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Innovative method of properties determination for tools covered with PVD coatings using computer simulation

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Analysis and modelling

ABSTRACT

Purpose: The goal of this work is to determine residual stresses of coats obtained in PVD process with the use of finite elements method and comparative analysis with results obtained by laboratory investigations.
Design/methodology/approach: Article introduces the usage of finite elements method for simulation of stresses measurement process in TiN Ti(C,N) and TiC coats obtained in magnetron PVD process on high-speed steel PM HS6-5-3-8. Modelling of stresses was performed with the help of finite element method in MARC environment, and the experimental values of stresses were determined basing on the $\sin^2\psi$.
Findings: The presented model meets the initial criteria, which gives ground to the assumption about its usability for determining the stresses in coatings, employing the finite element method using the MARC program. The computer simulation results correlate with the experimental results.
Research limitations/implications: To evaluate with more detail the possibility of applying these coatings in tools, further computer simulation should be concentrated on the determination of other properties of the coatings for example- microhardness.
Originality/value: From results of the simulation based on the finite element method is possible to compute the mechanical properties of coatings obtained in PVD process.
Keywords: Numerical techniques; Stresses; Computer simulation; Finite element method

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1. Introduction

Sintered high-speed steels are important group of engineer materials. They are in use in production of cutting off tools for hard treatment materials tooling. They work with large efficiency at required enlarged coefficients of work reliability. Numerous scientific investigations showed, that influence on considerable improvement of tools exploitation persistence has the covering of tools with thin layer with the help of physical of-settling from gas- phases PVD (physical vapour deposition) techniques [1-4].

Stresses should be considered as an important material data as they have an important effect on structural phenomena in materials and their other properties, like: hardness, cracking rate, fatigue resistance. Because of the functional quality of the coating used for the cutting tool flanks it is more advantageous that the coatings have the compression stresses, as heating the substrate up in the machining process should not lead to development of coating cracks, but only to reduction of the compression stress value, occurring in the coating [5, 6].

Finite elements method is at present one of most widely used practical methods of dissolving of all engineer problems. It finds use e.g. in such spheres of science as: solid mechanics fluid mechanics, biomechanics, material engineering, thermal analysis and magnetical and electrical analysis [8-10]. Finite elements method permits on time shortening of projecting and gives possibility to research the influence of each factors on the whole mathematical model. Usage of this method from economic point of view is well-founded because more than once it permits to avoid expensive laboratory investigations, and results obtained during simulation are reliable and approximate to real values [11, 13-21].

Model presented in the work makes possible fixing of stresses of TiN, Ti(C,N) and TiC coats obtained with PVD techniques in examined samples in dependencies of deposition circumstances.

2. Materials

The tests were carried out on the samples made of sintered high-speed steel PM HS6-5-3-8 type containing 1.28% C, 4.2% Cr, 5% Mo, 6.4% W, 3.1% V and 8.5% Co. The specimens were mechanically polished before putting the coatings down. Next, they were put into the single chamber vacuum furnace with the magnetron built in for ion sputtering from the distances of 125, 95 and 70 mm from the magnetron disk. The coating deposition process was carried out at temperatures of 460, 500 and 540°C. The Ti interlayer was put down in 6 minutes at the temperature relevant for this process, after which the next coating was put down within 60 minutes. Specifications of PVD process are presented in Tables 1 and 2.

Table 1.
Chemical composition of the investigated materials

Substrate	Coating								Process type
	Type	Process temperature, °C	Specimen distance from the magnetron disk, mm	Thickness, μm	Young's modulus, GPa	Poissn ratio	Thermal expansion coefficien, 1/K 10^{-6}		
sintered high speed steel PM HS6-5-3-8	TiN	540°C	125	2.3	520	0.26	9.5		PVD
			95	3.8	500				
			70	6.1	485				
		500°C	125	2.2	510				
			95	3.7	485				
			70	5	470				
		460°C	125	4.7	565				
			95	6.7	500				
			70	10	450				
	Ti(C,N)	540°C	125	1.9	640	0.22	9.4		
			95	3.5	550				
			70	5.5	520				
		500°C	125	3.5	580				
			95	6.0	480				
			70	9.1	400				
		460°C	125	4.0	540				
			95	6.4	460				
			70	10.1	400				
	TiC	540°C	125	2.6	400	0.19	7.8		
			95	4.6	370				
			70	6.9	360				
		500°C	125	2.6	420				
			95	4.2	400				
			70	6.6	350				
		460°C	125	2.5	440				
			95	3.9	400				
			70	6.4	385				

