Simulation of the effect of sintering on the integrity of diamond grains in grinding wheels

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This paper focuses on theoretical studies of the process of manufacturing diamond abrasive tools and of diamond grinding through 3D modelling of the stress–strain state of the components of the diamond layer of the grinding wheel. Modelling of the sintering process of diamond grinding wheels with metal-based binders is used in order to determine the conditions needed to maintain the integrity of the diamond grains in the diamond layer.

Keywords: binder, destructive stress, diamond grains, finite element method, metal inclusion, sintering

1. Introduction

Machining is the most prevalent manufacturing operation in terms of volume and expenditure. Machined components are used in almost every type of manufactured product. It has been estimated that machining expenditure contributes to approximately 5% of GDP in developed countries.[1, 2] Machining presents challenging and exciting intellectual problems that have fascinated researchers and practitioners for decades.

In modern engineering, problems of increasing the durability, reliability and efficiency of cutting tools are among the most important. Many of the final operations now use diamond grinding wheels. However, existing methods of manufacturing diamond tools have serious

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[1] E. Brinksmeier, J.C. Aurich and E. Govekar. Advances in modeling and simulation of grinding processes. *Annals of the CIRP* **55** (2006) 667–696.

[2] A.G. Mamalis, A.I. Grabchenko, V.A. Fedorovich, J. Kundrak and E.A. Babenko. Ways of simulation-based improvement in the performance of diamond-abrasive tools. *Journal of Machining and Forming Technologies* **4** (2012) 1–11.

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limitations associated with the application of a diamond layer and with the creation of the tool body.[1] The main disadvantages of the existing methods include: the possibility of diamond graphitization; low strength[1–4]; low adhesion of the diamond and binder; high power consumption; and a time-consuming process to produce the tool.

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. Today, improvement in the technologies for the synthesis of superhard materials related to the creation of stronger and heat- and wear-resistant materials,[3–5] as well as the application of new technologies for the production of the tool, partially solve this problem of deficient integrity. Our research focuses on the study of the combination of the components of the diamond wheel (binder, diamond grains with metallic inclusions and all possible types of coatings of the diamond grains) in order to achieve superior integrity.

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

The presence of large amounts of metal inclusions in the crystal leads to a reduction of strength and, especially, its thermal resistance. The sintering temperature of the diamond layer for tools that work under the most adverse conditions is 1000–1220 °C. Such sintering temperatures decrease the strength of the original diamond and reduce its efficiency.[1, 5] The formation of microcracks in the synthetic diamond during its manufacture may be due to the action of one or several mechanisms of thermal destruction. Destruction is due to a significant difference in the coefficients of thermal expansion (CTE) of the diamond and the metal inclusions. Heating to the sintering temperature leads to expansion of the metallic inclusions remaining in the diamond after synthesis; it creates an internal pressure in the cavity of the grains that causes destruction of the structure. Consequently, the initial cracking temperature in the crystals will depend on the thermal expansion coefficient of metal inclusions. The initial temperature of cracking will also depend on the amount and the nature of the inclusions and their location.

The solution to these problems cannot be seen in isolation from the processing conditions (processed material, cutting conditions and tool geometry), which largely determine the possibility and ways of destruction of diamond tools, especially those for high-speed grinding. While practising high-speed grinding, the important factor is the safety of the tool (its ability to withstand the significant shearing force), as well as changing the nature of the destruction of the diamond. At higher speeds (over 120 m/s), the formation of submicro cutting edges provides improved accuracy and a significant diminution of cutting forces during machining. Ensuring the formation of sharp edges should be a condition for the integrity of the diamond grains in the composite after sintering of the wheel.

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3 A.G. Mamalis, A.I. Grabchenko, V.A. Fedorovich and J. Kundrak. Simulation of effects of metal phase in a diamond grain and bonding type on temperature in diamond grinding. *International Journal of Advanced Manufacturing Technology* **58** (2012) 195–200.

4 N.V. Novikov, I.M. Androsov and A.L. Maistrenko. Technique of definition of strength and crack resistance of polycrystalline superhard materials. *Superhard Materials* **2** (1988) 33–37.

5 N.V. Novikov, A.L. Maistrenko and V.N. Kulakowski. *Breaking Strength of Superhard Composite Materials*. Kiev: Naukova Dumka (1993).

Using simulation we consider the connexion between the production and application of diamond tools. This allows the creation of a system to predict the behaviour of the tool and the quality of the machine part produced after the diamond grinding process.

2. Numerical simulation of the sintering process

Three-dimentional (3D) modelling of the fragment of the diamond layer was carried out using SolidWorks and models were imported to Abaqus Unified FEA to analyse the stress–strain state of the diamond layer. The modelling was based on the fundamental principles of the theory of the cutting of materials, heat conduction theory and the mechanics of failure. Planning of the model experiments and the processing of their results were undertaken on the basis of the theory of multifactorial experiments.

