

FEM application for modelling of PVD coatings properties

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Analysis and modelling

ABSTRACT

Purpose: The general topic of this paper is problem of determining the internal stresses of composite tool materials with the use of finite element method (FEM). The chemical composition of the investigated materials' core is corresponding to the M2 high-speed steel and was reinforced with the WC and TiC type hard carbide phases with the growing portions of these phases in the outward direction from the core to the surface. Such composed material was sintered, heat treated and deposited appropriately with (Ti,Al)N or Ti(C,N) coatings.

Design/methodology/approach: Modelling of stresses was performed with the help of finite element method in ANSYS environment, and the experimental values of stresses were determined basing on the X-ray diffraction patterns. The computer simulation results were compared with the experimental results.

Findings: Computer aided numerical analysis gives the possibility to select the optimal parameters for coatings covering in PVD process determining the stresses in coatings, employing the finite element method using the ANSYS software.

Research limitations/implications: It was confirmed that using of finite element method in stresses modelling occurring in advanced composite materials can be a way for reducing the investigation costs. In order to reach this purpose, it was used in the paper a simplified model of composite materials with division on zones with established physical and mechanical properties. Results reached in this way are satisfying and in slight degree differ from results reached by experimental method.

Originality/value: Nowadays the computer simulation is very popular and it is based on the finite element method, which allows to better understand the interdependence between parameters of process and choosing optimal solution. The possibility of application faster and faster calculation machines and coming into being many software make possible the creation of more precise models and more adequate ones to reality.

Keywords: Computational Materials Science; Finite Element Method; Stresses; Coatings PVD

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1. Introduction

Very common use of machining processes makes it necessary to intensify researches in area of proper materials selection as well

as in area of modern technologies for deposition of modern, avant-garde, wear-resistant coatings. Application of surface treatment technologies, as physical vapour deposition, has currently high development potential in area of methods for tool materials properties increase [1-2].

The adhesion of coating to the substrate is one of fundamental parameters, characterizing their functional properties. The character and distribution of internal stresses plays main part in determining of coating adhesion to properly prepared substrate. Researches of internal stresses, occurring on the surface of coated materials, as well as in the adhesion zone where coating meets the substrate, makes it possible to draw valuable conclusions concerning engineering process of the advisable structure and chemical composition of coatings [3-5].

The finite element method is currently commonly used in such branches of science, like: mechanics, biomechanics, mechatronics, materials engineering, and thermodynamics [6-9]. All types of simulations shorten the design process and give the possibility to investigate the particular factors on the entire model [10-18]. This is often impossible to achieve in real conditions or not justified economically. The finite element method makes it possible to understand the relationships among various parameters better and makes it possible to select the optimum solution [19-22].

Applying of this method contains many fields of contemporary industry and also modern technologies are supported by using of computers. MES system can be treated as one of program belonging to CAD/CAM/CAE group, which contain complex supporting of designing tools cycle, beginning with constructing up to realization of manufacture processes [23-24].

The general topic of this paper is the computer simulation with the use of finite element method (FEM) for determining the internal stresses of composite gradient tool materials. The chemical composition of the investigated materials' core is corresponding to the M2 high-speed steel and was reinforced with the WC and TiC type hard carbide phases with the growing portions of these phases in the outward direction from the core to the surface. Such composed material was sintered, heat treated and deposited appropriately with (Ti,Al)N or Ti(C,N) gradient coatings.

2. Investigation methodology

Stresses distribution test was done using computer programme called "Ansys" of „MSC.Software" company (Figs. 1, 2).

Analysis was carried out in four variants of materials. Individual variants differ from kind of used intensified carbon phase and kind of used PVD coating (Table 1). In order to achieve assumed purposes of this paper it was also assumed simplified model of gradient- structured materials with zones division including established mechanical and physical properties. For all zones of individual variants these properties were selected and put into computer programme that makes the analysis such as: Poisson ratio, Young's modulus, thermal expansion coefficient, density.

