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# Application of artificial neural networks in properties modelling of PVD and CVD coatings

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## ABSTRACT

**Purpose:** The aim of this paper is to describe the application of artificial neural networks in development of a model, which describes the influence of PVD and CVD coatings properties on the cutting edge durability from sintered carbides covered with these layers.

**Design/methodology/approach:** The input data used for the artificial neural networks were PVD and CVD coatings microhardness, thickness, grain size and their adhesion to the substrate. On the network's output is the durability of the PVD and CVD coatings coated on sintered carbide blades determined in technological cutting trials of grey cast iron.

**Findings:** Research results shows, that the greatest influence on the durability of coated sintered carbide blades is adhesion to the substrate. Smaller influence on blades durability has the size of grains. Other properties have a minor influence on the cutting tool.

**Practical implications:** The presented results indicates, that the coating material selection and design of PVD and CVD coatings deposition process should be implemented with taking into consideration in the first place the best coating's adhesion to the substrate.

**Originality/value:** The application of artificial neural networks for influence determination of PVD and CVD coatings microhardness, grain size, thickness and adhesion to the substrate on the durability of the sintered carbide blades covered with investigated coatings.

**Keywords:** Analysis and modelling; Computational Material Science; Working properties of materials and products; Mechanical properties; Thin and thick coatings

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## ENGINEERING MATERIALS PROPERTIES

## 1. Introduction

In recent years, in scientific and industrial environment an increasing interest in the production and application of multifunctional composites, and nanostructure gradient tools and machine parts coatings can be observed. Although the coating on the cutting tools blades are used for many years, their rapid development has occurred in the last decade. Currently, modified PVD (Fig. 1) and CVD (Fig. 2) coatings methods enable the production of machine parts and tools covered by these coatings with extreme tribological properties [1-7].

In the present two dominant parallel research directions in the thin coatings area can be distinguished. The first one is the development of new types of coatings or searching of usage possibilities for already known coatings. The second direction is related with the development technology of hard, wear-resistant coatings. It is the search for new methods of deposition and modernisation of existing coatings techniques [1-5,8-13]. Additionally, cognitive tests performed for better understanding and describing of protective coatings mechanisms are made. A study of this type allows the significant progress in the development of wear-resistant coatings production technology.

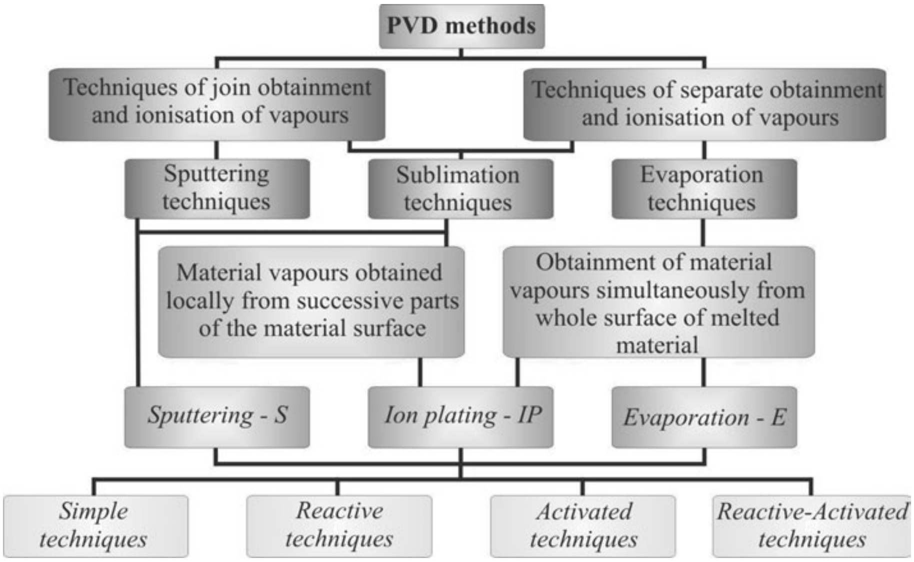

Fig. 1. Manufacturing technique classification for coatings obtained with use of PVD methods [6]

