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Application of artificial intelligence methods in PVD and CVD coatings properties modelling

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ABSTRACT

Purpose: The aim of this paper is the presentation of developed computational model build with use of artificial neural networks. This model describes the influence of PVD and CVD coatings properties on the cutting edge durability from sialon tool ceramics covered with these layers.

Design/methodology/approach: Obtained model has the ability to compute the durability of the PVD and CVD coatings coated on sialon tool ceramics blades determined in technological cutting trials of grey cast iron, basing on PVD and CVD coatings microhardness, thickness, grain size and their adhesion to the substrate.

Findings: Results of researches, performed with use of computational model, revealed, that the greatest influence on the durability of coated sialon tool ceramics blades have the adhesion to the substrate. Smaller influence on blades durability has the size of grains. Minor influence on the cutting tool from other properties was obtained.

Practical implications: Achieved results indicates, that the best coating's adhesion to the substrate for coating material selection and design of PVD and VD coatings deposition process should have priority in implementation.

Originality/value: Obtainment and utilisation of computational model builded with use of artificial intelligence methods.

Keywords: Artificial intelligence methods; Thin and thick coatings; PVD and CVD coatings

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METHODOLOGY OF RESEARCH, ANALYSIS AND MODELLING

1. Introduction

In recent years, scientific and industrial environments shows increased interest in production and application of multifunctional composites and nanostructured gradient tools and machine parts coatings. Although the coating on cutting tools blades have been used for years, their rapid development occurred in the last decade. Currently modified PVD and CVD methods enable the production of coatings exhibiting extreme tribological properties of elements covered by these coatings. However, there is no universal coating, suitable for different applications. Wide range of coatings requires appropriate selection of the coating depending on the application, the method of deposition and substrate type. At present we can distinguish two parallel lines of research in the area of thin coatings. The first line of research aims to develop new types of coatings, or finding new uses for already known coatings. The second line of research is related to the development of application technology of hard, wear-resistant coatings, the search for new methods of deposition, and modernization of existing techniques of deposition [1,2,6,7,9,10,13,15-27].

Protective coatings can be divided by type of chemical bonds in the dominant type of coating. Among all types of coating materials are the largest group of materials with a predominance of metallic bonds. These include nitrides and carbides of transition metals but also some of borides and silicides. In most of these phases are metallic-covalent bonds, producing in such materials high hardness and abrasion resistance with the resistance to brittle fracture, greater than the phase of covalent and ionic bonds. Another group of coating materials are the materials with a predominance of ionic bonds. To this group belong mainly oxides. The third group are the materials with a predominance of covalent bonds, which include diamond coatings and boron nitride. This group shows the highest hardness of material [1,2].

Artificial neural networks are modeling technique capable of mapping highly complex functions. They can be used wherever there are problems of prediction, classification or control. Neural networks are used to solve many practical problems. They are applied, among others, in medical diagnosis, quality control, for oil searches, coins grading, predicting the status of water in rivers and financial forecasting. Methods of artificial intelligence and, in particular, artificial neural networks are in the use, where the use of conventional mathematical tools would be time consuming and laborious. The advantages and effectiveness of the artificial intelligence determine their widespread use in the implementation of many technical tasks, including the application of expert human support in the process of making difficult and very complex decision. Intelligent systems used in materials science are often compositions of genetic algorithms, artificial neural networks and fuzzy systems components (Fig. 1). Such solutions are applied, for example in control systems, dynamic processes, where the multitude of factors may exceed the capabilities of digital and discrete systems. As examples of artificial neural networks application in materials science, papers published in recent years in the field of modeling and prediction of properties of steel and other metal alloys, modeling of hardenability of steel, plastic forming process optimization, analysis of properties of PVD and CVD, the design of new materials and selection of materials for existing and newly designed products can be presented. It should be noted that in the work cited here artificial intelligence methods are used only as a tool and not an essential part of the works topic [3-5, 7-9, 11,14].

