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FEM modelling of internal stresses in advanced PVD coatings

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Analysis and modelling

ABSTRACT

Purpose: The general topic of this paper is the computer simulation with use of finite element method (FEM) for determining the internal stresses of gradient and single -layer coatings (Ti,Al)N and Ti(C,N) deposited on the sintered tool materials, including cemented carbides, cermets and Al_2O_3+TiC type oxide tool ceramics by cathodic arc evaporation CAE-PVD method.
Design/methodology/approach: Internal stresses' models were performed with use of finite element method in ANSYS environment. The experimental values of stresses were were calculated using the X-ray sin2ψ technique. The computer simulation results were compared with the experimental results. Microhardness and adhesion as well as wear range were measured to investigate the influence of stress distribution on the mechanical and functional properties of coatings.
Findings: A more advantageous distribution of stresses in gradient coatings than in respective single-layer coatings yields better mechanical properties, and, in particular, the distribution of stresses on the coating surface has the influence on microhardness, and the distribution of stresses in the contact area between the coating and substrate has the influence on the adhesion of coatings.
Practical implications: Deposition of hard, thin, gradient coatings on materials surface by PVD method features one of the most intensely developed directions of improvement of the working properties of materials. Presently 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.
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. Influence of gradient structure of coatings on the mechanical and functional properties were investigated with use of finite element method.
Keywords: PVD coatings; Gradient coatings; Internal stresses

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1. Introduction

The finite element method is currently commonly used in such branches of science, like: mechanics, biomechanics, mechatronics, materials engineering, and thermodynamics [1-8]. All types of simulations shorten the design process and give the possibility to investigate the particular factors on the entire model. 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 Applying of this method contains many fields of contemporary industry and also modern technologies are supported by using of computers [1,4,18,20,22,23]. 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 [20].

Gradient PVD coatings can be deposited onto cutting tools made as well from the high speed steels, cemented carbides, cermets, and also from ceramic materials. In the development of new, contemporary materials the functionality is often improved by combining materials of different properties into composites [9-12,14].

In combination with the rapid development of new coating technologies, this has led to an accelerating increase in the use of coated components. Physical vapor deposited TiN coatings are widely used for machining of a wide variety of materials. Coatings based on (Ti,Al)N as well as Ti(C,N) were developed to provide better performance over titanium nitride since the incorporation of aluminum or carbon in TiN increased hardness, decreased coefficient of friction of the coatings [13-16]. Among wide range of PVD methods cathodic arc vapor deposition is widely used due to their ability to provide a dense and adherent thin coating at a relatively low temperature [17-19,21].

The general topic of this paper is the computer simulation with the use of finite element method (FEM) for determining the internal stresses of gradient and single -layer coatings (Ti,Al)N and Ti(C,N) deposited on the sintered tool materials, including cemented carbides, cermets and Al_2O_3+TiC type oxide tool ceramics by cathodic arc evaporation CAE-PVD method.

2. Methodology of research

The work presents the application of the finite elements method for the analysis of the distribution of internal stresses in the coatings obtained in the PVD process, as dependent on the parameters of the process and the material of the substrate and coating.

The model whereof objective is to determine the internal stresses in gradient and single-layer coatings (Ti,Al)N and Ti(C,N) on the substrate from cemented carbides, cermets and oxide tool ceramics, was elaborated using the finite elements method, assuming true dimensions of the specimen. The geometry of the insert with the deposited gradient and single-layer coatings as well as the calculations were carried out using the program ANSYS 12.0. On account of the predicted simulation range, parametric calculation files were elaborated which allowed to perform the analysis in a comprehensive way. We employed the experience involving computer simulation works in material engineering carried out for many years at the Division of Materials Processing Technology, Management and Computer Techniques in Materials Science of the Institute of Engineering Materials and Biomaterials of the Silesian University of Technology [11,14,16,20,22-26]. The geometrical model was subjected to discretization with the element of the PLANE 42 type for substrate material and external coating. The element of that type is applied for the modeling of spatial structures with the use of a flat (2-D) element of solids. It can be also applied for the modeling of the structures described by means of axial symmetry. It is a simpler and faster method, by the application of which we can avoid many errors which could have occurred when applying the network on spatial solids. This type of description generates radically smaller MES models as compared to the full 3D description, maintaining the understanding of the general description. The element of PLANE 42 type is defined by four basic nodes and can demonstrate such features as plasticity, creep, swelling, and it also enables the modeling of high bending and tension of the modeled objects. The true model was subjected to discretization, which is presented in Fig. 1. The calculation model consists of 12816 nodes and 11780 elements. In order to avoid errors in the calculation of internal stresses in the coatings, we applied variable quantities of finite elements. In the places where higher gradients of stresses were expected, the network is more condensed than in the areas where the stresses were expected to have values similar to one another. Therefore, in the coatings we applied smaller elements which better reflect the gradients of stresses, and in the substrate material the elements are increasing with the rise of the distance from the coatings. Figures 2 and 3 presents the real model of gradient and single- layer coatings.