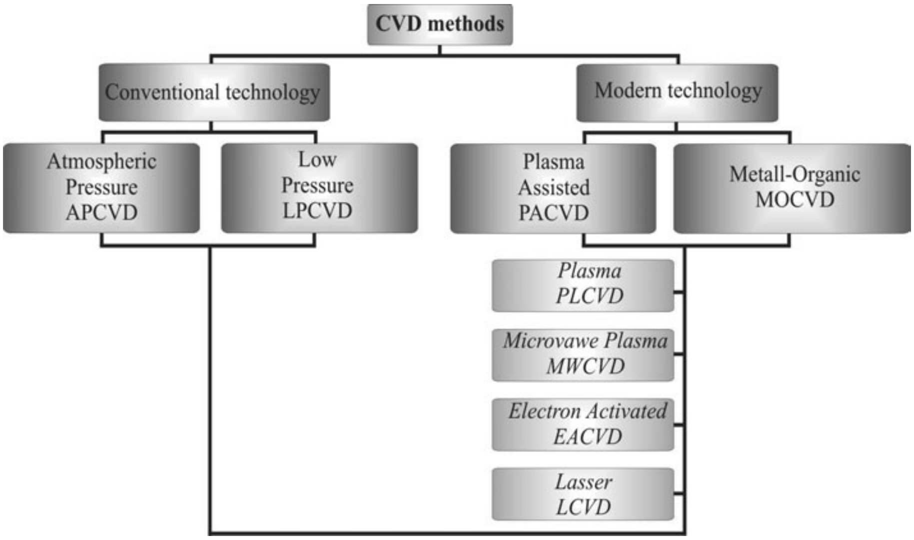

Fig. 2. Manufacturing techniques classification for coatings obtained with use of CVD methods [7]

Table 1.
Input data: ranges of coating thickness, microhardness, grain size and the critical load

| | Thickness, μm | Microhardness HV 0.05 | Grain size, nm | Critical load, N |
|---|---|---|---|---|
| Min. value | 1.8 | 2500 | 9.8 | 34 |
| Max. value | 8.4 | 3861 | 27.2 | 101 |

The dynamic development of research in the field of surface engineering is often aided by computerised techniques for data collecting and processing and for numerical simulations. Literature also provides many examples of materials computer science in surface engineering [14-18].

## 2. Methodology

The investigations were performed on sintered carbide cutting edges coated with PVD and CVD coatings, which are described among others in [1,19,20]. To build a model with use of artificial neural networks such properties as coating thickness, microhardness, grain size and adhesion to the substrate were used.

Coating thickness was measured by kalotest method. Microhardness was examined using a dynamic method Vickers method. Grain size was estimated with use of Scherrer method. The measure of coating adhesion to the substrate is the critical load [N], was determined by Scratch Test (Fig. 3).

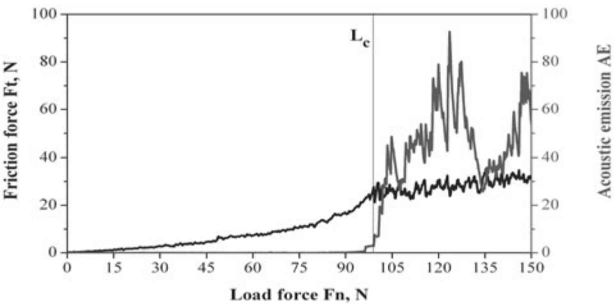

Fig. 3. Acoustic emission (AE) and friction force Ft as a function of the load Fn for Ti(C,N)+$Al_2O_3$+TiN coating obtained by CVD method on sintered carbides

In Table 1 applied ranges summary of coating thickness, microhardness, grain size and the critical load is presented.

For the coatings ranking in terms of inserts cutting ability coated with investigated coatings technological cutting trials on grey cast iron were performed. During the cutting process, the mean width of flank wear $VB_B$ was measured. The tests were stopped when the $VB_B$ value obtained the assumption criterion $VB_B$ = 0.20 mm. Tool life *T* is determined by time of continuous machining (determined by minutes) close to a threshold $VB_B$. Operations were carried out with a cutting speed $v_c$ of 180 m/min; feed rate $f_z$=0.2 mm/rev tooth; depth of a cut $a_p$=1 mm. The range of cutting ability is presented in Table 2.