The basic procedure in the simulation of the sintering process was to select a fragment of the diamond layer in the form of a cube with a number of diamond grains, bounded on all sides,[2, 4, 6] which is an acceptable approximation of the diamond wheel in general (Figure 1).

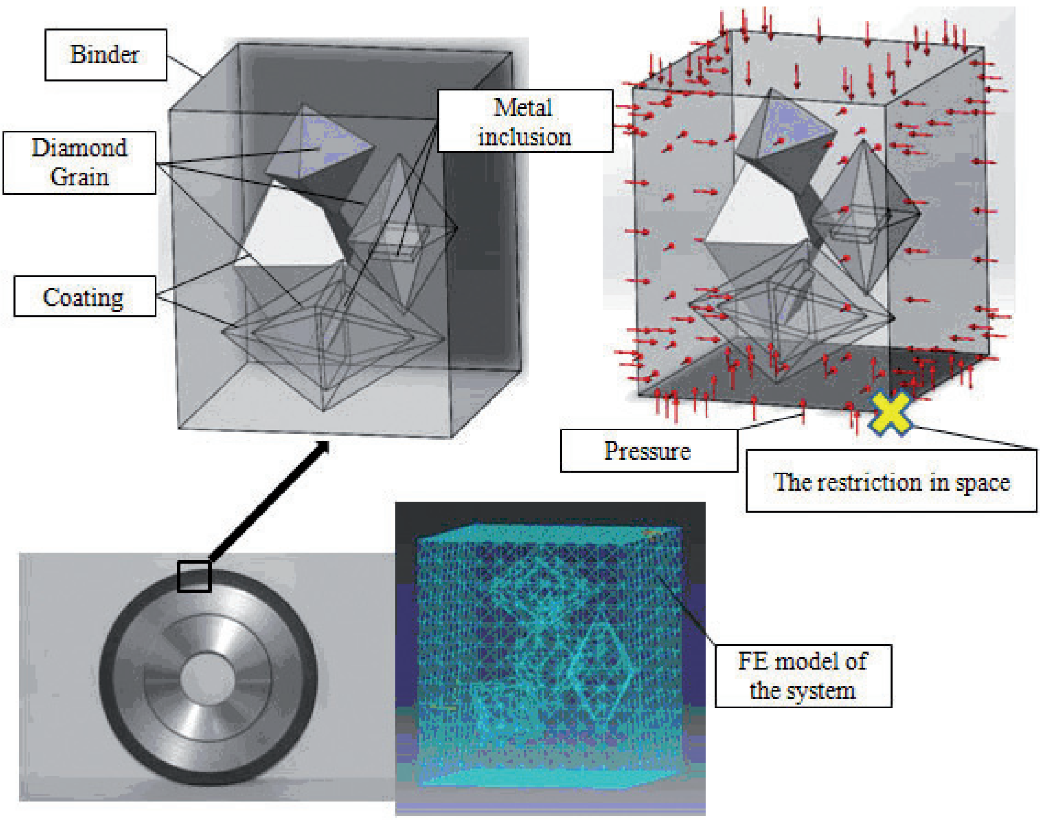

Figure 1. Concept of modelling of the sintering process of diamond wheels.

[6] N.V. Kozakova, E.V.Ostroverkh and G.L. Khavin. Method of calculating the temperature of brittle fracture of the “diamond crystal-metal inclusion”. *Cutting Tool and Process Systems* **59** (2001) 124–128.

Depending on the granularity considered, the grain sizes ranged from 50 × 30 × 30 to 500 × 300 × 300 micrometres, and the grains were modelled as octahedra, which represent the best convenient approximation to their real shape.[4, 8, 9] The presence of metal inclusions in the diamond grains was simulated with randomly oriented plates, whose volumes ranged from 5% to 20%, with one or two metal inclusions located on the periphery of the grain. The binder is represented as a cubic fragment with a size of 0.5 × 0.5 × 0.5 to 3 × 3 × 3 mm, depending on the size and concentration of the grains. We are interested in the stress–strain field distribution close to the diamond grains. Therefore, if the binder fragment considered will be not large enough, then the result of the calculation will be influenced by the imposed boundary conditions. During the simulation, the fragment of the diamond layer must be fixed in space. Applied loads cause the stresses at the place where the boundary conditions are applied. This causes uncertainty in modelling the process. Coatings on the diamond grains are presented in the form of a solid shell that repeats the shape of the grain. In calculations, the coating thickness varied from 15 to 50 μm.