One of the development directions in the field of cutting tools is to provide a high level of tools reliability, which is determined by constantly advancing automation and robotisation of machining processes. This implies toll designers and technologist to researches of new and more reliable solutions. Literature studies leave no doubt, improve the blades cutting properties through the use of hard, wear-resistant coatings, which are both thermal and chemical barrier is still an attractive and promising future direction of research and development and fulfills all kinds of economic and ecological criteria. In addition to the literature described relationships between structure and properties of coatings on particular interest is to know relations between properties and structure of the coating, and the lifetime of coated tools allowing them to design coatings exhibiting the best application properties. In addition to the literature described relationships between structure and properties of coatings particularly useful is understanding the relationship between properties and structure of the coating, and the lifetime of coated tools which allows to design coatings with the best application properties [2,6,7,9,10,13].

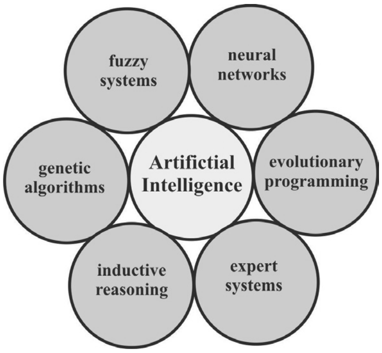

Fig. 1. Algorithms of artificial intelligence

The purpose of this study was to determine the influence of PVD and CVD properties on the durability of cutting blades durability of sialon ceramics tools.

2. Material and method

Studies presented in this paper comprised two stages. The first phase was laboratory investigatoins of sialon cutting tool ceramics coated with PVD and CVD coatings. The types of coatings are shown in Table 1. In the second stage, computational model of PVD and CVD coatings on the sialon substrate was build with use of artificial neural networks.

Table 1.
Coating types used for investigation

Coating	Type of coating
PVD	Ti(B,N)
	(Ti,Zr)N
	Ti(C,N) (1)
	Ti(C,N)+(Ti,Al)N
	Ti(C,N) (2)
	(Al,Ti)N
	(Ti,Al)N
	(Al,Cr)N
CVD	Ti(C,N)+Al_2O_3+TiN
	Ti(C,N)+TiN

Laboratory studies included mainly: investigations of particle size, and investigations of coating thickness and microhardness and investigations of coatings adhesion to the substrate.

Moreover, the structure of the coatings fractures on the scanning electron microscope was observed.

The evaluation of grain size in the investigated coatings was based on the diffraction patterns obtained by Grazing Incidence X-ray Diffraction (GIXRD) using the Scherrer method. This technique essentially consists in measuring of the diffraction line broadening at half its maximum intensity (the so-called half-width) (Fig. 2). Grain size was determined based on the formula:

$$B = \frac{0{,}9 \cdot \lambda}{D \cdot \cos\theta_B} \quad (1)$$

where:
D - grain size,
B - half-width, rad,
λ - X-ray wavelength, nm,
θ - the angle corresponding to the maximum Bragg reflection, º.

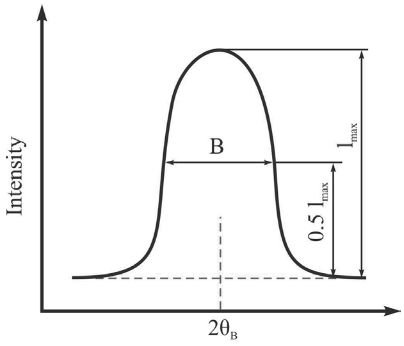

Fig. 2. Reflex profile with marked width B in the middle of the maximum intensity

Microhardness testing of produced coatings was performed with use of dynamic Vickers method, under-load - unload mode, in which the diamond indenter is loaded with constant force. This force is maintained for 10 s followed by unloading. The essence of investigations is to measure the depth of indentation, which does not exceed tenths of a micrometer, and where the base load does not exceed 0.5 N. This eliminates the influence of substrate on the measured coating hardness.

Coating thickness measurements were made using "kalotest" method, consisting in measurement of the characteristic size of the crater formed on the sample surface with the coating and by measuring the observed fractures with use of the scanning electron microscope.

Adhesion of coatings to substrates was evaluated based on investigations using scratch test on the Revetest CSEM device. This method consists of moving the Rockwell C diamond indenter over the surface of the sample at a constant speed with a linearly increasing loading force. Critical load Lc at which the loss of adhesion of the coating, was determined based on acoustic emission recorded during the measurement and observation of the cracks formed during investigation. Observations with use of light microscopy were performed. Detailed observations of occurred damages were performed with use of scanning electron microscope.

