Principles of 3D modelling of the production and application of diamond composite materials

A.G. Mamalis,[1,*] A.I. Grabchenko,[2] V.A. Fedorovich,[2] D.V. Romashov[2] and D.O. Fedorenko[2]

[1]*Project Centre for Nanotechnology and Advanced Engineering, NCSR "Demokritos", Athens, Greece*
[2]*Department of Integrated Engineering Techniques "M.F. Semko", National Technical University (Kharkov Polytechnic Institute), Kharkov, Ukraine*

Grinding is a common method for high-precision machining of machine parts. This article describes problems that arise during the operation of diamond abrasive tools, and discusses the results of simulation of the grinding process in the modes of high-speed processing and the natural self-sharpening of the tool.

Keywords: diamond wheel, grinding, finite element method, simulations

1. Introduction

The efficiency of the process of diamond grinding is determined by the qualitative characteristics of diamond wheels and the correctness of the choice of grinding conditions. The first condition is largely ensured at the stage of production of the diamond wheels, the second at the stage of their operation.

Currently, the most promising areas for improving the efficiency of the grinding process are to increase the speed of diamond-abrasive processing and to implement a naturally self-sharpening tool through rational choice of the parameters of the components of the wheel. High-speed grinding increases productivity, accuracy and surface quality.[1–3] The control of the

* Corresponding author. E-mail: mamalis@ims.demokritos.gr

1 M.J. Jackson, C.J. Davis, M.P. Hitchiner and B. Mills, High-speed grinding with CBN grinding wheels—applications and future technology. *Journal of Materials Processing Technology* **110** (2001) 78–88.

2 J.F.G. Oliveira, E.J. Silva, C. Guo and F.Hashimoto. Industrial challenges in grinding. *Annals of the CIRP* **58** (2009) 663–680.

3 M.J. Jackson, N. Barlow and K.K.B. Hon. Computer aided design of high-performance grinding tools. Proc. Inst. Mech. Engineers (London), Part B: *J. Engng Manufacture* **215** (2001) 583–588.

Nanotechnology Perceptions **8** (2012) 132–138
Received 4 July 2012

self-sharpening process can increase the cutting ability of the grinding wheel, which is otherwise reduced because of clogging and blunting of its working surface.[4,5]

Improving the efficiency of diamond abrasive tools is an important scientific and practical problem, the solution of which requires the development of science-based grinding modes and a rational choice of wheel components. The results from a great deal of theoretical and experimental research in the field of abrasive treatment testify to the efficacy of modelling for optimization of both the sintering and grinding processes.[2,3]

2. Principle

Simulating the complexity of the grinding process requires significant computational resources. Despite this, international experience provides evidence that processing (including high-speed grinding) simulation is an excellent tool for the evaluation and optimization of grinding processes and, consequently, for increasing our knowledge about them. [1–3,6,7] The development of computer technology opens perspectives for the development of complex research methodologies for grinding processes using three-dimensional (3D)-simulations.

In the present work, the main tools for correlating theoretical modelling to experimental grinding processes are analytical software packages based on the finite element method (FEM). Testing the adequacy of the model requires a large number of experiments; however, limitations of existing measurement methods do not allow the patterns of behaviour of a material to be established by varying a large number of parameters.

The present work has led to the development of a modelling technique that allows an adequate model of the grinding process using diamond wheels. Such a model is necessary for the prospective evaluation of the feasibility of using diamond-based technology and as a means to improve the cutting ability of grinding wheels.

Results for the improvement of diamond composite tools and the development of a coating of cutting diamond grains containing nanostructured diamond are also presented. They indicate the potential benefits of the deployment of nanostructured diamonds in the binding component. Note that the nanodiamond properties are unique in the sense that they differ from those of both hitherto known filling agents and other carbon materials. Furthermore, it should be noted that the sizes of the ultradispersed diamonds (UDD) are very small (4–6 nm).[8]

3. Results and discussion

A study of the effect of grinding wheel binder type, of the type of metal phase, and of the qualitative and quantitative composition of the diamond grains in the 3D system

---

4 L.L. Mishnaevskii. *Wear of Grinding Wheels*. Kiev: Naukova Dumka (1982).

5 L.V. Khudobin and A.N. Unyanin. *Minimization of Clogging of Grinding Wheels*. Ulyanovsk: ULSTU (2007).

6 V.V. Goldin, V.G. Zhuravskii and P.A. Pravilshchikov. CALS technologies and tolerant translators. *Automation and Remote Control* **68** (2007) 710–726.