During 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. The model takes into account heating from room temperature to the maximum sintering temperature and cooling back to room temperature. This corresponds to the process parameters of sintering.

The most important component for the stable operation of a grinding wheel in high-speed mode is the binder. The binders used in grinding wheels have several major functions: to hold the abrasive grains during processing; to wear at a desired rate relative to the wear rate of the diamond grains; and to resist centrifugal forces, especially at high processing speed.

This paper discusses the problem of the use of metal binders for diamond wheels in the range of processing speeds from 100 to 200 m/s. The technology of production of diamond wheels allows a variety of metals for these binders to be used. Therefore, there is a large range of types of binders for study. Also, diamond wheels with metal binders are common in the Ukraine, so there is a high demand for improvement of this tool. The same metal binder may cover a wide range of processing speeds, as defined by König et al.[10]

At the same time, the use of metal as the main component of the binder is the worst case from the viewpoint of maintaining the integrity of the diamond grains in the composite, since the sintering temperature go to 0.7–0.8 of the melting point of the metal, typically 500–830 °C.[4, 7, 9] Such conditions have a significant influence on the metal inclusions in synthetic diamond, promoting its cracking. However, our methodology can be used to predict diamond destruction with other types of binder.

The main input factors are the coefficient of thermal expansion (CTE) of the metal inclusion, the strength properties of the binder, the coating properties and the sintering temperature.

[7] M.J. Jackson and N. Barlow. Computer aided design of high-performance grinding tools. *Proceedings of the Institution of Mechanical Engineers (London), Part B: Journal of Engineering Manufacture* **215** (2001) 583–588.

[8] B. Brenner. *Industrial Diamond Tool and Method of Producing Same*. US Patent 2,411,867 (1946).

[9] N.V. Novikov. *Superhard Materials. Generation and Application* (monograph in 6 volumes). Kiev: National Academy of Sciences (2003–2007).

[10] W. König, F. Klocke and D. Stuff. High speed grinding with CBN wheels—boundary conditions, applications and prospects of a Future Oriented Technology. *1st French & German Conf. on High Speed Machining*, Metz, June 1997, pp. 207–218.

The levels of the factors for binder, metal inclusion and coating have been used for steel alloys, nickel alloys and copper alloys. This selection allows the exploration of a wide range of the most suitable materials with a single 3D model.

Since the sintering temperature of the metal binders almost reaches the melting point of the metal, it is appropriate to take into account the plastic properties of the components of the system (Figure 2).