Table 2.
Output data: The range of cutting ability of investigated coatings

| | Cutting ability, min |
|---|---|
| Min. value | 13 |
| Max. value | 58 |

For the construction of artificial neural networks the software package called Statistica Neural Network was used. Created numerical model of PVD and CVD coatings on sintered carbides wad developed. Two sets of descriptive vectors were obtained during data collection processes. The input set consists of four input descriptors, which are PVD and CVD coatings microhardness, thickness, grain size and their adhesion to the substrate.

The corresponding output set contains the durability of the PVD and CVD coatings coated on sintered carbide blades determined in technological cutting trials of grey cast iron. The whole set of collected vectors was divided into three subsets. First set, which was used for artificial neural networks training, was build of a half of available vectors.

A quarter of vectors was placed in a validation set used for neurons weight modification in the training process. Remaining vectors were used as testing set after teaching processes. The kind of the problem was determined as the standard, which means, that every vector is independent from another vector. The assignment of vectors to training, validation or testing set was random. Different architectures such as linear networks, radial base functions (RBF), regressive networks (GRNN) and multilayer perceptron (MLP) were applied in the training process. Best results wad obtained for multilayer perceptron with four input neurons, one hidden layer and one output neuron. This architecture (4:4-6-1:1) is presented on (Fig. 4).

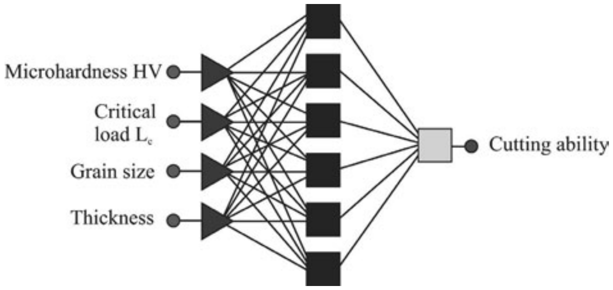

Fig. 4. Artificial neural network architecture of multilayer perceptron with one hidden layer

For the verification of networks usability in the aim of parameters prediction the following quality valuation parameters were used:

- average absolute error - difference between measured and predicted output values of the output variable;

- standard deviation ratio - standard deviation of errors for the output variable;
- Pearson correlation - the standard Pearson-R correlation coefficient between measured and predicted output values of the output variable. In Table 3 accepted evaluations of correlation forces are presented.

Table 3.
Evaluation of correlation force

| R | Correlation force |
|---|---|
| 0.0 ~ 0.2 | none |
| 0.2 ~ 0.4 | small |
| 0.4 ~ 0.7 | medium |
| 0.7 ~ 0.9 | strong |
| 0.9 ~ 1.0 | very strong |

## 3. Results

The paper presents the application of artificial neural networks to assess the impact of PVD and CVD coatings properties on the durability of carbide blades covered with these coatings. The average absolute error, standard deviation ratio and Pearson correlation coefficient for the training, validation testing sets are summarised in Table 4 shows, that all property models build with use of artificial neural networks are correctly simulated. The sensitivity analysis between input and output data (Table 5) shows that the blade durability has the greatest influence on coating adhesion to the substrate. In addition, the analysis of 3D charts shows, that the change of critical load, which is a measure of coating adhesion to the substrate has the greatest influence on the change of blades cutting ability (Figs. 5-14). Other properties, such as microhardness, coating thickness and grain size have a lesser impact on tested blades durability changes. However, it should be noted, that, among other properties, changing the grain size affects the most intensively the blade durability. In addition, the blade durability is inversely proportional to grain size. Change of microhardness and thickness of tested coatings have a minor influence on the cutting blade durability.

## 4. Summary

Based on experimental examinations results of multi-point inserts coated with PVD and CVD coatings computational model of the relationship between coating properties and inserts' cutting ability covered by these coatings have been developed using artificial neural networks. The model includes the impact of properties such as hardness, adhesion to the substrate, grain size and thickness of the coating on the durability of coated blades. The results are presented in 3D graphs. It was found that the greatest impact on the durability of the blades covered with coatings has the adhesion to the surface. Significant influence has also the grain size change. Other properties, hardness and thickness have small influence on the examined coated multi-point inserts stability. In addition, developed tool life models may be useful for prediction of coatings' operational properties based on knowledge of coatings' mechanical properties, without having to perform expensive and time-consuming cutting ability examinations.