In order to carry out the simulation of internal stresses in HS+WC/Ti(C,N), HS+WC/(Ti,Al)N, HS+TiC/Ti(C,N) and HS+TiC/(Ti,Al)N in PVD coated FGM, the following boundary conditions were applied:

- change of temperature in PVD process presents the cooling process of specimen from 500°C to ambient temperature of 20°C,

- for HS+WC/Ti(C,N), HS+WC/(Ti,Al)N, HS+TiC/Ti(C,N) and HS+TiC/(Ti,Al)N, materials properties were established on the basis of and Mat Web catalogue, which was presented in Tables 1 and 2

On the account of big difference between the thickness of three top layers and those which are in base of model, dimensions of each model were put in calculation programme by the use of scale.(Table 1). One millimeter in real model is one micrometer of model which was created in Ansys software.

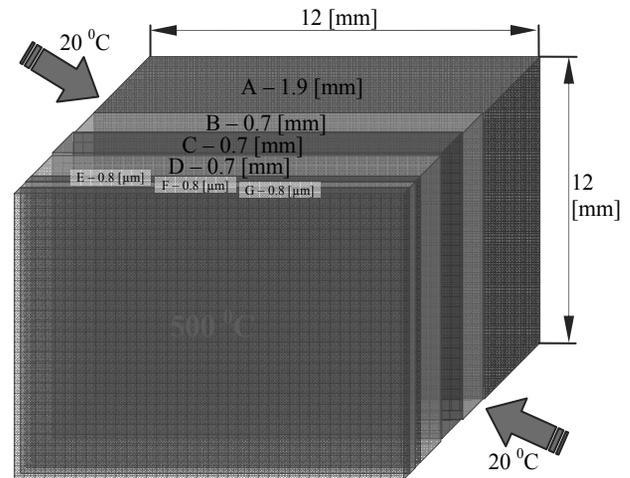


Fig. 1. Dimensioning model in SD section

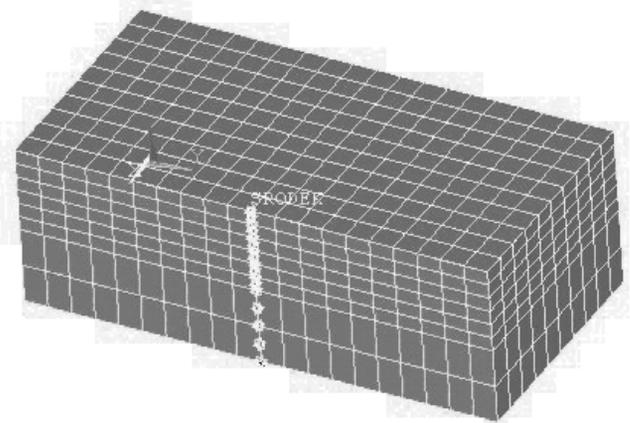


Fig. 2. Specimens model covered with coatings after meshing

Evaluation of the phase composition of the investigated coatings was made using the X'Pert PRO Panalytical X-ray diffractometer, equipped with a cobalt lamp as a radiation source. Measurements were made within the 2 θ angle range between 40-115°. Measurements of internal stresses in investigated gradient PVD coatings was made in two perpendicular directions with use of $\sin^2\psi$ method on X'Pert Stress software. Inclination angles ψ of samples towards primary beam was changed in range 0°-70°.

Table 1.
Arrangement of individual zones in models and material's data of individual models

Zone 1 (1.9mm)	HS 6-5-2			
Zone 2 (0.7mm)	HS 6-5-2 + 12%WC		HS 6-5-2 + 12%TiC	
Zone 3 (0.7mm)	HS 6-5-2 + 8%WC		HS 6-5-2 + 8%TiC	
Zone 4 (0.7mm)	HS 6-5-2 + 4%WC		HS 6-5-2 + 4%TiC	
Zone 5 (0.8 μ m)	TiN	TiN	TiN	TiN
Zone 6 (0.8 μ m)	Ti(C,N)	(0.7 Ti, 0.3 Al)N	Ti(C,N)	(0.7 Ti, 0.3 Al)N
Zone 7 (0.8 μ m)	TiC	(0.3 Ti, 0.7 Al)N	TiC	(0.3 Ti, 0.7 Al)N
	VARIANT 1 HS+WC/Ti(C,N)	VARIANT 2 HS+WC/(Ti,Al)N	VARIANT 3 HS+TiC/Ti(C,N)	VARIANT 4 HS+TiC/(Ti,Al)N
λ_x [W/m ² *K]	36.316	36.273	34.018	33.981
λ_y [W/m ² *K]	37.108	37.103	34.581	34.576
ρ [kg/m ³]	7752.179	7756.032	7395.515	7399.368
c [J/kg*K]	656.654	657.018	657.45	657.605