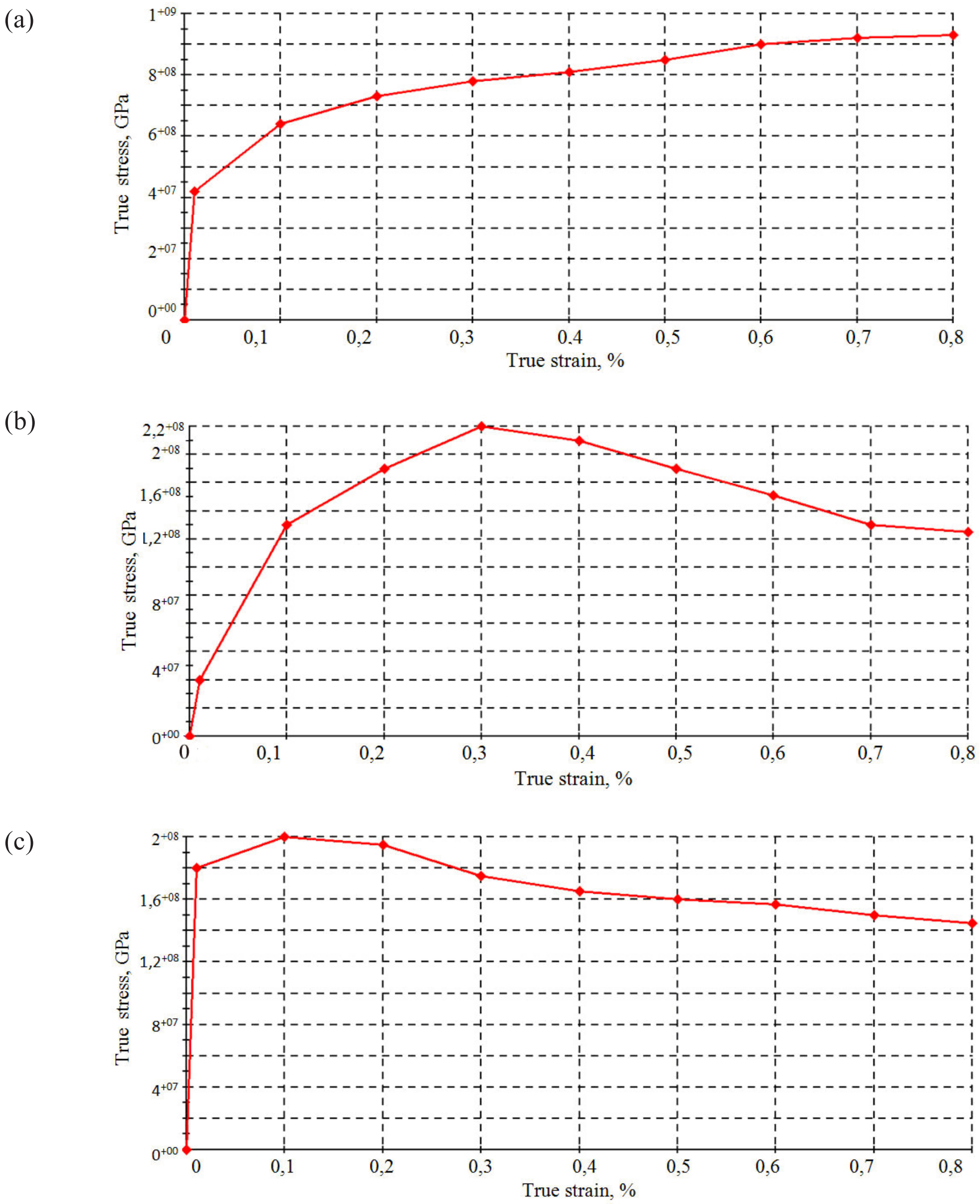

Figure 2. Plastic behaviour of the materials in the system studied: (a), steel alloy; (b), copper alloy; (c),

As the interest in this study is the distribution of stresses in the diamond grains at high temperatures, significant attention has been paid to the implementation of thermophysical properties of the diamond in the model, which improved agreement between simulation results and the model experiments. These calculations, including the thermophysical properties of materials and the plastic behaviour of the system, showed a difference of 15–20% compared with other modelling research in this area.[11–13, 9] The temperature dependence of the vibration properties of diamond were obtained using the quasiharmonic approximation (QHA) from Ivanova and Mavrin[14] and from Guo using molecular dynamics.[15] Figure 3 shows the temperature dependence of the coefficient of linear thermal expansion of diamond. The temperature dependences of the moduli of elasticity of the materials in the studied system are presented in Figure 4.

Important in this case is the selection of the destruction criterion, as it will greatly affect the magnitude of errors in the implementation of the model experiments. Today, based on the aggregation of a large amount of experimental data, specially designed studies and comparative analysis of the criteria for material types and stress–strain state, the most promising is the Pisarenko–Lebedev criterion: strain weakening the material, while the term $(1 \sim x)$ characterizes tensile stresses, which are responsible for the formation of microcracks at the fracture surface. At $x = 0$ (ideal brittle material) it takes the form corresponding to the criterion of maximum normal stress; at $x = 1$ (perfect plastic material) the criterion is converted into the energy equation of the theory of von Mises–Genki. The parameter x is determined by the result of two experiments carried out at different stress–strain states, such as tension–compression, tension–pure shear and so on.

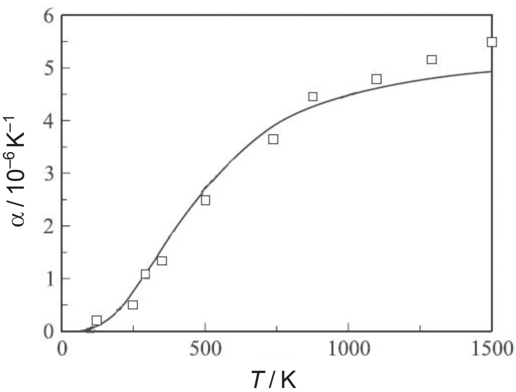

Figure 3. Temperature dependence of the coefficient of linear thermal expansion of diamond. Continuous line, quasiharmonic approximation;[14] squares, molecular dynamics.[15]

[11] J. Webster and M. Tricard. Innovations in abrasive products for precision grinding. *Annals of the CIRP* **53** (2004) 563–584.
[12] N.V Kozakova, N.F. Nakonechnyj and V.A. Fedorovich. 3D modeling to determine the optimal characteristics of diamond wheels. *High Technologies Engineering* **1** (2004) 81–86.
[13] H.K. Tönshoff, J. Peters, T. Inasaki and T. Paul. Modelling and simulation of grinding processes. *Annals of the CIRP* **41**/2 (1992) 677–688.
[14] T.A. Ivanova and B.N. Mavrin. Temperature dependence of thermal expansion and the frequency shift of the optical phonons in diamond from first principles. *Solid State Physics* **55** (2013) 143–146.
[15] J. Guo, B. Wen, R. Melnik, S. Yao and T. Li. Molecular dynamics study on diamond nanowires mechanical properties: strain rate, temperature and size dependent effects. *Diamond & Related Materials* **20** (2011) 551–555.