Table 2.
The summary data of the substrate and interface material used for computer simulation of stresses in the TiN, Ti(C,N) and TiC coatings

Material	Material thickness, μm	Young's modulus, GPa	Thermal expansion coefficient, 1/K 10^{-6}	Poisson ratio
Substrate (PM HS6-3-8)	4000	207	11.88	0.25
Interface (Ti)	1.1	113	8.6	0.34

3. Methodology and computer simulation

3.1. Investigation methodology

The chemical composition of the coatings was determined by Glow Discharge Optical Spectroscopy GDOS.

Examinations of the coating thickness were made using the ”kalotest” method, consisting the measurement of the characteristic parameters of the crater developed as a result of wear on the specimen surface caused by the steel ball with the diameter of 20 mm [2, 7, 12].

The microhardness tests of the coatings were carried out on the SHIMADZU DUH 202 ultra-microhardness tester. Young’s modulus was calculated using the HARDNESS 4.2 program being a part of the ultra-microhardness tester system, according to the formula [2, 7, 12]:

$$\frac{1}{E_r} = \frac{1-v_i^2}{E_i} + \frac{1-v_s^2}{E_s} \qquad (1)$$

where:
E_i – Young’s modulus of the indenter, kN/mm^2,
E_s – Young’s modulus of the specimen, kN/mm^2,
E_r – Reduced modulus of indentation contact,
v_i – Poisson ratio of the indenter,
v_s – Poisson ratio of the specimen.

Measurements of stresses for the analyzed coatings were made by $\sin^2\psi$ on the basis of X’Pert Stress Plus company’s programme, which contains, in a form of a database indispensable to calculate, values of material constants. In the method of $\sin^2\psi$, based on diffraction lines displacement effect for different ψ angles, appearing in the conditions of stress of materials with crystalline structure, a silicon strip detector was used at the side of diffracted beam. Samples inclination angle ψ towards the primary beam was changed in the range of 0-75° (Fig. 1) [22].

3.2. Numerical simulation model

Computer simulation of the stresses occurring in the PVD coating was performed using the finite element program MARC.

The real specimen’s dimensions were used for development of its model needed for determining the stresses in the coatings. The finite elements were used in computer simulation, basing on the 2D plane description, taking into account their central symmetry. The flat, axially symmetric PLANE 42 elements described by displacement in the nodes were used in simulation for the substrate, interface and the outer layer materials.

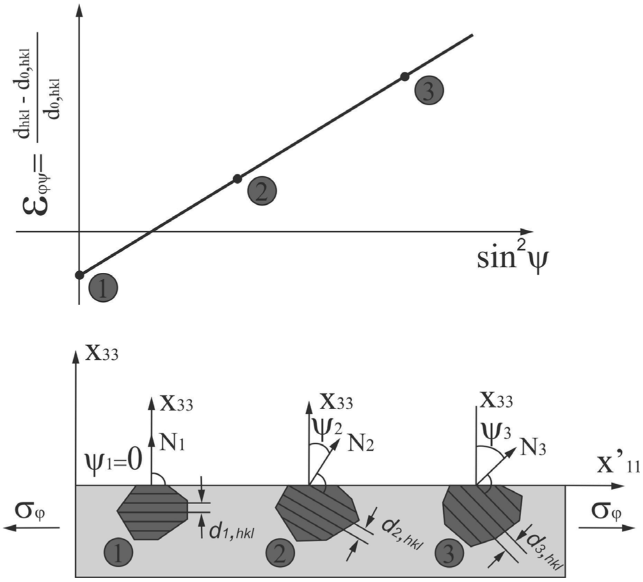


Fig. 1. Linear dependence in a classical method of $\sin^2\psi$ valid for assumptions of homogenous and plain stress state at points 1, 2, 3 correspond to measurements of values for interplanar distance at suitably - oriented grains of microstructure in different directions at y angle

The geometrical model of tested coating with an applied mesh of finite elements. Conditions of spreading in those samples and their mechanical properties, which were determined in experimental way and used in computer simulation.