In the aim of cutting inserts prioritisation in terms of functional properties, technological cutting tests were performed. Cutting ability examinations of sialon ceramic plates uncovered and covered with PVD and CVD coatings were performed with continuously rolling without the use of cutting fluids and cutting oils. Machining was performed at room temperature. As material, grey cast iron EN-GJL-250 with a hardness of approximately 215 HB was used. Cutting plates durability examinations were based on bandwidth consumption measurement on the flank face. The measurement of the average bandwidth consumption VB was performed with use of light microscope. Attempts were interrupted, when consumption criterion set for finishing VB = 0.2 mm was exceeded. Tool life is the time T [min], followed by a value exceeding the established criterion VB = 0.2 mm. Tool life is the time T [min], when measured value exceeding the established criterion VB = 0.2 mm.

On the basis of experimental results set a model of artificial neural networks (ANN) was build. This model allows the relationship obtainment between coating properties such as hardness, adhesion to the substrate, grain size and thickness on the cutting durability of tool blades coated with investigated coatings. Computational model was build with use of artificial neural network. Architecture of multi-layer perceptron (MLP) with one hidden layer was chosen. (Fig. 3).

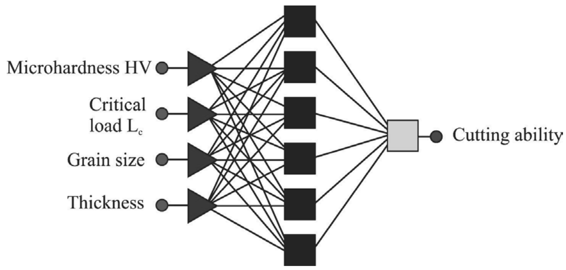

Fig. 3. Artificial neural network architecture of multilayer perceptron with one hidden layer

3. Results and discussion

3.1. Results of investigations

The results of the thickness and microhardness are presented in Table 2. Thickness of the coatings investigated is in the range from 1.3 to 7.0 microns. Microhardness of coatings obtained on the sialon ceramic tool is in a wide range from 2230 to 3600 HV0.05.

Table 2 presents the results of grain size. Researches shows that the smallest grains was observed in (Al,Ti)N coating, where the grain size is up to 8.2 nm. PVD coatings grain size is in the range 8.2-57 nm (Fig. 4), while the CVD coatings grain size is in the range 112-332 nm.

The value of critical load Lc which is a measure of the adhesion of PVD and CVD coatings to the surface with sialon ceramics are summarized in Table 2. In the case of PVD deposited on sialon ceramics substrate, the highest value of critical load Lc=112 N has a(Al,Ti)N coating, while the smallest Lc=13 N Ti(B,N) coating. It should be marked, that the high value of critical load Lc = 53 N to the sialon substrate has a (Al,Cr)N coating. Critical load in the case of CVD coatings obtained on sialon substrates is 43, and 72 N respectively for Ti(C,N)+ Al_2O_3+TiN and Ti(C,N)+TiN coating. In general, a wide range of critical load was obtained after investigation of coatings deposited on sialon tool ceramic substrate.

Results summary of cutting times are shown in Table 3. The results are comparative and are designed to create a ranking of coating durability. The results showed, that the highest service life T = 72 min were observed on sialon ceramic plates coated with (Al,Ti)N coating, while the lowest tool life T = 5 min on the same substrate shows Ti (B,N) and Ti(C,N) coatings.