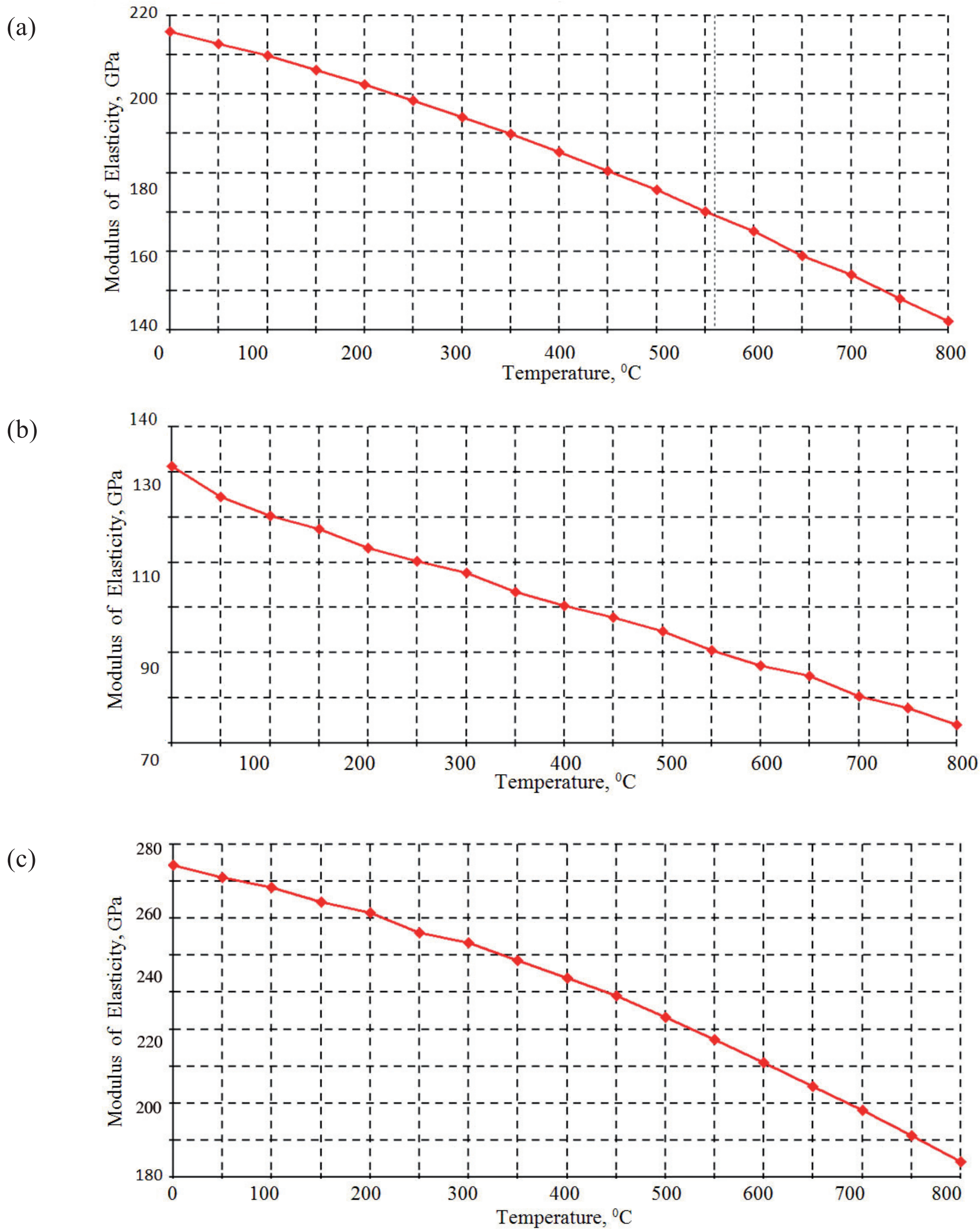

Figure 4. Temperature dependence of the modulus of elasticity: (a), steel alloy; (b), copper alloy; (c), nickel alloy.

The criterion can be applied to estimate the strength of structurally inhomogeneous materials (graphite, cast iron, brittle thermosetting plastics etc.). Thus, the parameters for calculating the strength and load capacity must be added to the compressive characteristics of the material or the parameter *x*.