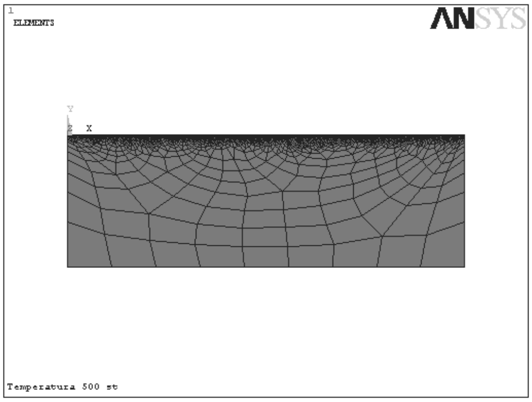

Fig. 1. True model subjected to discretization with deposited gradient and single-layer (Ti,Al)N and Ti(C,N) on different substrates

Since it was necessary to calculate internal stresses in the material of the chemical composition which was changing in the way perpendicular to the surface, the ideographic differentiation of the modeled gradient coatings was carried out into zones corresponding to the areas of similar chemical composition. The model with the spherical division of gradient coating was elaborated in the way ensuring that it was possible to determine the averaged internal stresses in the coating areas important in view of the applicability properties and to compare the obtained results with the calculations carried out for homogeneous coatings.

The following boundary conditions were accepted to simulate the eigen-stresses in the gradient single-layer coatings (Ti,Al)N and Ti(C,N) on different substrates:

- the temperature change of the PVD process is reflected by cooling the specimen from 500°C to the ambient temperature of 20°C,

- for the coatings (Ti,Al)N for the substrate from cemented carbides, cermets and oxide tool ceramics, the material properties were accepted basing on literature data [6] and MatWeb catalogue. The discrepancies in literature data involving the values of physical properties of particular materials result from different acquisition methods, from the differences in the structure and composition of the materials and from errors in the applied measurement method,

the substrate of the investigated specimen is immobilized due to depriving all nodes lying on this axis of all degrees of freedom.

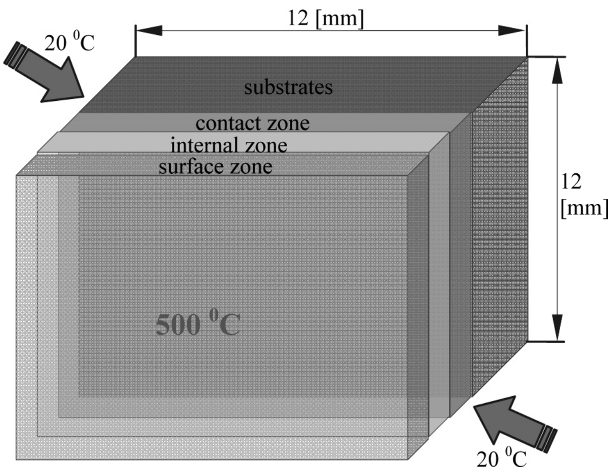

Fig. 2. Real model of gradient coatings

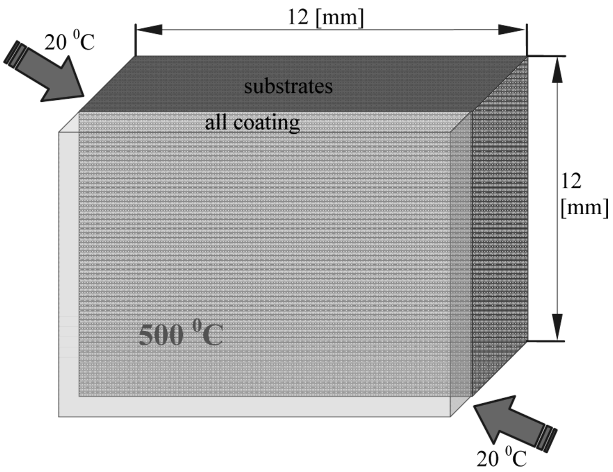

Fig. 3. Real model of single-layer coatings

With the temperature drop, from the coating deposition temperature (500°C) to the ambient temperature (20°C), internal stresses are generated both in the coating and in the substrate material, connected principally with different thermal expansion of particular materials. The distribution of these stresses is also connected with the geometry of the specimen and with thermal transfer during the cooling process. In effect of non-uniform cooling of the specimen material in the particular areas, the distribution of stresses on the coating surface and their concentration in the corners of the specimen is different.

To verify the results of computer simulation, the values of internal stresses in the investigated single-layer and gradient coatings were calculated using the X-ray $\sin^2\psi$ technique.

3. Results

The deposition of single-layer and gradient coatings resistant to wear of the type (Ti,Al)N and Ti(C,N) on the investigated sintered tool materials results in the rise of roughness parameter R_a which is within the range from 0.11-0.27 µm, and is higher than in the case of material surfaces without coatings (Table 1).

The deposited PVD coatings are characterized by good adhesion to the substrate within the range L_c=40-65 N. In general, the deposition of wear resistant gradient coatings of the type (Ti,Al)N and Ti(C,N) on the investigated sintered tool materials results in a considerable rise of microhardness in the area around the surface, which, combined with the good adhesion of the coating to the substrate obtained in effect of the application of gradient structure of the coating, yields good functionality properties of these materials, confirmed during machining tests (Table 1).

The hardness of the substrate material (Table 1) is 1755 HV for cemented carbides, 1850 HV for cermet and 2105 HV for oxide ceramics. The deposition of the coatings (Ti,Al)N and Ti(C,N) on the investigated sintered tool materials results in a considerable rise of microhardness in the area around the surface within the range of 2600-3200 HV. It was demonstrated that the gradient coatings have higher hardness than the single-layer coatings, independent of the substrate material.