Table 2.
Properties of investigated coatings

Coating	Thickness, μm	Microhardness, HV 0.05	Grain size, nm	Critical load L_c, N	Tool life T, min
Ti(B,N)	1.3	2676	57	13	5
(Ti,Zr)N	2.3	2916	13.6	21	5.5
Ti(C,N) (1)	1.5	2872	21.3	25	5
Ti(C,N)+(Ti,Al)N	1.4	2786	24	36	6
Ti(C,N) (2)	1.8	2843	18.7	26	9
(Al,Ti)N	3.0	3600	8.2	112	72
(Ti,Al)N	5.0	2961	40	21	9
(Al,Cr)N	4.8	2230	16.7	53	50
Ti(C,N)+Al_2O_3+TiN	7.0	2669	266.5 [1)] / 324 [2)]	43	3
Ti(C,N)+TiN	2.8	2746	332 [1)] / 112 [3)]	72	15

[1)] TiN layer; [2)] Al_2O_3 layer; [3)] Ti(C,N) layer

Table 3.
Regression statistics of artificial neural network trained for prediction of PVD and CVD coatings properties deposited onto sialon ceramics

Network architecture	Regression statistics	Data sets		
		Training Set	Validation Set	Testing Set
MLP3 4:4-6-1:1	Average absolute error	2.57	2.17	2.74
	Standard deviation ratio	0.14	0.10	0.19
	Pearson correlation	0.99	0.99	0.98

Table 4.
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 sialon ceramics

Data sets	Statistics	Microhardness	Critical load L_c	Grain size	Thickness
Training	Range	4	1	2	3
	Error	2.78	20.30	18.45	5.11
	Ratio	1.33	9.71	8.82	2.44
Validation	Range	4	1	2	3
	Error	3.08	27.12	15.26	4.89
	Ratio	2.49	21.96	12.36	3.96

a) b)

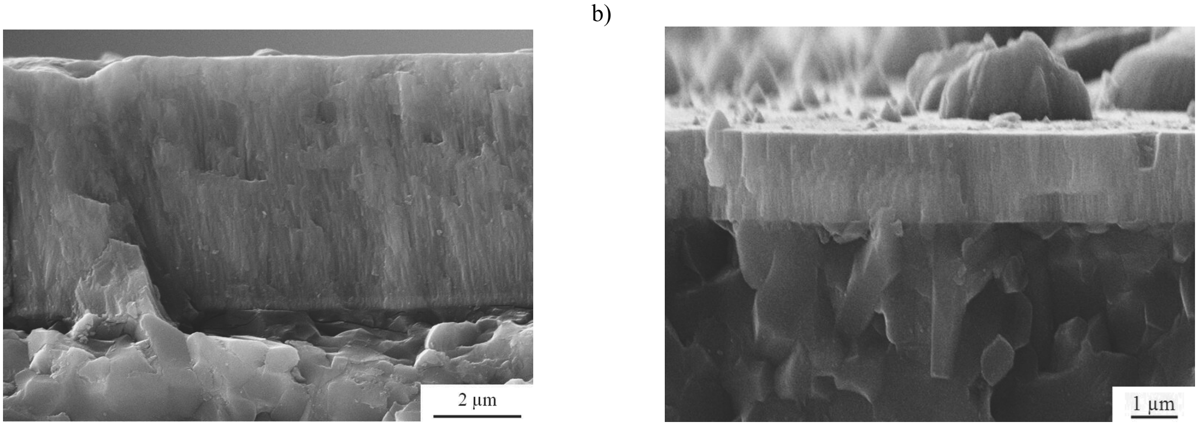

Fig. 4. Fracture of the coatings deposited onto the sialon ceramics substrate: a) (Ti,Al)N, b) (Ti,Zr)N