According to the results of compression tests:[5, 16]

$$\sigma_k = \frac{P}{d\,t}, \qquad (1)$$

where σ_k is the average strength over the section in the specimen under diametrical compression and incorporates diameter d, height t and destructive force P. For the transition from σ_k to σ_p the expression:

$$\sigma_p = B\,\sigma_k, \qquad (2)$$

is used, where B is a coefficient depending on the choice of destruction criterion and σ_p is the ultimate strength of the material. Taking the Pisarenko–Lebedev criterion into account and equation (2) leads to the dependence:

$$\sigma_p = \frac{0.41\sigma_k\,\sigma_c}{\sigma_c - 1.89\sigma_k}, \qquad (3)$$

where σ_c is the ultimate strength under uniaxial compression.

Figure 5 shows the distribution of stresses in the system under the worst and best possible combinations of components of the composite. The lowest stress observed is with the combination of nickel-based binder (elastic modulus = 2.44×10^{11} N/m^2), iron-based inclusion (CTE = 1.32×10^{-6} K^{-1}, and coatings with properties similar to those of copper alloys (elastic modulus = 1.02×10^{11} N/m^2). Stresses which exceed the strength limits of the diamond are located on the borders of inclusions and cause the development of internal cracks in the grain, which confirms the results.[12, 8, 17, 13]

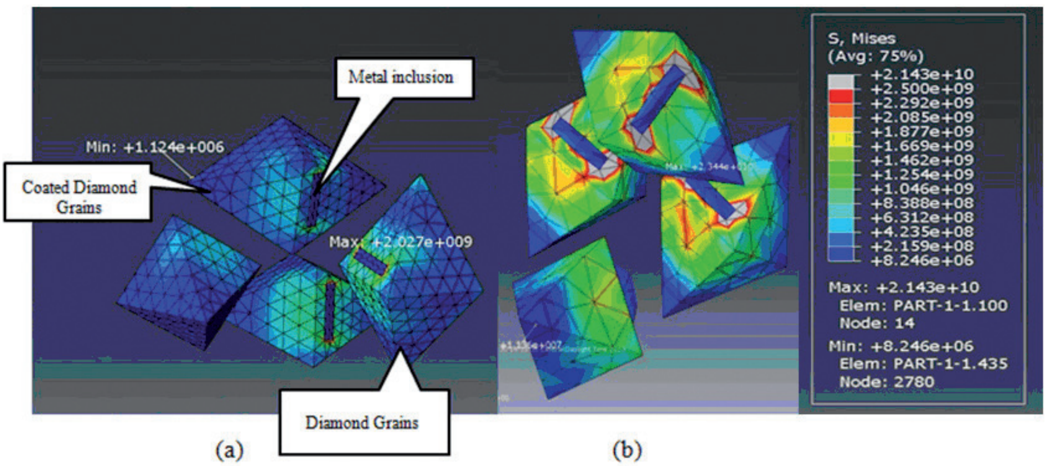

Figure 5. Distribution of stresses around the inclusions in the diamond grains: (a), maximum stress (2 GPa); (b), maximum tensile stress exceeds the strength of the diamond (8.2 GPa).

[16] L. Devin. Determination of tensile strength of polycrystalline superhard materials. *Superhard Materials* **2** (1988) 24–28.

[17] R.-L Hecker, I.-M Ramoneda and S-Y. Liang. Analysis of wheel topography and grit force for grinding process modeling. *Journal of Manufacturing Processes* **5** (2003) 13–23.

It is established that an increase in the binder strength causes the growth of stresses.[12, 8, 18, 17, 6] The explanation of this is that the increased stress in the binder enhance the effect on stress in the grain. However, previous studies did not take into account the plastic behaviour of the binder material and the temperature dependence of the physical and mechanical properties, which leads to significant adjustments to these conclusions (Figure 6).

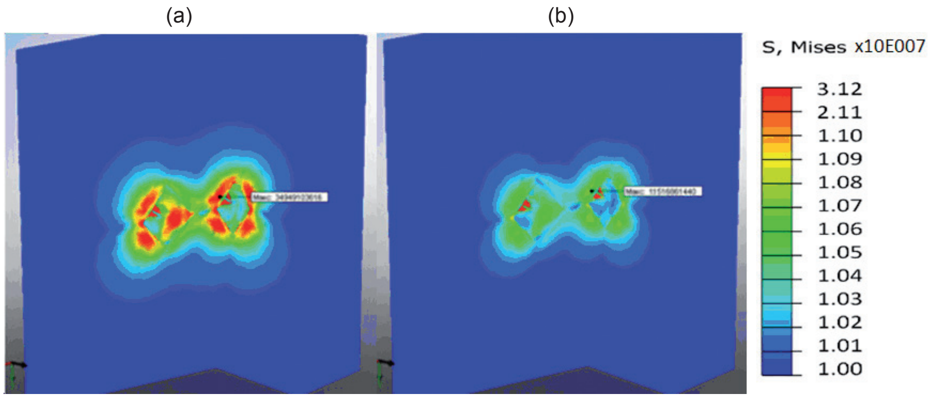

Figure 6. Stress fields in the "diamond grains–metal inclusion–binder" system. Variant with 4.4 carat/cm^3 grain concentration. Sintering in the system: (a) modulus of elasticity of binder = 2.44×10^{11} N/m^2, CTE of metal inclusion = 3.16×10^{-5} K^{-1}; (b) modulus of elasticity of binder = 1.85×10^{11} N/m^2, CTE of metal inclusion = 1.32×10^{-5} K^{-1}.