In case of single-layer (Ti,Al)N coatings deposited on cemented carbides, cermets and on sintered oxide ceramic substrates, the occurrence of compressive stresses with average absolute value (σ=170-410 MPa was stated (Table 4, Figs. 4, 6, 8).

As the result of performed simulation it was observed, that for all used types of substrates, the replacement of single layer (Ti,Al)N coatings by gradient (Ti,Al)N coating, takes effect on significant reduction of absolute value of stresses in the contact zone (Tables 3, 4, Figs. 4-9).

Reduction of internal stresses' absolute values in the contact zone of the gradient coatings with the substrate takes profitably effects on improvement of coatings adhesion. Too high compressive stresses' value can be a reason of too high tensile stresses ocurring under the coating reducing fatigue resistance of the element [3,8,20]. Increase of gradient coatings adhesion in comparison with adhesion of single-layer coatings was confirmed as a result of "scratch tests" done and may be one of main factors making influence on much better wear resistance results obtained during machining tests in comparison to single-layer coatings. (Table 1).

Table 1.
Characteristics of the investigated materials

Substrate	Coating	Coating thickness, μm	Roughness, R_a, μm	Microhardness, HV	Critical Load, L_c, N	Tool life t, min
Cemented carbide*	uncoated	-	0.13	1755	-	2.5
	(Ti,Al)N	2.2	0.14	2750	52	20.0
	gradient (Ti,Al)N	2.6	0.14	3000	56	25.5
	Ti(C,N)	1.5	0.13	2600	44	5.0
	gradient Ti(C,N)	2.7	0.11	2850	64	5.0
Cermet**	uncoated	-	0.06	1850	-	2.5
	(Ti,Al)N	1.5	0.13	2900	54	19.5
	gradient (Ti,Al)N	3.0	0.12	3150	63	22.0
	Ti(C,N)	1.5	0.12	2950	42	8.0
	gradient Ti(C,N)	2.6	0.11	2950	60	9.5
Al_2O_3+TiC***	uncoated	-	0.10	2105	-	12.5
	(Ti,Al)N	1.6	0.27	3170	53	21
	gradient (Ti,Al)N	3.2	0.24	3200	65	40
	Ti(C,N)	1.3	0.23	2850	40	15
	gradient Ti(C,N)	2.1	0.21	2950	55	19

* phase composition: WC, TiC, TaC, Co,
** phase composition: TiCN, WC, TiC, TaC, Co, Ni,
*** phase composition: Al_2O_3, TiC.

Table 2.
Properties of individual materials

Coating / Substrate	Coating zone	Physical properties		
		Young's modulus, [GPa]	Thermal expansion coefficient, $[10^{-6} \cdot K^{-1}]$	Poisson ratio
(Ti,Al)N gradient	Surface zone	420	6.1	0.23
	Internal zone	480	7.1	0.21
	Contact zone	510	8.5	0.26
(Ti,Al)N	-	480	7.1	0.21
Cemented carbides	-	500	7.9	0.22
Cermet	-	450	9.0	0.22
Al_2O_3+TiC	-	400	8.0	0.21

Table 3.
Results of computer simulation of internal stresses in the analysed gradient PVD coatings

Substrate	Coating	Computer simulation results of internal stress, [MPa]		
		Surface layer	Middle layer	Contact area
Cemented carbide	(Ti,Al)N	-350	-220	130
	Ti(C,N)	-150	160	280
Cermet	(Ti,Al)N	-570	-350	-100
	Ti(C,N)	-300	-50	50
Al_2O_3+TiC	(Ti,Al)N	-380	-250	100
	Ti(C,N)	-170	120	240

Table 4.
Results of computer simulation of internal stresses in the analysed single-layer PVD coatings

Substrate	Coating	Computer simulation results of internal stress, [MPa]
Cemented carbide	(Ti,Al)N	170
	Ti(C,N)	150
Cermet	(Ti,Al)N	-410
	Ti(C,N)	15
Al_2O_3+TiC	(Ti,Al)N	-180
	Ti(C,N)	150

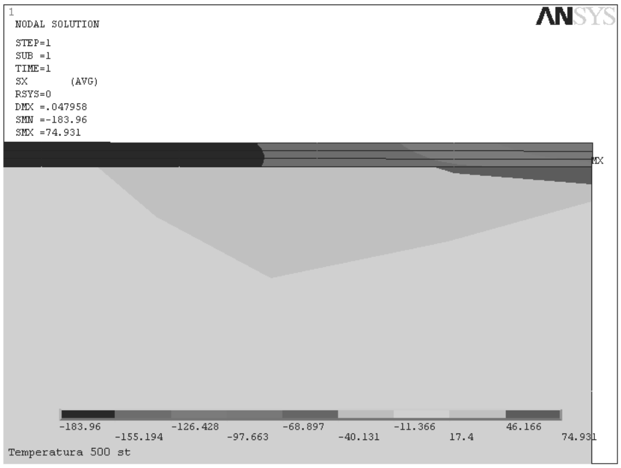

Fig. 4. Distribution of the simulated compression stresses in the single-layer (Ti,Al)N coating deposited on to cemented carbide substrate