Table 4.
Regression statistics of artificial neural network trained for prediction of PVD and CVD coatings properties deposited onto sintered carbides

| Network architecture | Regression statistics | Data sets | | |
|---|---|---|---|---|
| | | Training Set | Validation Set | Testing Set |
| MLP3 4:4-5-1:1 | Average absolute error | 4.68 | 4.38 | 4.32 |
| | Standard deviation ratio | 0.31 | 0.27 | 0.36 |
| | Pearson correlation | 0.95 | 0.97 | 0.93 |

Table 5.
Results of sensitivity analysis of input data for output data of artificial neural network trained for prediction of PVD and CVD coatings properties deposited onto sintered carbides

| Data sets | Statistics | Microhardness HV 0.05 | Critical load $L_c$ | Grain size | Thickness |
|---|---|---|---|---|---|
| Training | Range | 4 | 1 | 2 | 3 |
| | Error | 5.57 | 22.14 | 6.63 | 6.38 |
| | Ratio | 0.92 | 3.66 | 1.10 | 1.05 |
| Validation | Range | 4 | 1 | 3 | 2 |
| | Error | 4.25 | 20.49 | 6.80 | 7.12 |
| | Ratio | 0.86 | 4.13 | 1.37 | 1.43 |

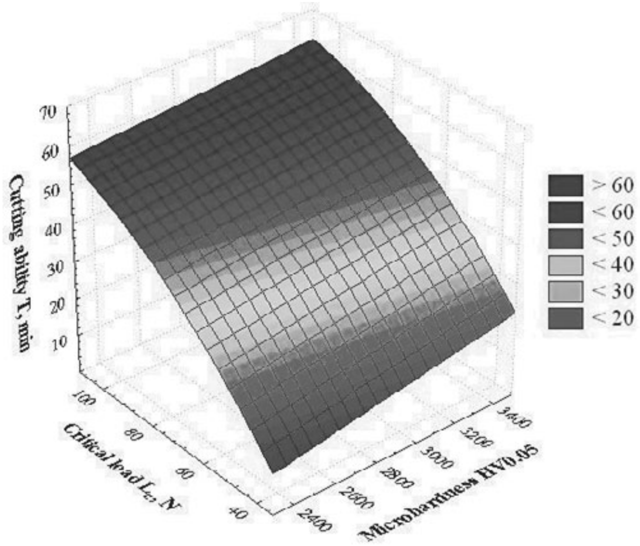

Fig. 5. Evaluation of the PVD and CVD coatings critical load and the microhardness influence of tool life T for sintered carbide tools coated with PVD and CVD coatings determined by artificial neural networks at a fixed coating thickness 2.5 microns and particle size 9.8 nm

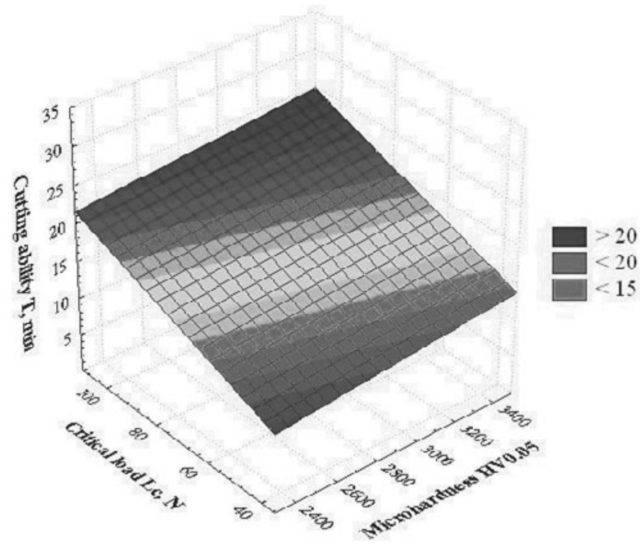

Fig. 6. Evaluation of the PVD and CVD coatings critical load and the microhardness influence of tool life T for sintered carbide tools coated with PVD and CVD coatings determined by artificial neural networks at a fixed coating thickness 2.5 microns and particle size of 420 nm