7 B. Karpuschewski, M. Wehmeier and I. Inasaki. Grinding monitoring system based on power and acoustic emission sensors. *Annals of the CIRP* **49** (2000) 235–240.

8 A.G. Mamalis, A.I. Grabchenko, V.A. Fedorovich, J. Kundrak, Y. Babenko and T. Dovbiy. Chemical deposition of nickel with inclusion of ultradispersed diamonds. *Nanotechnol. Perceptions* **7** (2011) 218–222.

"workpiece–grain–metal phase–binder" was accomplished. In addition, the influence of thickness, composition, and of geometric shape of the grain coverings was determined.

Since the processing is performed at high speeds, there is a risk of structural failure under the influence of significant centrifugal forces; therefore, it is necessary at the design stage to take into account these features. Our study was performed in two stages: first, the calculation of tool design; and second, the calculation pertaining the layer of diamond fragments. Figure 1 shows the stress distribution diagrams in the composite diamond tool investigated.

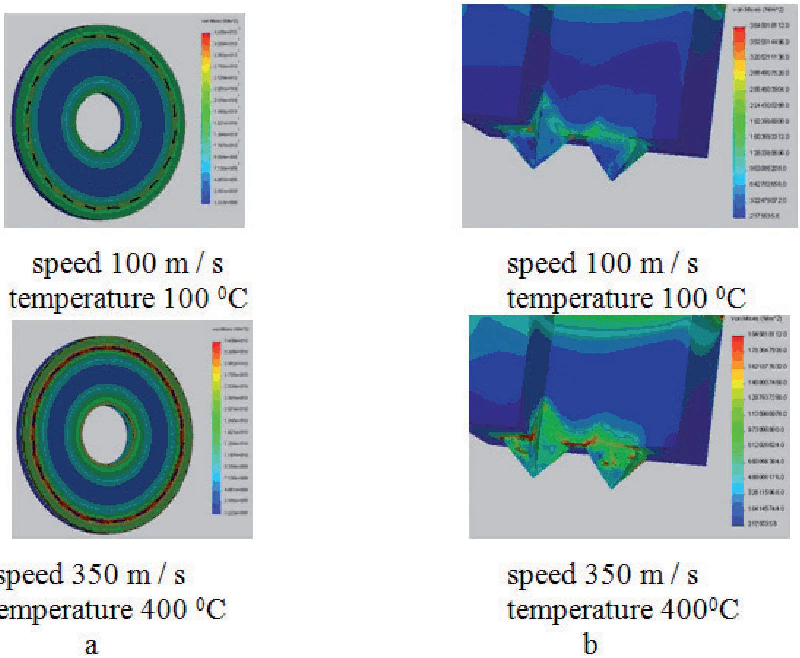


Figure 1. Stress (σ) distribution in a composite diamond tool (σ_{max}= 3.45 GPa). (a) structural test of the grinding wheel; (b) testing of a single piece of composite diamond layer.

After defining the necessary properties of diamond wheels for grinding it is necessary to establish a productive combination of properties for the manufacture of these tools. It has been determined that temperature may be a decisive factor in the process of destruction of the diamond grains. This conclusion has been made on the basis of the calculation of the stress–strain state. Since the tensile strength of diamond is lower than its compressive strength, the criterion for fracture was obtained by calculating the maximum tensile stress for diamonds of different brands and grits. Figure 2 shows the simulation of the manufacturing process of the diamond composite material, indicating the worst-case by using a metal binder, in which case the temperature has a huge impact on the destruction process.