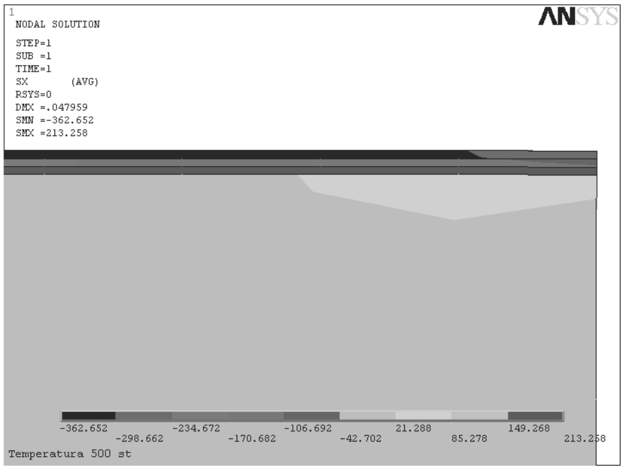

Fig. 5. Distribution of the simulated compression stresses in the gradient (Ti,Al)N coating deposited on to cemented carbides substrate

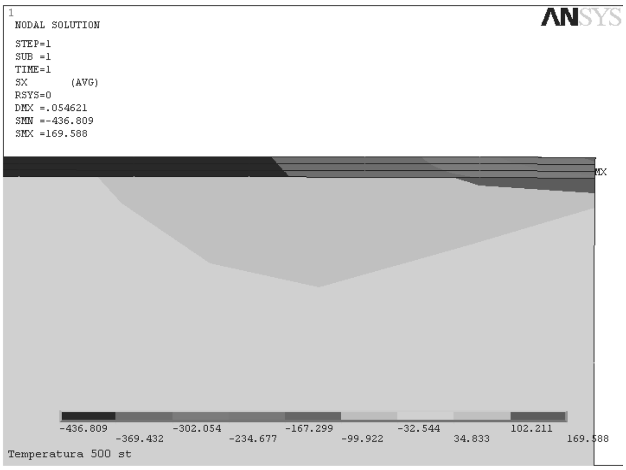

Fig. 6. Distribution of the simulated compression stresses in the single-layer (Ti,Al)N coating deposited on to cermet substrate

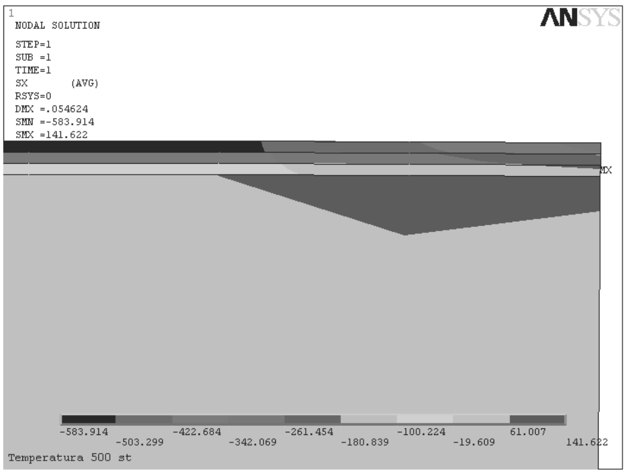

Fig. 7. Distribution of the simulated compression stresses in the gradient (Ti,Al)N coating deposited on to cermet substrate

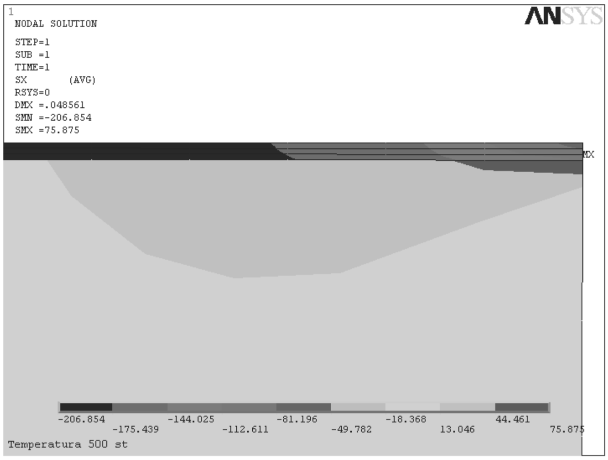

Fig. 8. Distribution of the simulated compression stresses in the single-layer (Ti,Al)N coating deposited on to Al_2O_3+TiC type oxide tool ceramics substrate

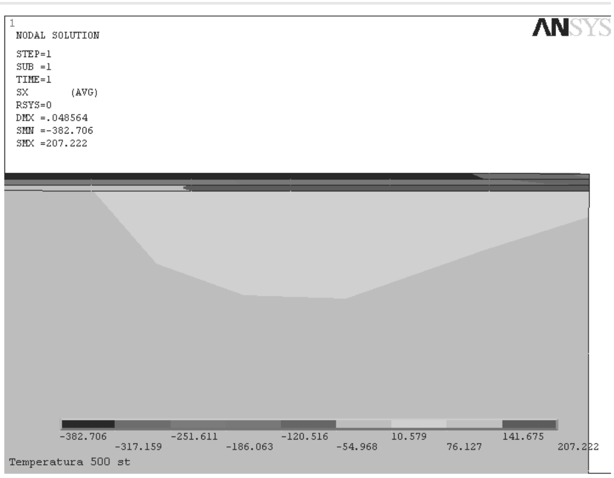

Fig. 9. Distribution of the simulated compression stresses in the gradient (Ti,Al)N coating deposited on to Al_2O_3+TiC type oxide tool ceramics substrate