Table 2.
Properties of individual layers

	Poisson ratio	Young's modulus. [GPa]
HS 6-5-2 + 12%TiC	0.29	241
HS 6-5-2 + 8%TiC	0.30	233
HS 6-5-2 + 4%TiC	0.30	225
HS 6-5-2 + 12%WC	0.31	172
HS 6-5-2 + 8%WC	0.30	183
HS 6-5-2 + 4%WC	0.30	195
HS 6-5-2	0.30	215
(0.3 Ti, 0.7 Al)N	0.27	480
(0.7 Ti, 0.3 Al)N	0.23	420
TiC	0.19	390
Ti(C,N)	0.24	410
TiN	0.26	510

Table 3.
Computer simulation results of stresses for all variants in particular zones [MPa]

	VARIANT 1 HS+WC/Ti(C,N)	VARIANT 2 HS+WC/(Ti,Al)N	VARIANT 3 HS+TiC/Ti(C,N)	VARIANT 4 HS+TiC/(Ti,Al)N
Zone 1 (1.9mm)	(-) 230-998	(-) 150-998	(-) 180-950	(-) 190-1000
Zone 2 (0.7mm)	(-) 150-752	(-) 100-620	(-) 100-680	(-) 100-750
Zone 3 (0.7mm)	(-) 100-473	(-) 100-470	(-) 100-460	(-) 100-400
Zone 4 (0.7mm)	(-) 100-368	(-) 100-363	(-) 100-368	(-) 100-334
Zone 5 (0.8 μ m)	(-) 100-540	(-) 260-700	(-) 100-550	(-) 100-654
Zone 6 (0.8 μ m)	(-) 220-660	(-) 220-750	(-) 210-660	(-) 270-839
Zone 7 (0.8 μ m)	(-) 316-821	(-) 340-820	(-) 320-815	(-) 300-869

3. Investigations results

Using experimental results and assumed data given in Table 3 internal stresses were modelled using ANSYS software, with the finite element method. Figures 3-10 present obtained results of numerical analysis gathered as distribution maps of stresses in HS+WC/Ti(C,N), HS+WC/(Ti,Al)N, HS+TiC/Ti(C,N) and HS+TiC/(Ti,Al)N in PVD coated FGM.

Figure 11 presents displacement of the sample in 100 s, whereas the Figure 12 presents displacement of the sample during analysis in time function for $t=100$ s. Distribution of stresses being reduced HMH in 100 s of cooling and also displacement of samples elements at 300 multiplicity of magnification what was shown in the Figure 13 and Figure 14 presents distribution of stresses in cooling function 0-3000 s for successive zones of sample cross-section.

Figure 15 presents x-ray diffraction pattern on the basis of which were calculated internal stresses in the coatings, interlayers and in substrate materials.

Value stress error in the simulated model is 3%. The comparative analysis was carried out of the results of computer simulation of stresses with the experimental results.

Table 3 presents calculated results of stresses range value in individual zones for all analyzed variants of material.

On the basis of result analyses obtained by simulation it was stated that stresses range value in particular zones are very much the same depending on material variant what should be associated with almost the same physical properties of analyzed material variants. In all analyzed cases it was stated the presence of compress stresses with little or medium value which might have positive influence on functional properties of tested materials.

The biggest span of stresses range was found in zone 1. It is partly connected with geometry of analyzed samples and physical properties of applied materials and also with the biggest thickness of zone 1 in given simplified model of gradient- structural materials.

The inside of zone 1 characterizes by relatively high value of compress stresses (from (-)950 MPa in case of variant HS+TiC/Ti(C,N) to 1000 MPa in case of variant HS+TiC/ Ti, Al)N) within the side surface zone the stresses show medium value, while side edges characterise by little stresses value.