On the basis of these simulations, multifactorial dependencies were obtained and a mathematical description of the sintering process of the diamond composite layer was formulated, which clearly describes the behaviour of the investigated system for a particular range of the properties of its components, chosen according to the most widely used types of grinding wheels (the parameters have the same values in the experiments concerning the

Metallic binder
Sintering temperature: 400 ºC
Elastic modulus of binder 4.4×10^{11} N/m^2
Elastic modulus of coating 1.1×10^{11} N/m^2
Maximum value of σ_{equiv}: 1.25 GPa

Metallic binder
Sintering temperature: 700 ºC
Elastic modulus of binder 4.4×10^{11} N/m^2
Elastic modulus of coating 1.1×10^{11} N/m^2
Maximum value of σ_{equiv}: 2.01 GPa

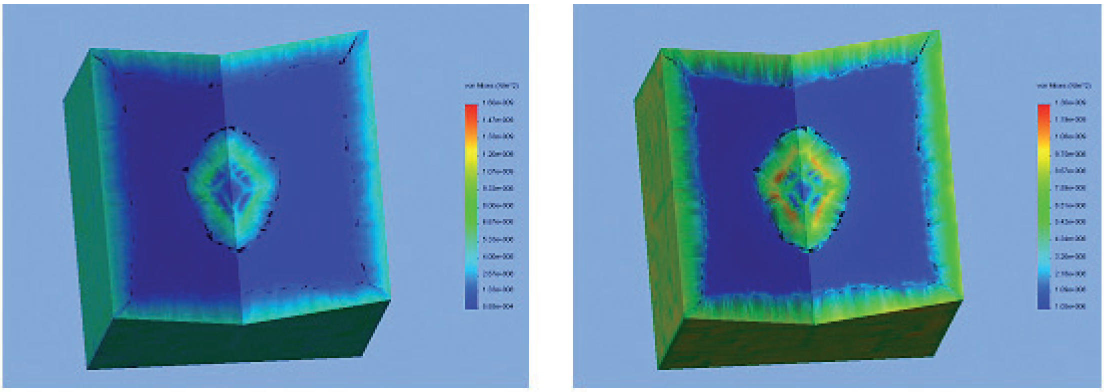


Figure 2. Influence of binder properties and process conditions of sintering on the integrity of the diamond tool.

production and exploitation of the diamond composite layer). The mathematical model used to describe the process has the general form:

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

The specific model to describe the process of sintering is:

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

where the chosen factors were: sintering temperature $X_4 = 400–800$ °C; coefficient of thermal expansion of metallic inclusions in the grains $X_1 = 0.5 \times 10^{-5} - 1.7 \times 10^{-5}$ K^{-1}; elastic modulus of binder $X_2 = 1.9 \times 10^{11} - 6.9 \times 10^{11}$ N m^{-2}; elastic modulus of coating $X_3 = 1.1 \times 10^{11} - 9 \times 10^{11}$ N m^{-2}. In Figure 3, a diagram of the stress dependence of the modulus of elasticity Y of the binder on the sintering temperature, calculated according to equation (2), is shown.