In order to carry out the simulation of internal stresses in Ti+TiN, Ti+Ti(C,N) and Ti+TiC coatings, the following boundary conditions were applied:

- symmetry axis of sample is fixed on the whole length by taking away the all degrees of freedom from nodes which are on this axis.
- change of temperature in PVD process presents the cooling process of specimen from 540, 500 and 460°C to ambient temperature of 20°C,
- for TiN, Ti(C,N) and TiC coating, interface Ti and a substrate (sintered high-speed steel PM HS6-5-3-8), materials properties were established on the basis of and Mat Web catalogue, which was presented in Tables 1 and 2.

Figure 2 presents the geometrical form of sintered high-speed steel PM HS6-5-3-8 test piece with the deposited Ti+TiN, Ti+Ti(C,N) and Ti+TiC coatings. The geometrical model of the investigated coating overlaid with the finite elements’ mesh is presented in Figure 3.

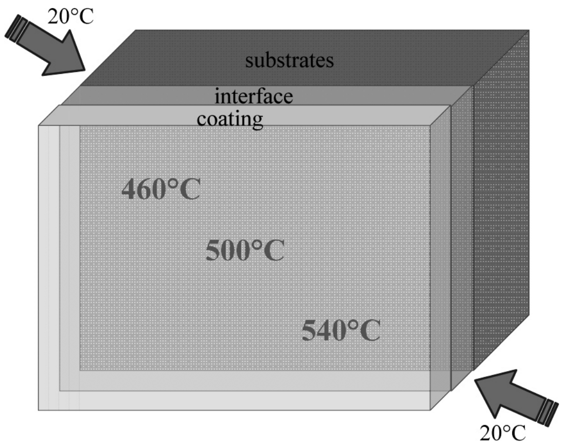


Fig. 2. Real model of coatings

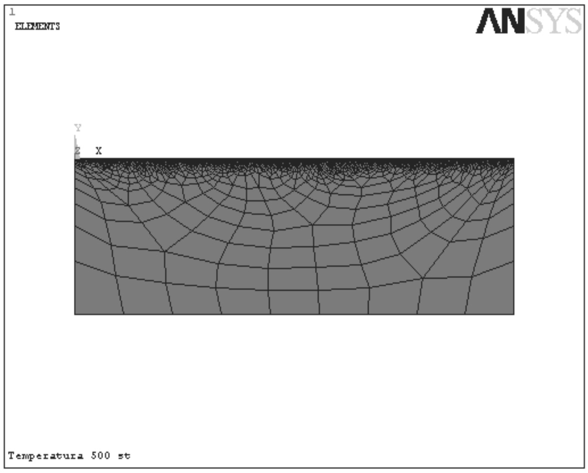


Fig. 3. Specimens model of sintered high-speed steel covered with coatings after meshing

To avoid the error in the calculation of internal stresses in coatings applied variable size of finite elements, in places where the larger value of stresses was expected the mesh is more concentrated than in the area where the stresses should take similar values, so smaller elements are used in the coatings.

4. Results

Using methods of X-ray qualitative phase analysis found that under the assumptions on the surface of the test sintered high-speed steel PM HS6-5-3-8 was covered by Ti + TiN , Ti+TiC and Ti + Ti (C, N) coatings. Diffraction images used for measuring residual stresses of the analysed coatings deposited on sintered high speed steel are shown in Figures 4 and 5.