The smallest span of stresses range was found in zone 4, which is real surface zone of substrate for deposited PVD coatings. The stresses within this zone show the lowest value among analysed zones (maximum up to (-)368 MPa in case of variant HS+WC/Ti(C,N) and HS+TiC/Ti(C,N)). The surface distribution of stresses changes in relation to bigger depth of zone 1 where the highest value occur around the middle of analyzed piece of sample, while the lowest value occur exactly in the middle and peripheries of zone 4 (Fig. 7).

The maximum stresses value ascends while changing of analyzed zone towards the surface of the sample (zone 5-7) (Figures 8-10) and reach the level over 800 MPa in zone 7, in area near to edges (Fig. 10). Concentration of compress stresses

in edges might has influence on higher microhardness of tested material and also contributing to improvement of its functional properties.

Calculated value of internal stresses in tested high-speed steel matrix composites deposited with gradient PVD coatings change gradually towards surface of coatings. Thanks to application of gradient substrates and also gradient coatings, it was achieved small difference of stresses between zone 4, which is real zone of substrate surface for PVD coating, and zone 5 which is first coating zone. It contributes to more coating adhesion to substrate of material and benefits functional properties of tested materials.

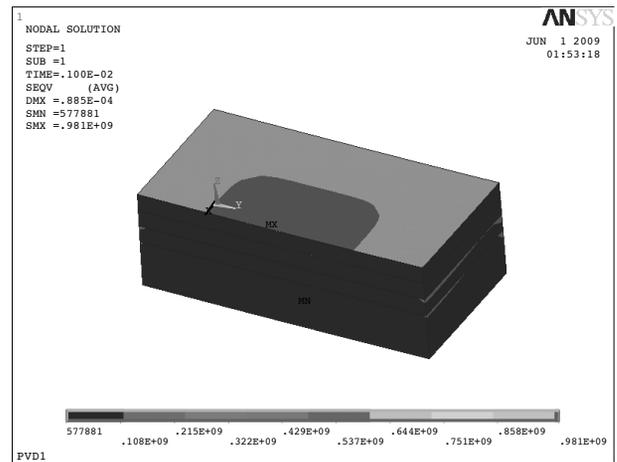


Fig. 3. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) coating [MPa]

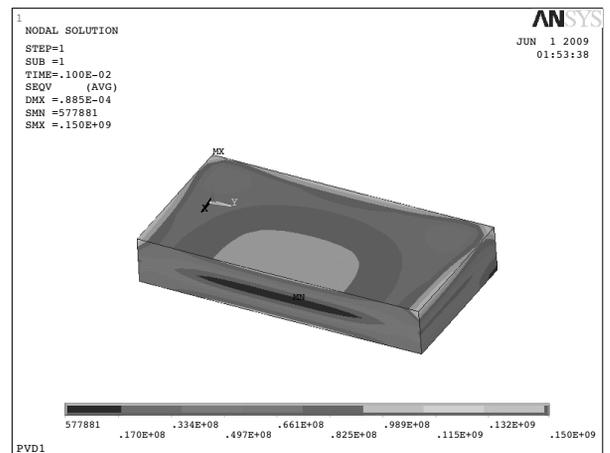


Fig. 4. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) coating (in first zone) [MPa]

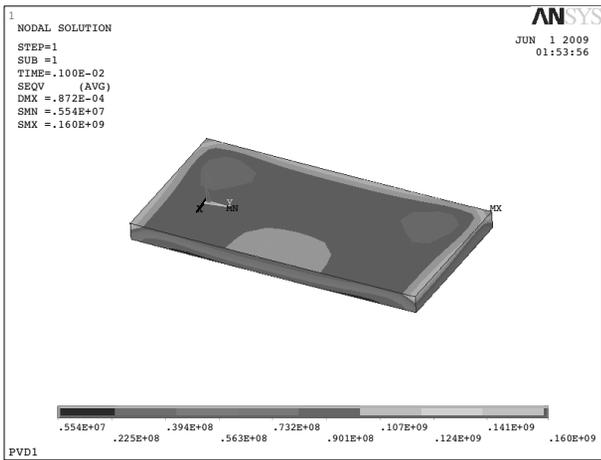


Fig. 5. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) coating (in second zone) [MPa]