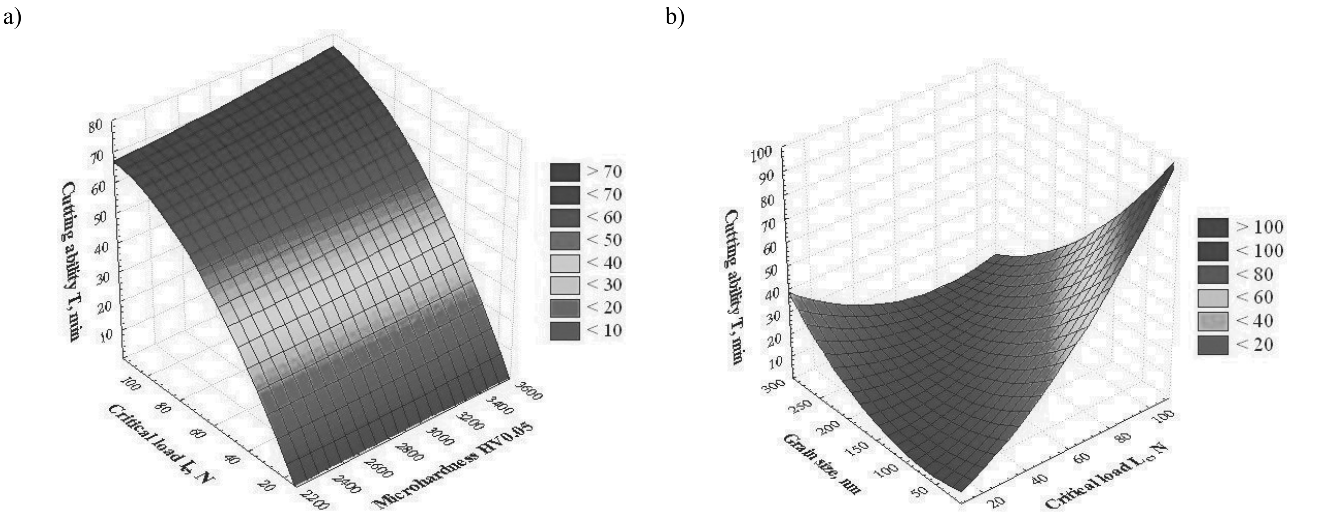

Fig. 5. a) Evaluation of the PVD and CVD coatings critical load and the microhardness influence of tool life T for sialon ceramics tools coated with PVD and CVD coatings determined by artificial neural networks at a fixed coating thickness 3.0 microns and particle size 8.2 nm; b) Evaluation of the PVD and CVD coatings particle size and the critical load influence of tool life T for sialon ceramics tools coated with PVD and CVD coatings determined by artificial neural networks with a fixed thickness of 3.0 microns and coating microhardness 3600 HV 0.05

3.2. Results of analysis using performed with use of artificial neural networks

This paper presents the application of artificial neural networks to estimate the influence of coatings investigated properties on the sialon ceramics blades durability. Mean absolute error, standard deviation and Pearson correlation coefficient for the learning, validation and testing sets are summarized in Table 3. Obtained results indicate, that artificial neural networks computations are correct. Sensitivity analysis of input data to output data (Table 4) shows that the tool life has the greatest influence on adhesion of coatings to the substrate. Change of the critical load, which is a measure of the coatings adhesion, the greatest impact on the change of tool life (Fig. 5). Other properties such as hardness, coating thickness and grain size have a lesser impact on investigated blades durability. It should be marked that, among other properties, the change in grain size most intensively affects the change of investigated stability of the blades (Fig. 5b), and the blades durability is inversely proportional to grain size. Change of microhardness and coating thickness of investigated coating has small influence on investigated cutting tool durability.

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References

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

[2] F. Čuš, M. Soković, J. Kopač, J. Balič,Model of complex optimization of cutting conditions, Journal of Materials Processing Technology 64 (1997) 41-52.

[3] L.A. Dobrzański, R. Honysz, Application of artificial neural networks in modelling of quenched and tempered structural steels mechanical properties, Journal of Achievements in Materials and Manufacturing Engineering 40/1 (2010) 50-57.

[4] L.A. Dobrzański, M. Krupiński, J.H. Sokolowski, Methodology of automatic quality control of aluminium castings, Journal Of Achievements in Materials and Manufacturing Engineering 20 (2007) 69-78.

[5] L.A. Dobrzański, R. Maniara, J.H. Sokolowski, W. Kasprzak, M. Krupinski, Z. Brytan, Applications of the artificial intelligence methods for modeling of the ACAlSi7Cu alloy crystallization process", Journal of Materials Processing Technology 192-193 (2007) 582-587.

[6] L.A. Dobrzański, D. Pakuła, Comparison of the structure and properties of the PVD and CVD coatings deposited on nitride tool ceramics, Journal of Materials Processing Technology 164-165 (2005) 832-842.

[7] L.A. Dobrzański, M. Staszuk, R. Honysz, Application of artificial neural networks in properties modelling of PVD and CVD coatings, Archives of Computational Materials Science and Surface Engineering 2/3 (2010) 141-148.