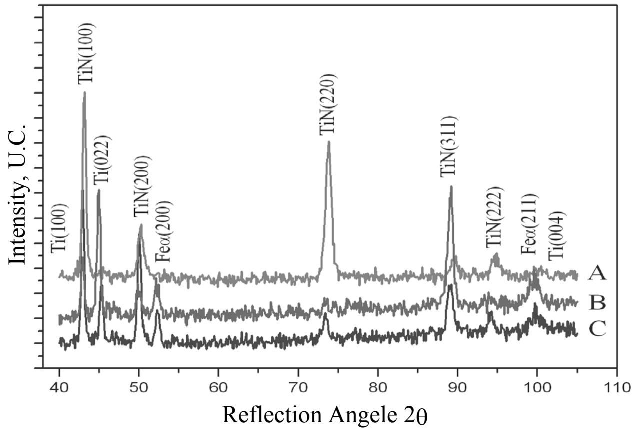


Fig. 4. Diffraction patterns of the sintered high-speed steel PM HS6-5-3-8with the TiN coatings obtained at the distance of 1) 125, 2) 90, 3) 75 mm of the specimens from the magnetron disk: A – Process temperature 460°C, B – Process temperature 500°C, C – Process temperature 560°C

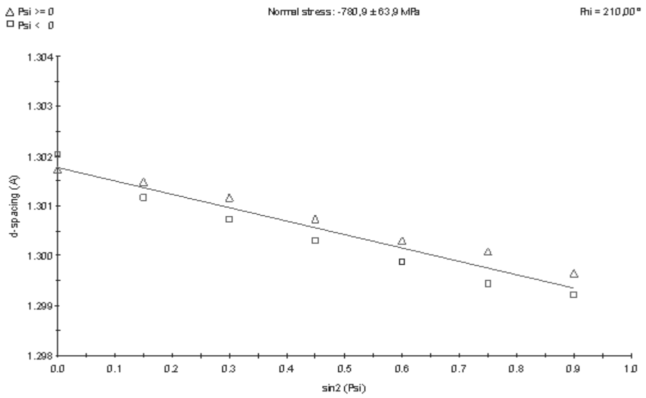


Fig. 5. Changes of interplanar distance of d reflex(3,1,1) of TiN layer (coating thickness g=2.3 μm, process temperature 540°C) a function of $\sin^2\psi$ (stresses measurement made by $\sin^2\psi$ method for different φ values of samples setting towards goniometer axis, TiN coating obtained on a substrate of sintered high-speed steel PM HS6-5-3-8

Due to the fact that the magnetron disks are made from titanium alloy with the chemical composition of 90% Ti, 5.7% Al, 1.4% Cr, 2.0% Mo, defined by X-ray phase analysis phase of TiN, TiC and Ti (C, N), could be determined (Ti, Al, Cr, Mo) N, (Ti, Al, Cr, Mo) C, (Ti, Al, Cr, Mo) (C, N)what has been confirmed in researches in the spectrometer and emission spectrometer as a result of the chemical composition of the magnetron disk. Chemical composition analysis shows the presence of Al, Cr and Mo in the studied coatings, which the cumulative average concentration is 3-10% depending on the atomic conditions for obtaining the coating, wherein the total concentration of Cr and Mo does not exceed 1%.

In the Figures 6-8 were presented the results of numerical analysis using finite element collected as maps stress distribution on the edge and in the centre of analysed coatings in MARC program.

Numerical analysis showed the presence of compressive stress on the surface of the analysed coatings which was confirmed by experimental studies

a) b)