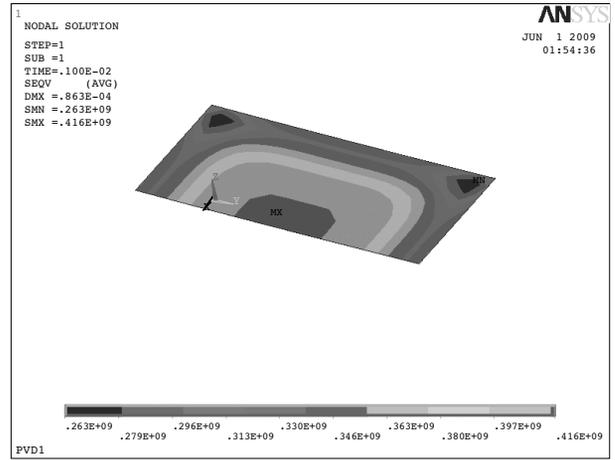


Fig. 8. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) coating (in fifth zone) [MPa]

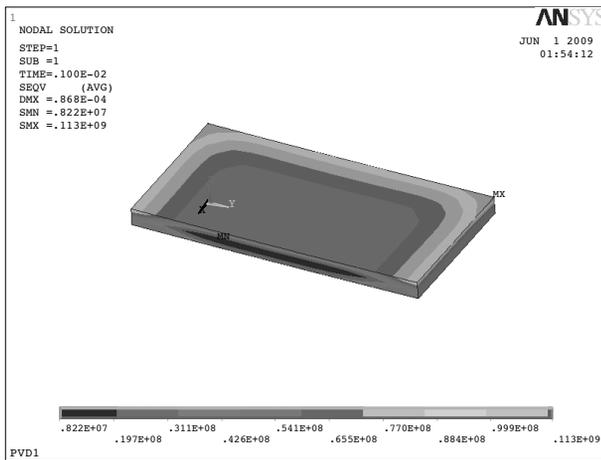


Fig. 6. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) coating (in third zone) [MPa]

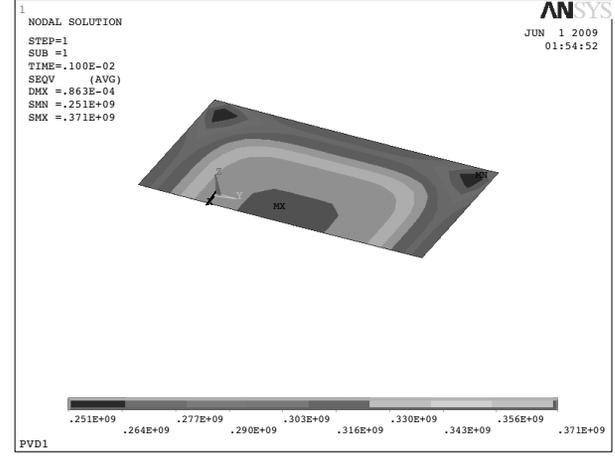


Fig. 9. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) coating (in sixth zone) [MPa]

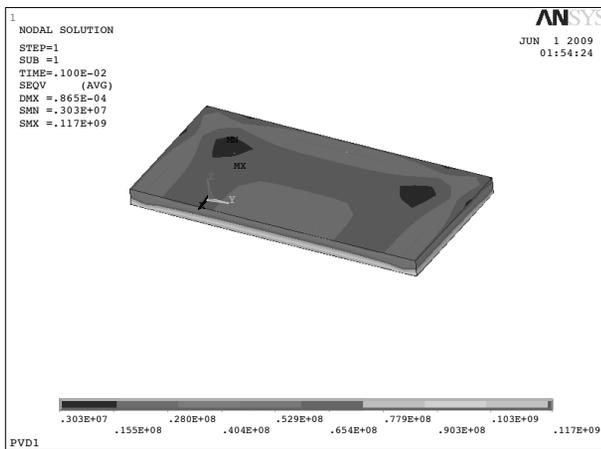


Fig. 7. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) coating (in fourth zone) [MPa]

