14] has been found to provide good results while capturing the essential components of ceramic response to ballistic impacts.[13, 14] It should be noted that any constitutive equation embodies assumptions, some of which are tied to the scale of the model. For example, the initiation of failure in ceramic materials is, to a great extent, linked to the presence of microscopic defects.[13, 14] Thus, a representative constitutive model must embody this effect to some degree. The key to any model is achieving the correct balance between accurate representations of the physical phenomenon while maintaining some degree of computational efficiency. The JH-2 model achieves this through representation of the initiation and propagation of failure via a damage variable.

The strength of the material is determined by the equation[13]

$$\sigma^* = \sigma_i^* - D(\sigma_i - \sigma_f) \qquad (3)$$

where σ^* is the current normalized strength, σ_i is here the intact material's strength, D the material damage (total) and σ_f the fractured material's strength.

Simulation modelling has established that in excess of a speed of 120 m/s, the diamond abrasive grains become sharp. The reason for this phenomenon is, in our opinion, the destruction of the blunted grains upon impact with the workpiece. When operating at high speeds the binder becomes so rigid that the grains cannot be dampened by shock and collapse, leading to the formation of brittle sharp edges. Figure 7 shows results of calculations of the specific consumption of diamond grains during processing. The result is the possibility of a theoretical prediction of the grinding performance of different materials, as well as of judging the quality of the surface layer of the residual stresses and deformations in the workpiece.

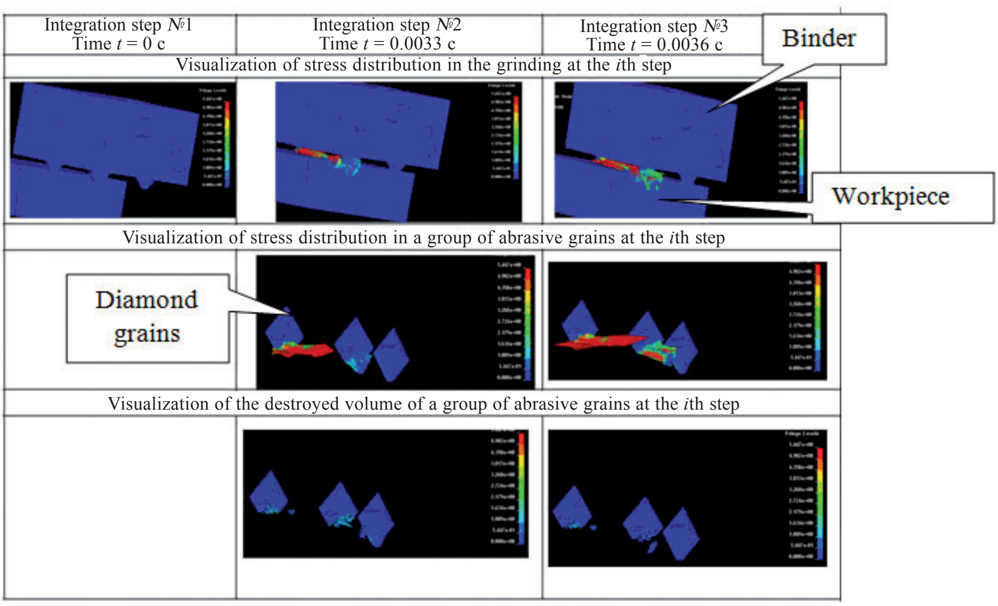

Figure 7. Theoretical estimation of damage in working grain (see text).

4. Conclusion

Using these techniques we have been able to establish the mutual influences of all major components of the diamond composite material and the sintering process on themselves. Interesting results for the choice of coating for the diamond grains, minimizing the destructive temperature factor, were obtained: the cheaper diamond grains with a high value of metallic inclusions can still be used. It has been demonstrated that reducing the concentration of diamond grains in the wheel reduces the effect of the pressures during sintering. A high concentration of grains requires a special orientation of the grains in the wheel. This improves performance because of the greater number of grains taking part in the actual processing.