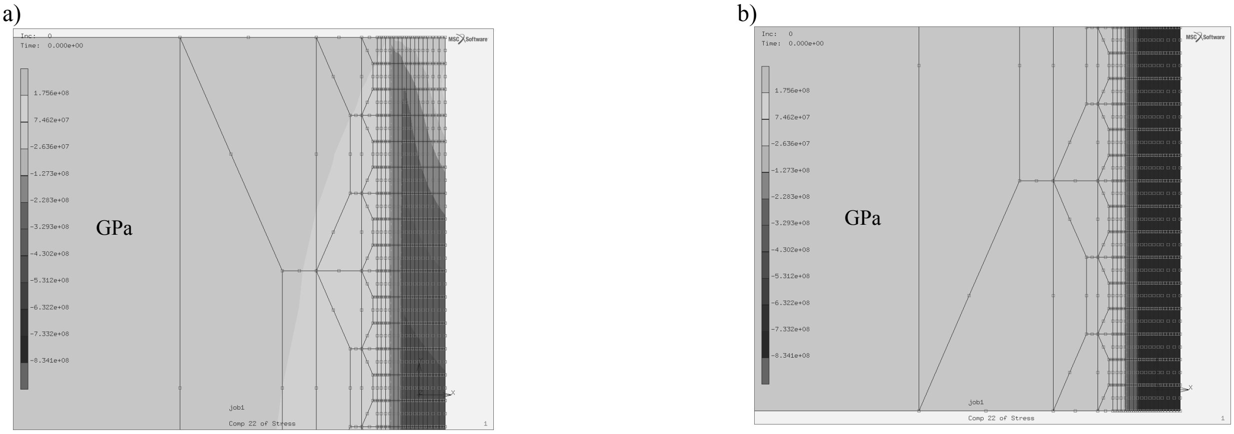


Fig. 6. Distribution of the simulated compression stresses in the TiN coating. (coating thickness g=2.3 μm, process temperature 540°C. a) Stress distribution of the edge, b) Stress distribution of the centre

a) b)

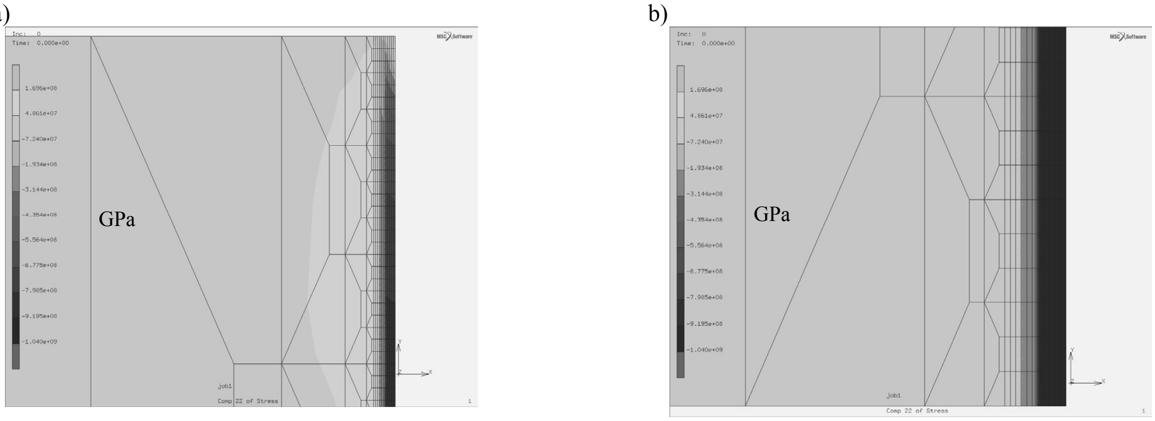


Fig. 7. Distribution of the simulated compression stresses in the Ti(C,N) coating. (coating thickness g=1.9 μm, process temperature 540°C. a) Stress distribution of the edge, b) Stress distribution of the centre

a) b)

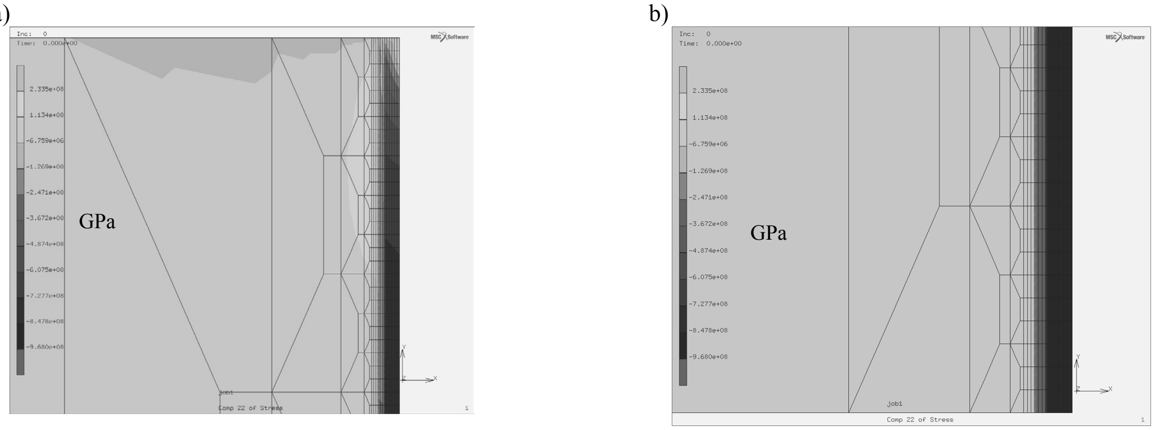


Fig. 8. Distribution of the simulated compression stresses in the TiC coating. (coating thickness g=2.6 μm, process temperature 540°C. a) Stress distribution of the edge, b) Stress distribution of the centre