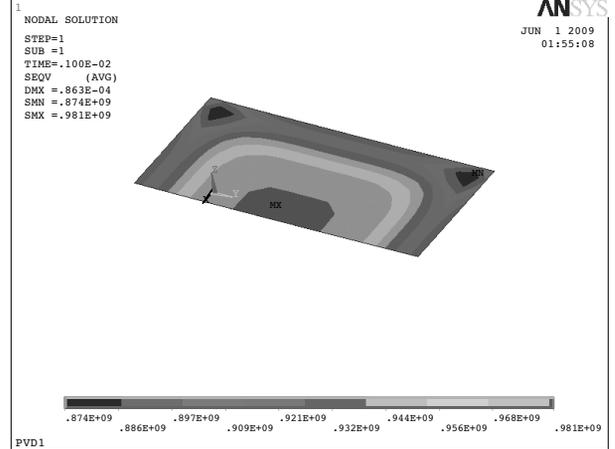


Fig. 10. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) coating (in seventh zone) [MPa]

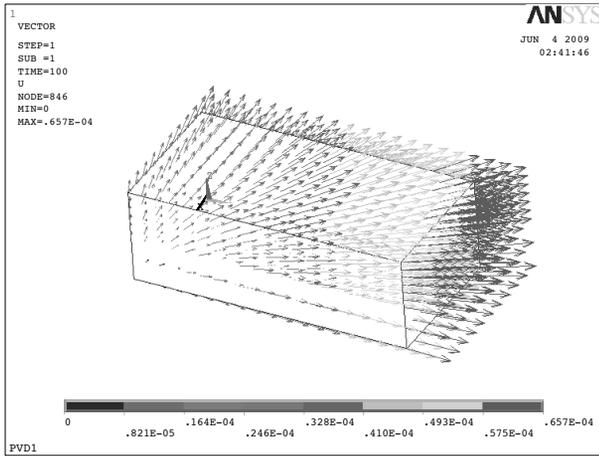


Fig. 11. Displacement of sample in 100 s

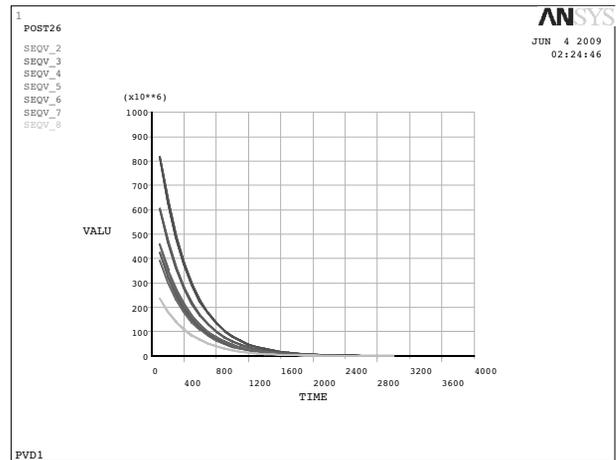


Fig. 14. Distribution of stresses in cooling function 0-3000 s for successive zones of sample cross-section

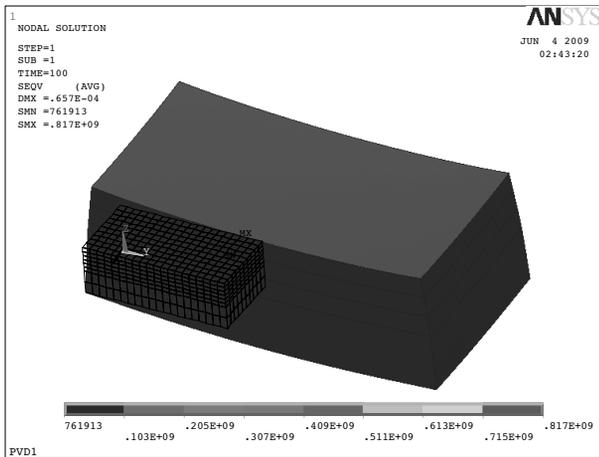


Fig. 13. Distribution of reduced stresses HMH in 100 s of cooling and also displacement of sample's elements at 300 multiplicity of magnification