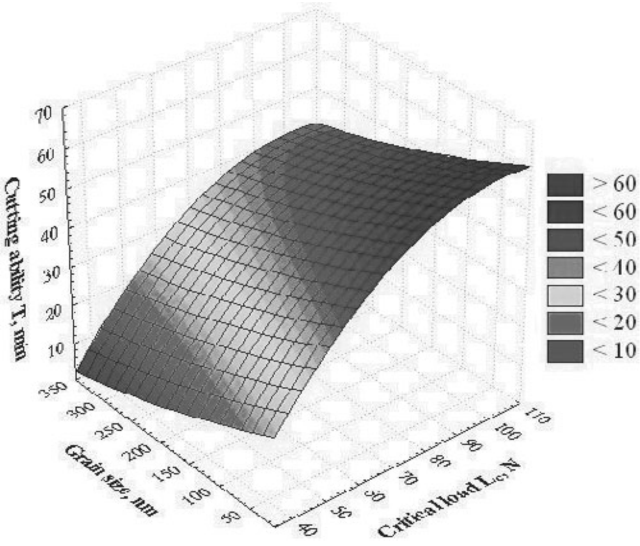

Fig. 7. Evaluation of the PVD and CVD coatings particle size and the critical load influence of tool life T for sintered carbide tools coated with PVD and CVD coatings determined by artificial neural networks with a fixed thickness of 2.5 microns and coating microhardness 3600 HV 0.05

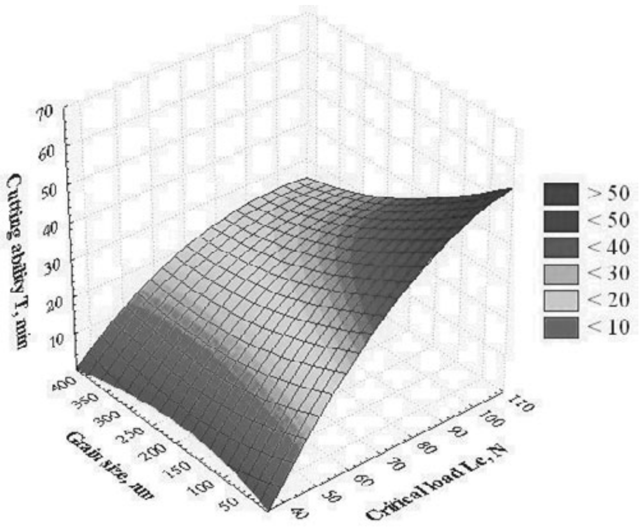

Fig. 8. Evaluation of the PVD and CVD coatings particle size and the critical load influence of tool life T for sintered carbide tools coated with PVD and CVD coatings determined by artificial neural networks with a fixed thickness of 2.5 microns and coating microhardness 2300 HV 0.05

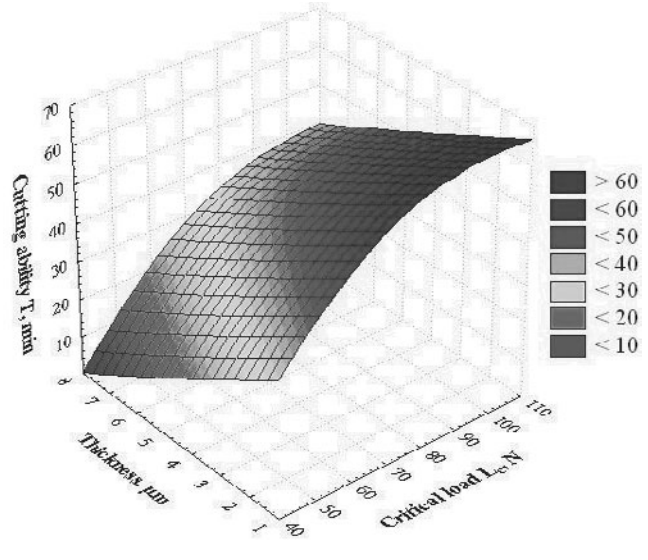

Fig. 9. Evaluation of the PVD and CVD coatings thickness and the critical load influence of tool life T for sintered carbide tools coated with PVD and CVD coatings determined by artificial neural networks with a fixed grain size of 9.8 nm microhardness 3600 HV 0.05