In the case of two-layer Ti + TiN coatings, it was found that the internal stress value includes in the range (-)633- (-)834 MPa while the highest stress value was obtained for the coating thickness of 2.3 µm. obtained at 540°C with a sample at a distance of 125 mm from the magnetron disk.

For coatings, Ti + Ti (C, N) found that internal stresses are in the range (-)548- (-)1040 MPa, and the highest value obtained for residual stresses in coatings obtained at 540°C with a sample at a distance of 125 mm from the magnetron disk and with a coating thickness of 1.9 µm.

For the Ti + TiC coatings obtained at a distance of 125 mm from the magnetron disk, at 540°C and 2.6 µm coating thickness was obtained the maximum value of residual stresses and value of residual stresses for this coating is in the range (-)774- (-)1045 MPa.

Comparison of the results of residual stresses obtained by simulation and experimental method are summarized in Tables 3-5 and Figure 9.

Table 3.
Comparison of obtained results for TiN coatings

Temperature of the process, °C	Distances of themagnetron disk, mm	Thickness coatings TiN, µm	Stresses Ti+TiN, of the centre, MPa MARC	Experimental stresses Ti+TiN, of the centre, MPa $\sin^2\psi$
540	125	2.3	-834	-781±64
	95	3.8	-801	-780±43
	70	6.1	-774	-740±52
500	125	2.2	-739	-760±33
	95	3.7	-700	-689±30
	70	5	-700	-710±25
460	125	4.7	-761	-781±44
	95	6.7	-725	-740±40
	70	10	-633	-647±31

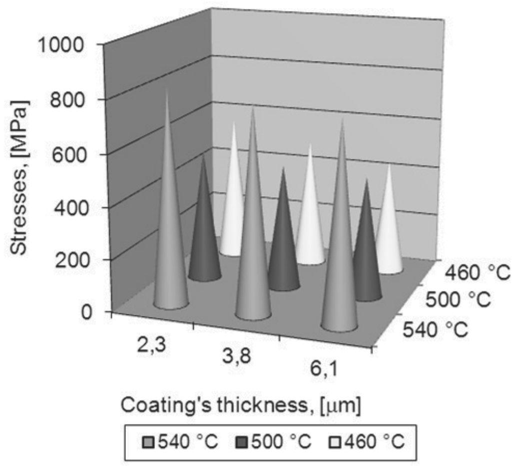
Table 4.
Comparison of obtained results for Ti(C,N) coatings

Temperature of the process, °C	Distances of themagnetron disk, mm	Thickness coatings TiN, µm	Stresses Ti+ Ti(C,N), of the centre, MPa MARC	Experimental stresses Ti+ Ti(C,N), of the centre, MPa $\sin^2\psi$
540	125	1.9	-1040	-1010±49
	95	3.5	-894	-920±36
	70	5.5	-892	-910±41
500	125	3.5	-869	-861±37
	95	6	-719	-730±55
	70	9.1	-598	-612±45
460	125	4	-632	-610±39
	95	6.4	-549	-530±30
	70	10.1	-548	-529±40

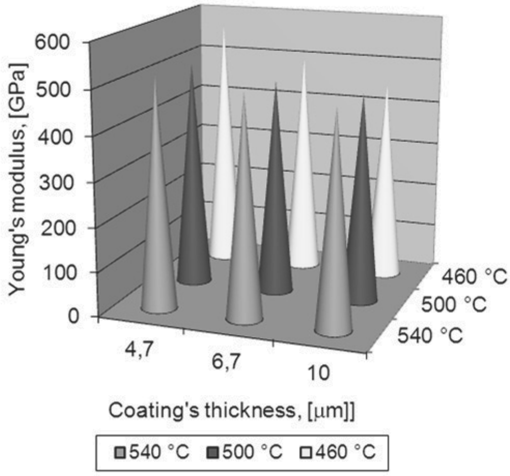
Table 5.
Comparison of obtained results for TiC coatings