As already mentioned, there is a significant difference between the coefficients of thermal expansion of diamond and of the metal inclusions. Figure 7 shows the dependence of maximum stress *vs* temperature with different types of metal inclusions.

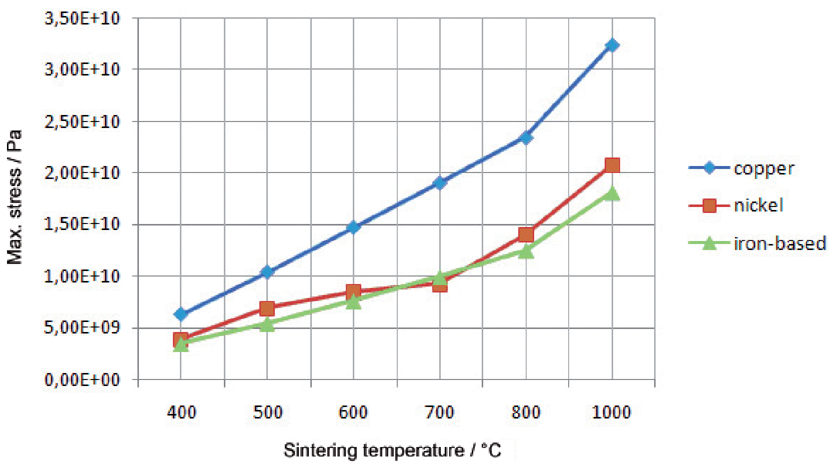

Figure 7. Maximum stress *vs* temperature for different types of metal inclusions.

[18] T.W. Hwang, C.J. Evans and S. Malkin. High speed grinding of silicon nitride with electroplated diamond wheels, Part 2: Wheel topography and grinding mechanisms. *Journal of Manufacturing Science and Engineering* **122** (2000) 42–50.

On the basis of the simulations, multifactorial dependencies and the mathematical description of the sintering process of the diamond composite layer were obtained.[19]

To describe the process, the mathematical model used was:

$$Y = b_0 + \sum b_i X_i + \sum b_{i,j} X_i X_j + \sum b_{ii} X_i^2 + \ldots \quad (4)$$

where Y is the calculated value of the output parameter (maximum stress), X are the variables (independent factors with the greatest impact on the output parameter), b_i the coefficients of the equation for the corresponding variables, and i, j number the factors that have the greatest effect on the output parameter

Independent factors are the sintering temperature of the diamond wheels, the coefficient of thermal expansion of the metal inclusions, the binder strength of the diamond wheel and the coating strength of the diamond grains.

After a significant number of simulation experiments the mathematical dependencies between the major factors affecting the properties of the components of the diamond layer were found (Figures 8 and 9).

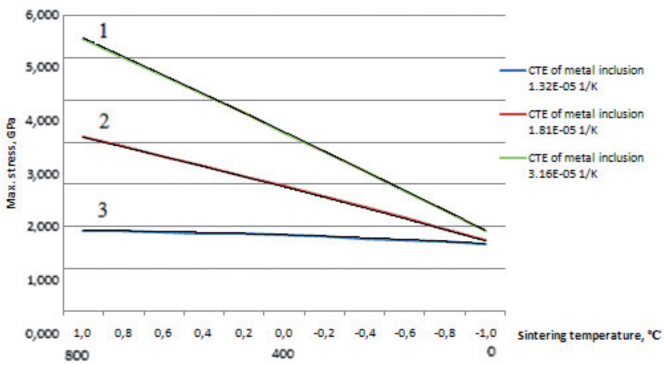

Figure 8. Stress dependence of the max. stress *vs* modulus of elasticity of binder by varying the sintering temperature: curve 1, $y = -0.001x^2 - 0.215x + 3.443$; curve 2, $y = -0.001x^2 - 0.109x + 2.165$; curve 3, $y = -0.001x^2 - 0.003x + 0.956$.