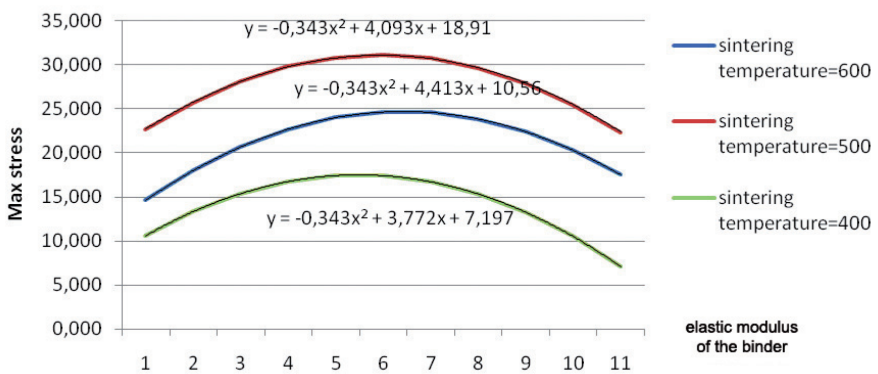


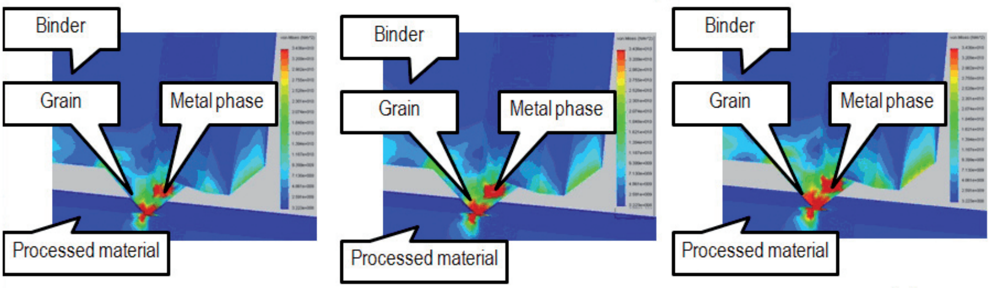
Figure 3. Stress dependence of the elasticity modulus of the binder / N m^{-2} on the sintering temperature / °C .

Using this model, a favourable range of parameters for the manufacturing process of the diamond composite layer can be defined. With the same method, a combination of properties of the coating and the properties of the binder, which can significantly reduce the influence of the temperature factor, can be determined. It may be noted that these diagrams can be selected to determine the effect of each factor on the stress distribution. In the same way, the degree of influence of any factor is determined (e.g., it was found that *no* significant change of the elastic modulus of the grain coating makes it possible to use cheaper synthetic diamonds with significant metal inclusions).

Additionally, mathematical models of the process of diamond abrasive machining were obtained using finite element simulations. Some preliminary results on the use of different types of diamond compositions and rational processing speeds are given. Figure 4 shows the influence of mechanical parameters of components of the wheel on its 3D stress–strain state.

INFLUENCE OF ELASTIC MODULUS ON 3D STRESS–STRAIN STATE OF THE SYSTEM

Reduced stress diagrams at a peripheral speed of 160 m/s; value of the coefficient of thermal expansion (CTE) 1.7×10^{-5} K^{-1}, thermal load 600 °C



value of elastic modulus 2×10^{11} N/m^2 | value of elastic modulus 9.8×10^{10} N/m^2 | value of elastic modulus 6.9×10^{10} N/m^2

Figure 4. Finite element model (FEM) simulation of the single grain microcutting process.

In these simulations the theory of multifactorial experiment planning (Figure 5) was also employed.

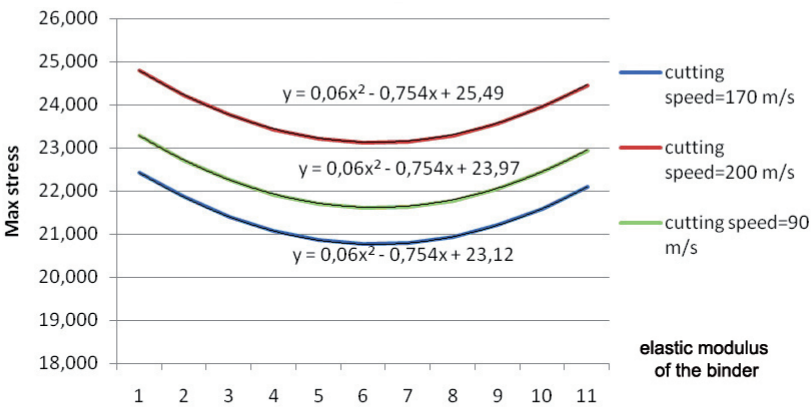


Figure 5. Stress dependence of the elasticity modulus of the binder / N m^{-2} on the cutting speed.