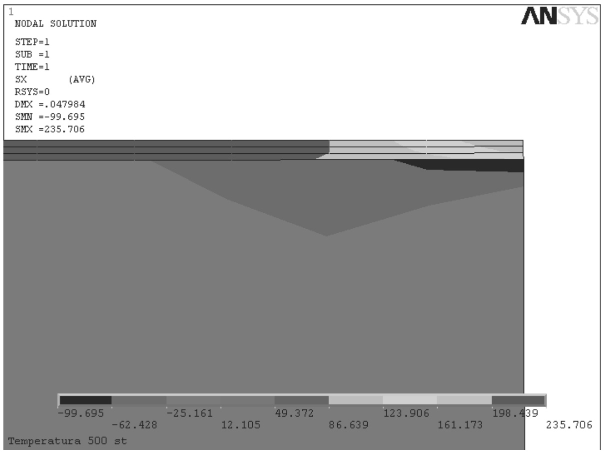

Fig. 10. Distribution of the simulated compression stresses in the single-layer Ti(C,N) coating deposited on to cemented carbide substrate

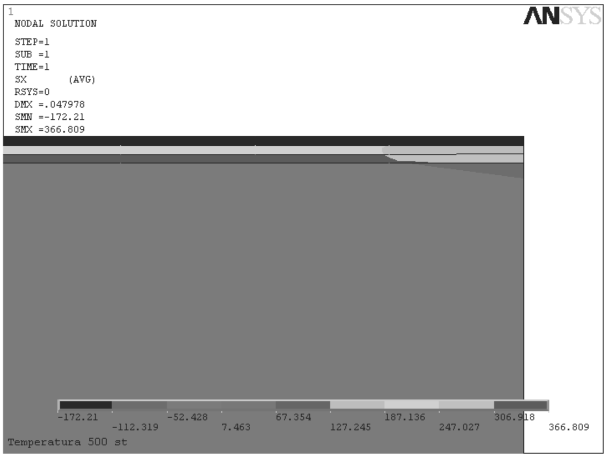

Fig. 11. Distribution of the simulated compression stresses in the gradient Ti(C,N) coating deposited on to cemented carbides substrate

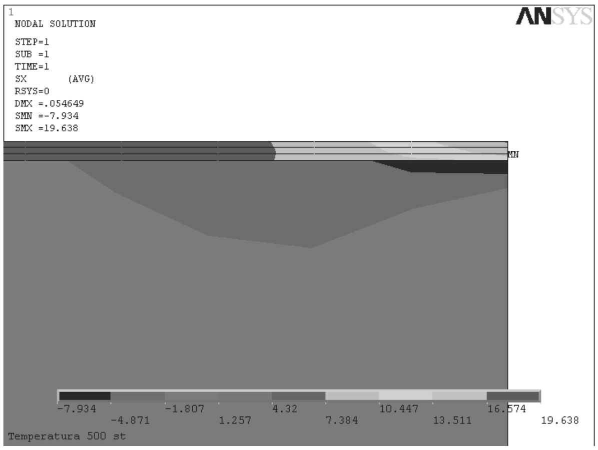

Fig. 12. Distribution of the simulated compression stresses in the single-layer Ti(C,N) coating deposited on to cermet substrate

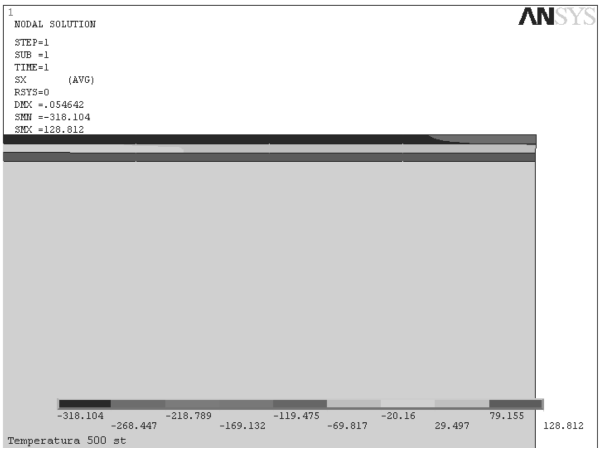

Fig. 13. Distribution of the simulated compression stresses in the gradient Ti(C,N) coating deposited on to cermet substrate

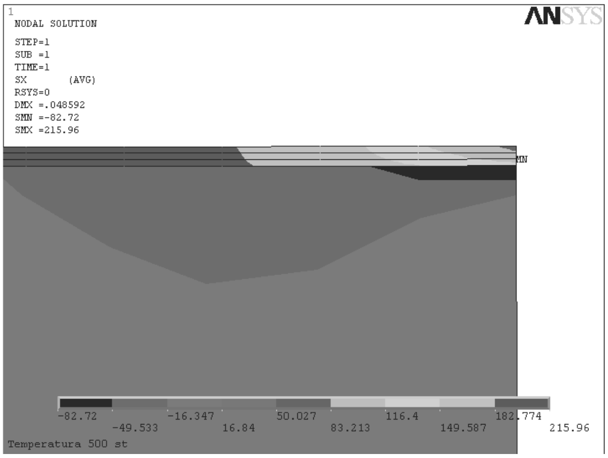

Fig. 14. Distribution of the simulated compression stresses in the single-layer Ti(C,N) coating deposited on to Al_2O_3+TiC type oxide tool ceramics substrate