[8] L.A. Dobrzański, J. Trzaska, Application of neural networks for prediction of critical values of temperatures and time of the supercooled austenite transformations, Journal of Materials Processing Technology 155-156 (2004) 1950-1955.

[9] 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.

[10] K. Lukaszkowicz, J. Sondor, A. Kriz, M. Pancielejko, Structure, mechanical properties and corrosion resistance of nanocomposite coatings deposited by PVD technology onto the X6CrNiMoTi17-12-2 and X40CrMoV5-1 steel substrates, Journal of Materials Science 45 (2010) 1629-1637.

[11] W. Sitek, L.A. Dobrzański, Application of genetic methods in materials' design, Journal of Materials Processing Technology 164-165 (2005) 1607-1611.

[12] W. Sitek, L.A. Dobrzański, J. Zacłona, The modelling of high-speed steels' properties using neural networks, Journal of Materials Processing Technology 157-158 (2004) 245-249.

[13] T. Tański, K. Labisz, Electron microscope investigation of PVD coated aluminium alloy surface layer, Solid State Phenomena 186 (2012) 192-197.

[14] J. Trzaska, L.A. Dobrzański, A. Jagiełło, Computer programme for prediction steel parameters after heat treatment, Journal of Achievements in Materials and Manufacturing Engineering 24/2 (2007) 171-174.

[15] M. Soković, J. Kopač, L.A. Dobrzański, J. Mikuła, K. Gołombek, D. Pakuła, Cutting characteristics of PVD and CVD - Coated ceramic tool inserts, Tribology in Industry 28/1-2 (2006) 3-8.

[16] D. Pakuła, L.A. Dobrzański, K. Gołombek, M. Pancielejko, A. Křiž, Structure and properties of the Si3N4 nitride ceramics with hard wear resistant coatings, Journal of Materials Processing Technology 157-158 (2004) 388-393.

[17] 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.

[18] D. Pakuła, L.A. Dobrzański, A. Križ, M. Staszuk, Investigation of PVD coatings deposited on the Si3N4 and sialon tool ceramics, Archives of Materials Science and Engineering 46/1 (2010) 53-60.

[19] D. Pakuła, Structure and properties of multicomponent coatings deposited onto sialon tool ceramics, Archives of Materials Science and Engineering 52/1 (2011) 54-60.

[20] A.D. Dobrzańska-Danikiewicz, K. Gołombek, D. Pakuła, J. Mikuła, M. Staszuk, L.W. Żukowska, Long-term development directions of PVD/CVD coatings deposited onto sintered tool materials, Archives of Materials Science and Engineering 49/2 (2011) 69-96.

[21] L.A. Dobrzański, M. Staszuk, PVD and CVD gradient coatings on sintered carbides and sialon tool ceramics, Journal of Achievements in Materials and Manufacturing Engineering 43/2 (2010) 552-576.

[22] Yin-Yu Chang, Da-Yung Wang, Characterization of nanocrystalline AlTiN coatings synthesized by a cathodic-arc deposition process, Surface and Coatings Technology 201 (2007) 6699-6701.

[23] G.S. Fox-Rabinovich, J.L. Endrino, B.D. Beake, A.I. Kovalev, S.C. Veldhuis, L. Ning, F. Fontaine, A. Gray, Impact of annealing on microstructure, properties and cutting performance of an AlTiN coating, Surface and Coatings Technology 201 (2006) 3524-3529.

[24] W. Grzesik, Z. Zalisz, S. Król, Tribological behaviour of TiAlN coated carbides in dry sliding tests, Journal of Achievements in Materials and Manufacturing Engineering 17/1-2 (2006) 181-184.

[25] W. Grzesik, Z. Zalisz, S. Król, Tribological behaviour of TiAlN coated carbides in dry sliding tests, Journal of Achievements in Materials and Manufacturing Engineering 17/1-2 (2006) 181-184.

[26] B.A. Movchan, K.Yu Yakovchuk, Graded thermal barrier coatings, deposited by EB-PVD, Surface and Coatings Technology 188-189 (2004) 85-92.

[27] M. Pancielejko, W. Precht, Structure, chemical and phase composition of hard titanium carbon nitride coatings deposited on HS 6-5-2 steel, Journal of Materials Processing Technology 157-158 (2004) 394-298.