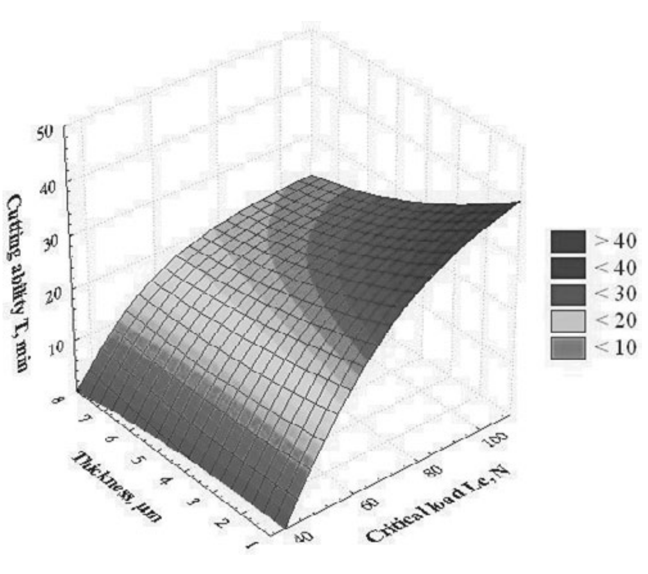

Fig. 10. Evaluation of the PVD and CVD coatings thickness and the critical load influence of tool life T for sintered carbide tools coated with PVD and CVD coatings determined by artificial neural networks with a fixed 350 nm grain size and microhardness of 2355 HV 0.05

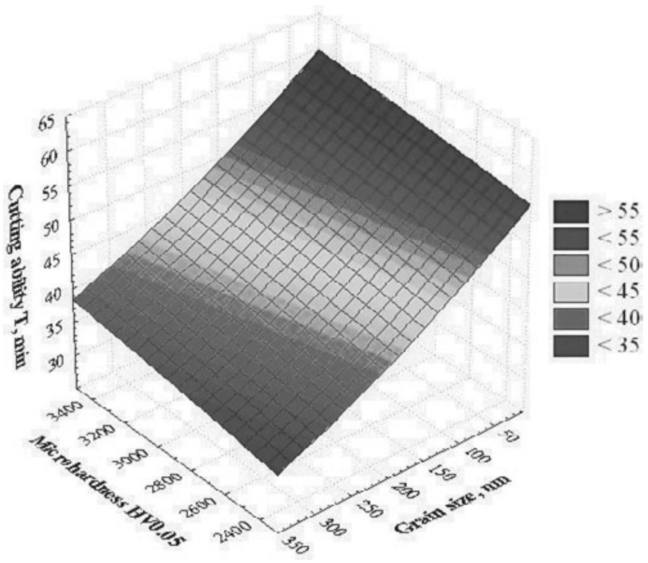

Fig. 11. Evaluation of the PVD and CVD coatings microhardness and grain size influence of tool life T for sintered carbide tools coated with PVD and CVD coatings determined by artificial neural networks with a fixed thickness of 2.5 microns and the critical load $L_c = 100$ N