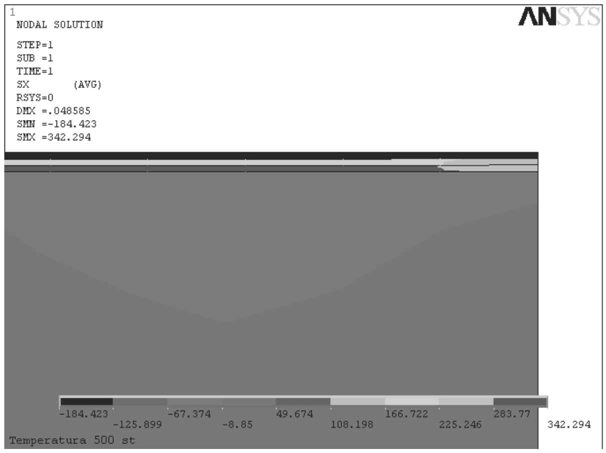

Fig. 15. Distribution of the simulated compression stresses in the gradient Ti(C,N) coating deposited on to Al_2O_3+TiC type oxide tool ceramics substrate

It was found that thanks to use of gradient coating in all examined substrates, compressive stresses in surface layer of coating were obtained. Moreover, increase of compressive stress' values on the surface of gradient coatings in comparison to single-layer coatings was observed (Table 3, 4, Figs. 5, 7, 9). Occurrence of 350-570 MPa values of compressive stresses, on the surface of gradient coatings has advantageous influence on their mechanical properties, especially on microhardness what was confirmed as a result of microhardness measurements (Fig. 16-18).

In the case of Ti(C,N) coatings we can observe the rise of tensile stresses in the contact area after the replacement of the single-layer coating with the gradient one (Tables 3,4, Figs. 11-15). In spite of this, higher adhesion has been demonstrated in the case of gradient Ti(C,N) coatings than in the case of respective single-layer coatings. It can be connected with the character of surface topography and the size of coating grains with respect to the roughness of the substrate (Table 1), which, combined with the presence of tensile stresses, can result within certain limits in the positive influence of such stresses on the adhesion due to anchoring of the coating in a relevantly developed surface of the substrate [28].

Due to the application of gradient coatings on all investigated substrate materials, we obtained compressive stresses in the surface layer of the coating having a direct contact with the machined material during the operation process (Table 3). In the case of Ti(C,N) coatings we can observe the change in the character of stresses on the coating surface from tensile stresses, occurring on the surface of single-layer coatings, to compressive stresses occurring on the surface of gradient coatings (Tables 3, 4, Figs. 11-15). The generation of compressive stresses in the surface layer brings about better resistance to cracking, and through the rise of hardness, improves the resistance to wear. The generation of compressive stresses in the surface layer (Figs. 19-21) can prevent the formation of cracks when the element in the operational conditions is subjected to stresses generated by external forces. Yet, an excessive value of compressive stresses can lead to adhesive wear and can bring about the formation of too high tensile stresses under the coating, lowering the fatigue resistance of the element [1,3,6,20]. Volvoda [21] pointed out the relation between the value of stresses and the hardness of the layer of titanium nitrides obtained in effect of magnetron sputtering, demonstrating that with the rise of compressive stresses the hardness of the obtained layer is progressively increasing. Basing on the carried out research, it was demonstrated that the occurrence of compressive stresses on the surface of gradient coatings of the investigated materials has a positive influence on their mechanical properties, in particular on the microhardness (Table 1).

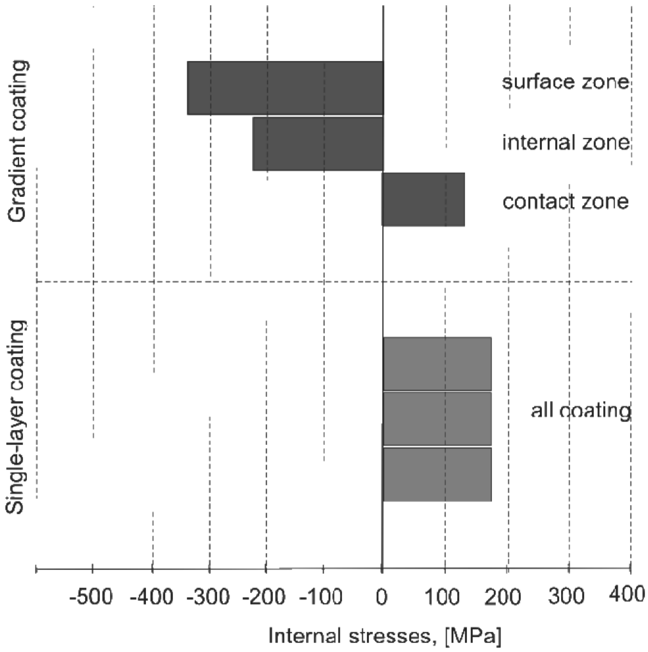

Fig. 16. Schematic distribution of stresses in the (Ti,Al)N coatings deposited on cemented carbides obtained by computer simulation