Equation (1) has the following specific form for describing the process of grinding:

$$Y = 55.91 - 0.02X_1 - 0.07X_2 - 6.79X_3 + 0.51X_4 + 0.001X_1X_2 + 0.01X_1X_3 - 0.001X_1X_4 - 0.02X_2X_3 + 0.06X_2X_4 + 0.32X_3X_4 - 3.83X_1^2 - 3.25X_2^2 - 12.05X_3^2 - 9.52X_4^2 . \quad (3)$$

The chosen factors were: the cutting speed (X_4); the coefficient of thermal expansion of metallic inclusions in the grains (X_1); the elastic modulus of the binder (X_2); and the temperature (X_3). Some results are shown in Figure 5.

Furthermore, numerical simulations were performed using an explicit dynamics solver (LS-DYNA), in order to calculate the performance and dynamic behaviour of the grinding process (Figure 6). Simulation modelling has established that above a speed of 120 m/s the diamond abrasive grains become sharp. The reason for this phenomenon, in our opinion, is the destruction of the blunted grains by impact with the workpiece. When operating at high speeds, the binder becomes so rigid that the shock on the grains cannot be dampened and they collapse, with the formation of brittle sharp edges.

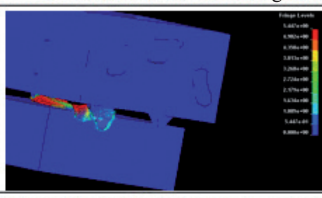
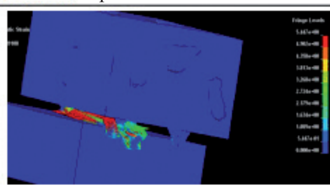
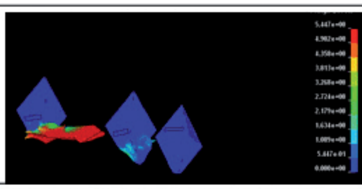
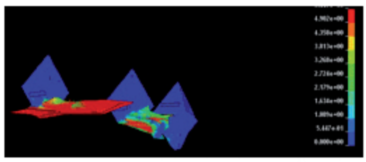
Integration step №1 Time $t = 0$ c	Integration step №2 Time $t = 0.0033$ c	Integration step №3 Time $t = 0.0036$ c
Visualization of stress distribution in the grinding at the *i*th step		
		
Visualization of stress distribution in a group of abrasive grains at the *i*th step		
		
Visualization of the destroyed volume of a group of abrasive grains at the *i*th step		
		

Figure 6. Illustration of theoretical definition of damage in a working grain.

After analysing the behaviour of the main composite materials used in grinding, the idea of introducing nanostructured additives in the binder and coating of the diamond grains, see Figure 7, was further advanced.[8]

Investigations of the samples of the diamond-bearing layer of the grinding wheel, based on the organic bonding agent B2-01[8] and diamond grains obtained by nickel–diamond coating,

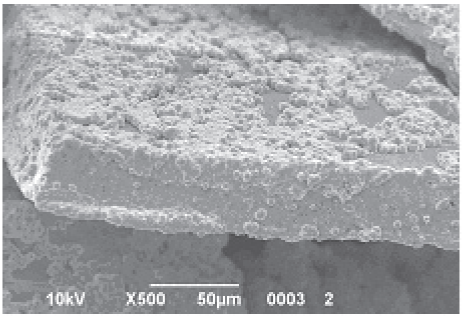


Figure 7. Diamond grain with nickel–diamond surface coating.

have been conducted. The composition of the diamond-bearing layer and its concentration varied during manufacture of the samples. Tests of the physico-mechanical properties of the particular brand of organic bonding agent used were carried out, whilst computer simulations of the behaviour of these binders and coatings of diamond grains during grinding are planned for the subsequent stage of investigation.

4. Conclusions

A new scientific approach to modelling the process of diamond grinding has been proposed, which takes into account the main features of life-cycle engineering of diamond tools: development, production and operation. Certain patterns useful for the selection of optimal characteristics of diamond composite layers for the grinding process were identified. The efficacy of high-speed grinding processing of superhard materials was demonstrated.