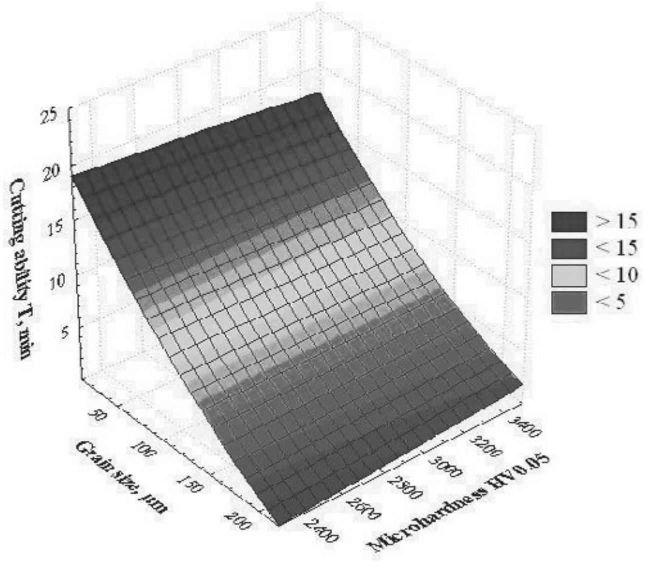

Fig. 12. Evaluation of the PVD and CVD coatings microhardness and grain size influence of tool life T for sintered carbide tools coated with PVD and CVD coatings determined by artificial neural networks with a fixed thickness of 1.8 microns and the critical load $L_c = 35$ N

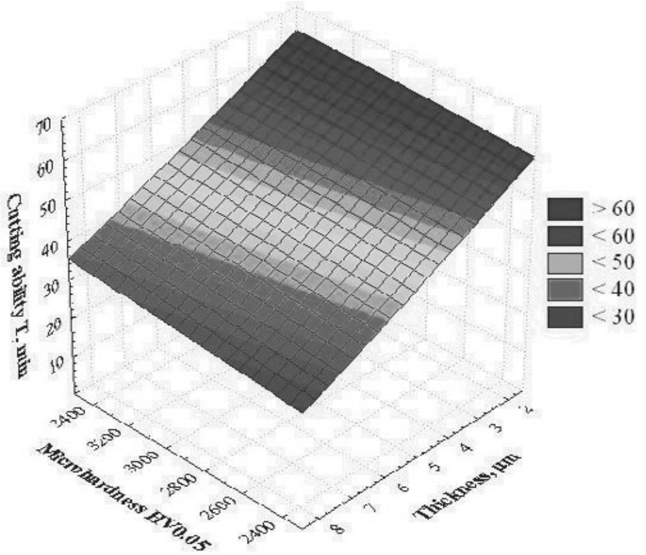

Fig. 13. Evaluation of the PVD and CVD coatings microhardness and the thickness influence of tool life T for sintered carbide tools coated with PVD and CVD coatings determined by artificial neural networks with a fixed critical load $L_c$ = 100 N and particle size 9.8 nm

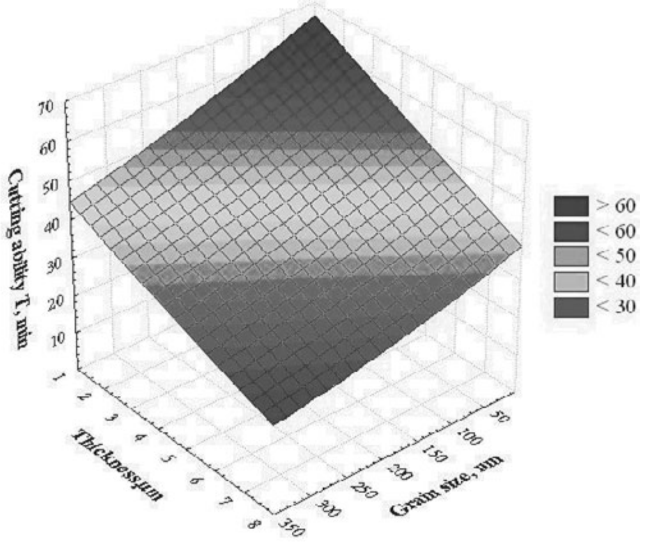

Fig. 14. Evaluation of the PVD and CVD coatings thickness and grain size influence of tool life T for sintered carbide tools coated with PVD and CVD coatings determined by artificial neural networks at a fixed and microhardness of 3600 HV and the critical load $L_c$ = 100 N

## Additional information

Selected issues related to this paper were presented at the 18th International Scientific Conference on Achievements in Mechanical and Materials Engineering AMME`2010.