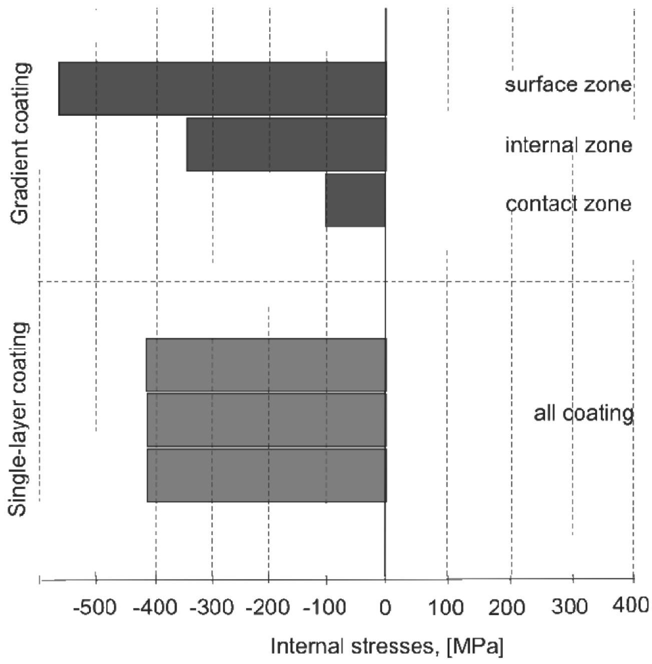

Fig. 17. Schematic distribution of stresses in the (Ti,Al)N coatings deposited on cermet substrates obtained by computer simulation

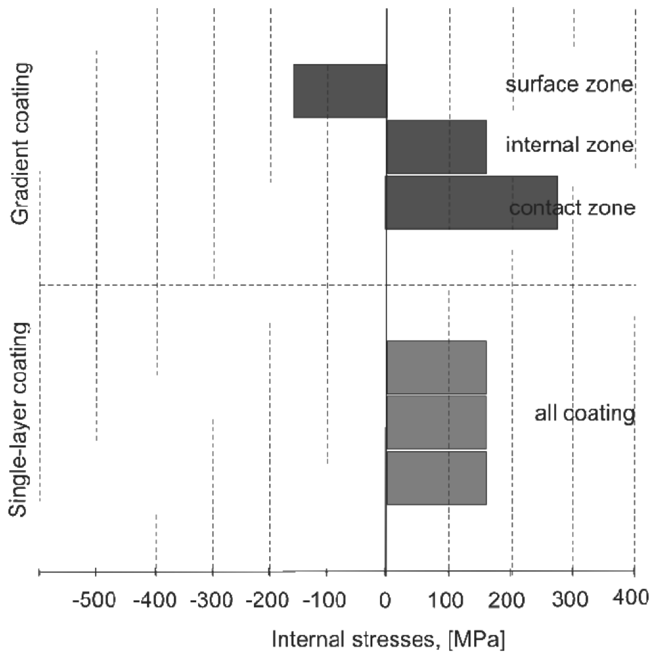

Fig. 19. Schematic distribution of stresses in the Ti(C,N) coatings deposited on cemented carbides obtained by computer simulation

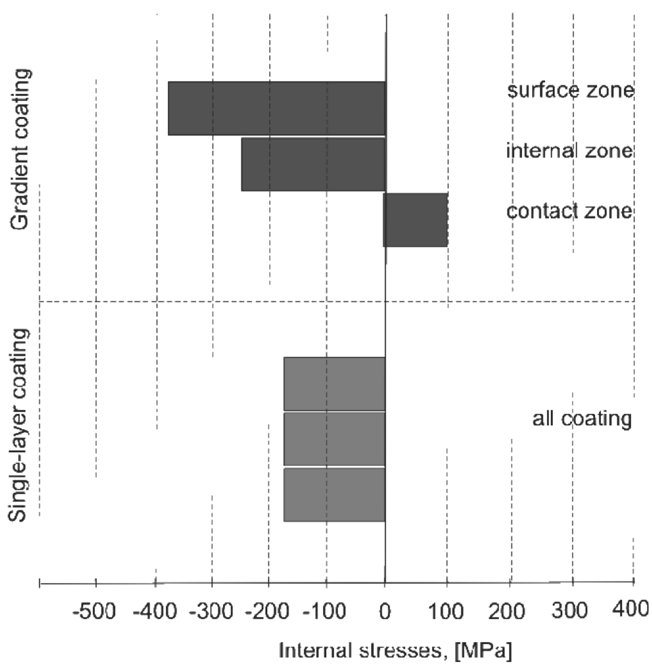

Fig. 18. Schematic distribution of stresses in the (Ti,Al)N coatings deposited on Al_2O_3+TiC type oxide tool ceramics substrate obtained by computer simulation