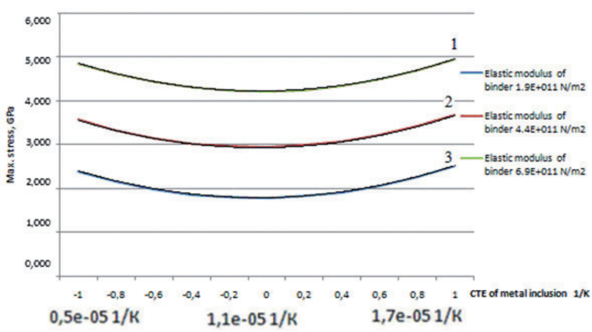

Figure 9. Stress dependence of the max. stress *vs* coefficient of thermal expansion of metallic inclusions using the different types of binders: curve 1, $y = 0.013x^2 - 0.157x + 2.5719$; curve 2, $y = 0.013x^2 - 0.157x + 1.925$; curve 3, $y = 0.013x^2 - 0.156x + 1.347$.

[19] G.I. Krasovskiy and G.F. Filaretov. *Experiment Planning*. Minsk: Publishing House of the Belarusian State University (1982).

Using these techniques we can define a favourable range of parameters for the manufacturing process of the diamond composite, which can significantly reduce the influence of the temperature factor.

The resulting mathematical model to describe the sintering process is:

$$Y = 31.09 - 0.39X_1 - 0.17X_2 - 2.29X_3 + 3.60X_4 + 0.85X_1X_2 + 0.85X_1X_3 + 0.85X_1X_4 + 0.61X_2X_3 + 1.60X_2X_4 + 0.38X_3X_4 - 12.89X_1^2 - 8.60X_2^2 + 14.50X_3^2 - 10.03X_4^2 \quad (5)$$

3. Discussion

Calculations have shown that the tear resistance is the determining factor in the destruction of diamond grains. Each grade (type) of diamond grain corresponds to a certain value of the maximum strength, which decreases with decreasing numeric index of the grade (type) and when exceeded indicates the destruction of the grain; also each grade (type) of diamond grain corresponds to a certain volume content of inclusions that may engender significant changes in the stress–strain state of the diamond grain (Figure 5).

A few propositions for reducing the effect of destructive stress on the diamond grain have been verified by computational methods. The first calculations have been devoted to the simplest option, reducing the concentration of diamond grains in producing the tool. The high values of stresses 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 particles in the composite, the lower the ability to compress, which means more stress is caused by the same pressure on the system. However, during the sintering of diamond wheels with metallic binders the temperature reaches 0.7–0.8 of the melting temperature, and taking account of plasticity in the calculations showed a significant reduction in the stresses acting on the grain inside the composite. These stresses (maximum values are less than 2 GPa) are contractile and do not approach the ultimate strength of the diamond, which suggests the possibility of manufacturing a diamond layer for high-speed grinding with a higher concentration of diamond grains with a minimum amount of damaged grains having strong metal bonds. (Figure 6). The concentration of 100% of the weight of diamonds in the diamond layer will be 4.4 carat/cm^3, 75% will be 3.3 carat/cm^3 and 200% will be 8.8 carat/cm^3. Using finite element simulations, mathematical models of the process of diamond abrasive machining were obtained. Preliminary results on the use of different types of diamond composites and rational processing speeds could thus be provided.

Test calculations have established that the optimal sintering temperature range is from 300 to 500 °C. However, when using the iron-based metal inclusion (with a CTE close to 1.32×10^{-5} K^{-1}) and copper alloy-based coatings of the diamond grains (elastic modulus close to 1.02×10^{11} N/m^2) destructive stress does not occur in the grains at temperatures up to 800 °C (Figures 5–7).

The best combination of diamond–metal composition is using binder with the nickel-based alloys (elastic modulus close to 2.44×10^{11} N/m^2) and coated grains with the copper-based alloys (modulus of elasticity close to 1.02×10^{11} N/m^2). It is possible to use grains with a large amount of metal inclusions, which are cheaper and easier to produce (Figures 8 and 9).

4. Conclusions

In summary, the main simulation results pertaining to optimization of sintering of the diamond wheel are:

- A 3D methodology for determining the optimal properties of the sintered diamond–metallic composites of diamond grinding wheels for high-speed grinding has been developed .
- The technique of 3D modelling of the diamond layer allows analysis of the stress–strain state of the system diamond grains–metal inclusion–coating–binder taking into account the thermomechanical properties of the components of the sintered composition.
- The mathematical dependencies of the influence of the main factors (properties of binder, coating, metal inclusion, the strength properties of the grains and the sintering regimes) on the integrity of diamond grains in the composite has been established.
- It is shown that the plastic behaviour of binder has a significant impact on the stress–strain state of sintering zone around the diamond grains in the composite. It was found that using metal binders it is possible to use a larger range of concentrations of diamond grains during sintering of the composite (30% more compared with the recommendations given in previous studies).

Acknowledgments

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