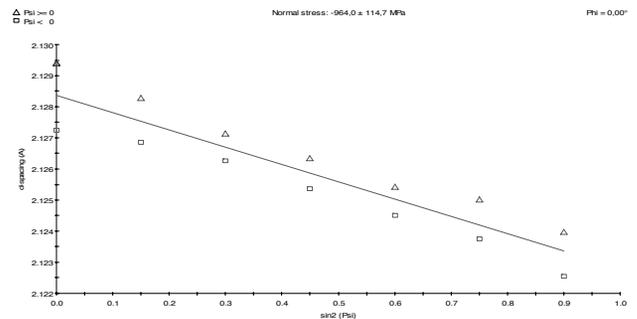


Fig. 15. Change of interplanar distance d for (200) reflection of Ti(C,N) coating in function of $\sin^2 \psi$

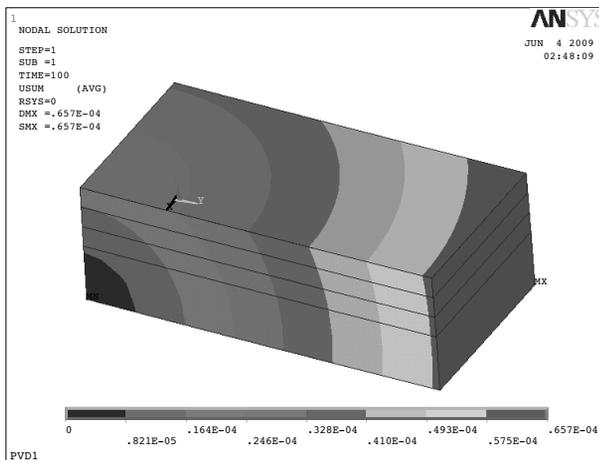


Fig. 12. Displacement of sample during analysis in time function for $t= 100$ s

4. Conclusions

New generation of the composite tool materials with the core sintered with the matrix obtained using the powder metallurgy of the chemical composition corresponding to the HS6-5-2 high-speed steel reinforced with the WC and TiC type hard carbide phases providing of high properties characteristic of cemented carbides with the high ductility characteristic of steel. It can be achieved mostly because of the possibility of ensuring the change of the chemical composition and properties by using growing portions of hard phases in the outward direction from the core to the surface. It can have an impact on fabrication costs thanks to savings made on the hard carbide phase, used in the tool surface layer only. Additional reinforcing of the surface achieved by PVD depositing of (Ti,Al)N or Ti(C,N) coating makes it possible improve the efficiency of tools made from developed materials and to widen their range of application.

Internal stresses occurred in analyzed materials 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.

Developed model of internal stresses occurred in analyzed materials meets the initial criteria, which gives ground to the assumption about its usability for determining the stresses in gradient coatings as well as in gradient substrates, employing the finite element method using the ANSYS software. It was confirmed that using of finite element method in stresses modelling occurring investigated materials can be a way for reducing the investigation costs. In order to reach this purpose, it was used in the paper a simplified model of advanced composite tool materials materials with division on zones with established physical and mechanical properties. Results reached in this way are satisfying and in slight degree differ from results reached by experimental method. However for achieving better calculation accuracy in further researches it should be developed given model which was presented in this paper.

In all tested cases it was stated occurring compress stresses characterise by little or medium value which might have positive influence on functional properties of tested materials.

The smallest span of stresses range it was found in surface zone of substrate for applied PVD coatings. It was stated that maximum value of stresses gradually ascends towards the surface of sample and reach the level over (~)800 MPa in area near to edges. Concentration of compress stresses in edges might has influence on higher microhardness of tested material contributing also to improvement of its functional properties.

Thanks to applied structure of substrates and coatings it was possible to reach minimum difference of stresses between surface of substrate and PVD coating. It contributes to higher coating adhesion with substrate of material and positively influence on functional properties of tested materials.

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