Temperature of the process, °C	Distances of themagnetron disk, mm	Thickness coatings TiN, µm	Stresses Ti+ TiC, of the centre, MPa MARC	Experimental stresses Ti+ TiC, of the centre, MPa $\sin^2\psi$
540	125	2.6	-1045	-1030±34
	95	4.6	-966	-946±64
	70	6.9	-963	-976±39
500	125	2.6	-1013	-999±51
	95	4.2	-964	-980±36
	70	6.6	-845	-833±40
460	125	2.5	-973	-990±38
	95	3.9	-883	-868±29
	70	6.4	-774	-781±31

a)



b)



c)

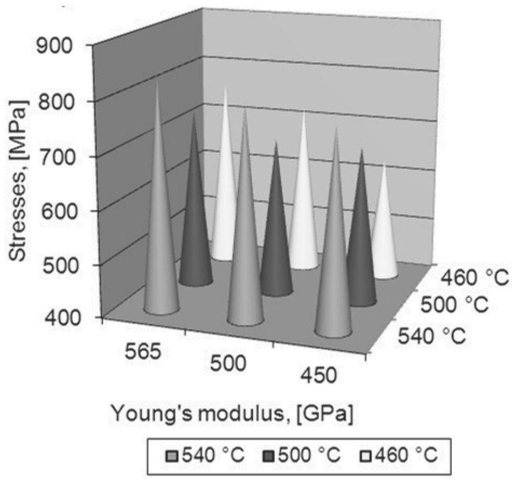


Fig. 9. Effect of PVD deposition conditions on the value of the stresses occurring in the TiN coatings. a)dependency between Young's modulus and stresses in coatings; b) dependency between Coating's thickness and Young's modulus; c) dependency between Young's modulus and stresses in coatings

All results presented in the work were analysed statistically by calculating average value for each series of measurements, standard deviation, variance and confidence intervals assuming a significance level = 0.05.

5. Conclusions

Stresses should be considered as an important material data as they have an important effect on structural phenomena in materials and their other properties, like: hardness, cracking rate, fatigue resistance. Because of the functional quality of the coating used for the cutting tool flanks it is more advantageous that the coatings have the compression stresses, as heating the substrate up in the machining process should not lead to development of coating cracks, but only to reduction of the compression stress value, occurring in the coating .

Of the basis of researches results it was found that using advanced technique of calculation among others thing the finite elements method MES, can be exploited as tools using in surface engineering to coatings characterizing. This method allows to realize complex analysis proceeding during processes of coatings spread and also analysis of phenomena occur as an effect of final process. One has to indicate that such analysis need knowledge of many quantities as physical and mechanical properties of substrate material and coating and also its parameters of spread. As a result of this mentioned above method allows to create a model which describes inner stresses in relation to parameters of process and also to kind of substrate material and to coatings.

Taking into consideration the data referring to the substrate, interface, and outer coating material properties (Young's modulus, Poisson ratio, thermal expansion coefficient) one can determine stresses in the investigated specimens. The computer simulation results correlate with the experimental results. The presented model meets the initial criteria, which give ground to the assumption about its usability for determining the stresses in coatings, employing the finite element method using the FEM programs.

On the basis of numerical analysis of a sample of model with covered PVD coatings was found that the value of the residual stresses on the surface of coatings depends on the type of coating and the conditions of their deposition noted that:

- With the increase of coating's thickness reduces the value of Young's modulus,
- With the increase of Young's modulus increases the stresses in coatings,
- With increasing of coating's thickness the value of stresses decrease,
- With increasing temperature of PVD process increases the value of stresses in coatings,

As a result of experimental researches and computer simulation of formed residual stresses in Ti+TiN, Ti+Ti(C,N) and Ti+TiC coatings which were applied on the substrate of sintered high-speed steel PM HS6-5-3-8 in PVD process, it was found the occurrence of compressive stresses what ensures the rise of strength properties.

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