## References

[1] L.A. Dobrzański, M. Staszuk, M. Pawlyta, W. Kwaśny, M. Pancielejko, Characteristics of Ti(C,N) and (Ti,Zr)N gradient PVD coatings deposited onto sintered tool materials, Journal of Achievements in Materials and Manufacturing Engineering 31/2 (2008) 629-634.

[2] L.A. Dobrzański, K. Gołombek, E. Hajduczek, Structure of the nanocrystalline coatings obtained on the CAE process on the sintered tool materials, Journal of Materials Processing Technology 175 (2006) 157-162.

[3] L.A. Dobrzański, K. Gołombek, J. Mikuła, D. Pakuła, Multilayer and gradient PVD coatings on the sintered tool materials, Journal of Achievements in Materials and Manufacturing Engineering 31/2 (2008) 170-190.

[4] D. Pakuła, L.A. Dobrzański, K. Gołombek, M. Pancielejko, A. Křiž, Structure and properties of the $Si_3N_4$ nitride ceramics with hard wear resistant coatings, Journal of Materials Processing Technology 157-158 (2004) 388-393.

[5] Dongli Zou, Dianran Yan, Lisong Xiao, Yanchun Dong, Characterisation of nanostructured TiN coatings fabricated by reactive plasma spraying, Surface and Coatings Technology 202 (2008) 1928-1934.

[6] T. Burakowski, T. Wierzchoń, Engineering of metal surface, WNT, Warsaw, 1995.

[7] P. Kula, Surface engineering. Monograph, Technical University of Lodz publishing house, Lodz, 2000.

[8] W. Pawlak, B. Wendler, Multilayer, hybrid PVD coatings on Ti6Al4V titanium alloy, Journal of Achievements in Materials and Manufacturing Engineering 37/2 (2009) 660-667.

[9] K.T. Wojciechowski, R. Zybala, R. Mania, J. Morgiel, DLC layers prepared by the PVD magnetron sputtering technique, Journal of Achievements in Materials and Manufacturing Engineering 37/2 (2009) 726-729.

[10] M. Betiuk, M. Szudrowicz, Ion etching and ion assisted in PAPVD-Arc process - AIDA ions source, Engineering Materials 5 (2005) 277-280 (in Polish).

[11] I. Dörfel, W. Österle, I. Urban, E. Bouzy, Microstructural characterization of binary and ternary hard coating systems for wear protection, Part I: PVD coatings, Surface and Coatings Technology 111 (1999) 199-209.

[12] N.M. Mustapha, R.P. Howson, Reactive filtered arc evaporation, Vacuum 60 (2001) 361-368.

[13] S. Hogmark, S. Jacobson, M. Larsson, Design and evaluation of tribological coatings, Wear 246 (2000) 20-33.

[14] A. Śliwa, J. Mikuła, K. Gołombek, L.A. Dobrzański, FEM modelling of internal stresses in PVD coated FGM, Journal of Achievements in Materials and Manufacturing Engineering 36/1 (2009) 71-78.

[15] W. Kwaśny, A modification of the method for determination of surface fractal dimension and multifractal analysis, Journal of Achievements in Materials and Manufacturing Engineering 33/2 (2009) 115-125.

[16] W. Kwaśny, W. Sitek, L.A. Dobrzański, Modelling of properties of the PVD coatings using neural networks, Journal of Achievements in Materials and Manufacturing Engineering 24/2 (2007) 163-166.

[17] M. Rajendra, M. Patrikar, Modeling and simulation of surface roughness, Applied Surface Science 228 (2004) 213-220.

[18] S. Guessasma, G. Montavon, Ch. Coddet, Modelling of the APS plasma spray process using artificial neural networks: basis, requirements and an example, Computational Materials Science 29 (2004) 315-333.

[19] L.A. Dobrzański, M. Staszuk, J. Konieczny, W. Kwaśny, M. Pawlyta, Structure of TiBN coatings deposited onto cemented carbides and sialon tool ceramics, Archives of Materials Science and Engineering 38/1 (2009) 48-54.

[20] L.A. Dobrzański, M. Staszuk, K. Gołombek, A. Śliwa, M. Pancielejko, Structure and properties PVD and CVD coatings deposited onto edges of sintered cutting tools, Archives of Metallurgy and Materials 55/1 (2010) 187-193.