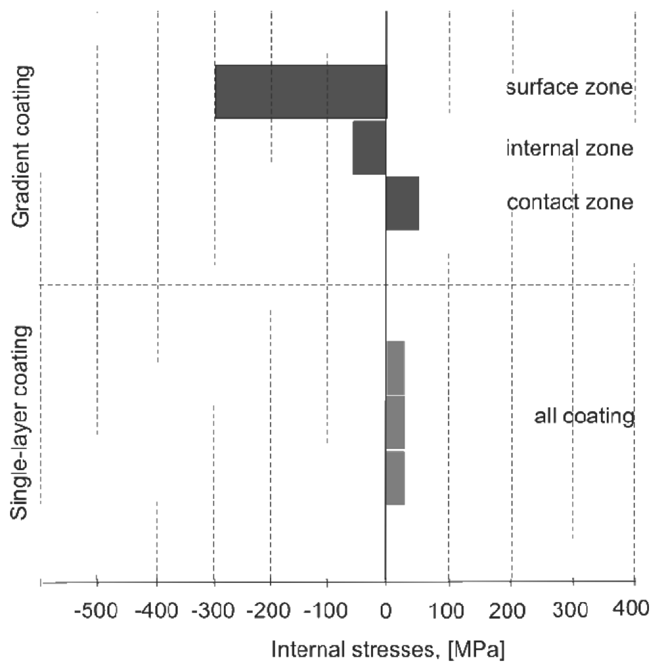

Fig. 20. Schematic distribution of stresses in the Ti(C,N) coatings deposited on cermet substrates obtained by computer simulation

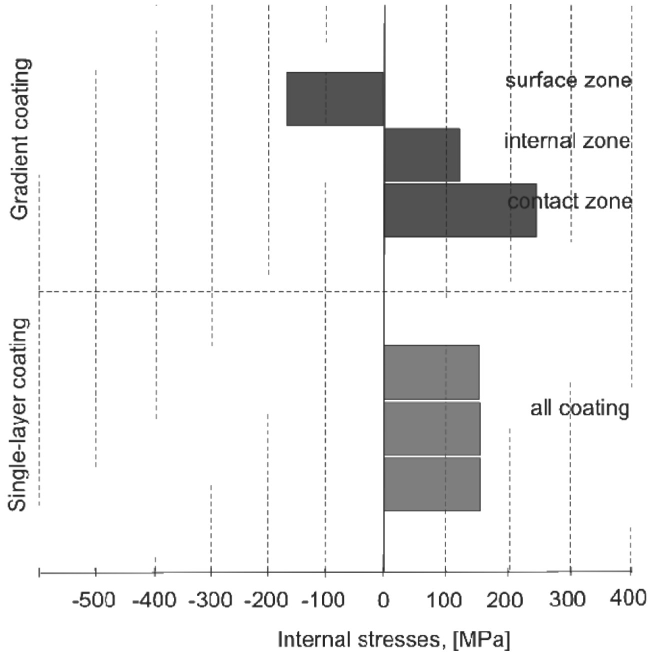

Fig. 21. Schematic distribution of stresses in the Ti(C,N) coatings deposited on Al_2O_3+TiC type oxide tool ceramics substrate obtained by computer simulation

To verify the results of computer simulation, the values of eigen-stresses in the investigated single-layer and gradient coatings were calculated using the X-ray $\sin^2\psi$ technique (Table 5).

4. Conclusions

The results of the computer simulation with the use of finite element method (FEM) for determining the internal stresses of gradient and single-layer coatings (Ti,Al)N and Ti(C,N) deposited on the sintered tool materials, including cemented carbides, cermets and Al_2O_3+TiC type oxide tool ceramics by cathodic arc evaporation CAE-PVD method are given in the paper.

Many aspects pertaining to forming of coatings, including also the process conditions effect on their properties, still remain inexplicable in spite of the enormous interest paid in them by many industrial centres and research laboratories.

Developing an appropriate model allows the prediction of properties of PVD coatings, which are also the criterion of their selection for specific items, based on the parameters of technological processes. In addition, developed model can to a large extent eliminate the need for expensive and time-consuming experimental studies for the computer simulation.

In the case of Ti(C,N) coatings we can observe the rise of tensile stresses in the contact area after the replacement of the single-layer coating with the gradient one. In spite of this, higher adhesion has been demonstrated in the case of gradient Ti(C,N) coatings than in the case of respective single-layer coatings. It can be connected with the character of surface topography and the size of coating grains with respect to the roughness of the substrate, which, combined with the presence of tensile stresses, can result within certain limits in the positive influence of such stresses on the adhesion due to anchoring of the coating in a relevantly developed surface of the substrate.

A more advantageous distribution of stresses in gradient coatings than in respective single-layer coatings yields better mechanical properties, and, in particular, the distribution of stresses on the coating surface has the influence on microhardness, and the distribution of stresses in the contact area between the coating and substrate has the influence on the adhesion of coatings.

Table 5.
Results of experimental internal stresses using the X-ray $\sin^2\psi$ technique of the analysed PVD coatings

Substate	Coating	Internal stresses σ [MPa]
Cemented carbide	(Ti,Al)N	212±42
	(Ti,Al)N gradient	-395±45
	Ti(C,N)	-
	Ti(C,N) gradient	-
Cermet	(Ti,Al)N	-459±49
	(Ti,Al)N gradient	-647±77
	Ti(C,N)	-
	Ti(C,N) gradient	-
Al_2O_3+TiC	(Ti,Al)N	-228±48
	(Ti,Al)N gradient	-456±76
	Ti(C,N)	122±52
	Ti(C,N) gradient	-235±65

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