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# FEM modelling of internal stresses in PVD coated FGM

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**Analysis and modelling**

## ABSTRACT

**Purpose:** The general topic of this paper is problem of determining the internal stresses of composite gradient 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) gradient coatings.

**Design/methodology/approach:** Modelling of stresses was performed with the help of finite element method in PATRAN 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:** 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 PATRAN software. The computer simulation results correlate with the experimental results.

**Research limitations/implications:** It was confirmed that using of finite element method in stresses modelling occurring in gradient- structured 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 gradient- structured 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.

**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; FGM

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## 1. Introduction

Recent development of the gradient tool materials pertains mostly to the cobalt matrix sintered carbides. Low amount of information in literature on gradient materials fabricated basing on high-speed steels is caused with the complexity of problems that occur in the sintering and heat treatment processes, and with refraining from this research in favour of the sintered carbides mentioned above. Employing the high-speed steel as the gradient materials matrix yields, however, the possibility to control the matrix properties with heat treatment. Development of a new generation of the composite gradient 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 gradients of the chemical composition and properties, cutting simultaneously fabrication costs thanks to savings made on the hard carbide phase, used in the tool surface layer only [1,2].

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. Coating composites like (Ti,Al)N are designed to specifically get better properties such as tribological, electrical, optical, electronic, chemical and magnetic [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 " Patran" of „MSC.Software" company. The models with given boundary conditions were created in Patran programme however the calculations were done in one of integrated calculation modulus called "Nastran" (Figs. 1, 2).

Analysis were 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 2 and 3.

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 Patran software.

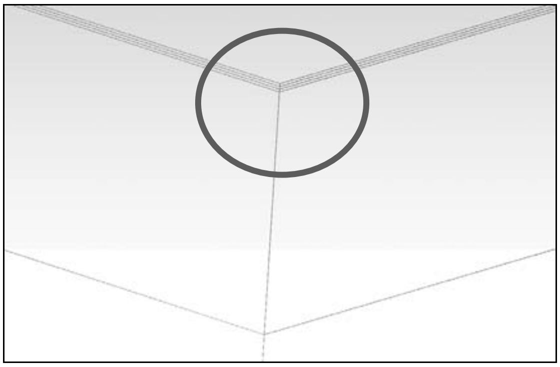

Fig. 1. Real model with noticeable zones

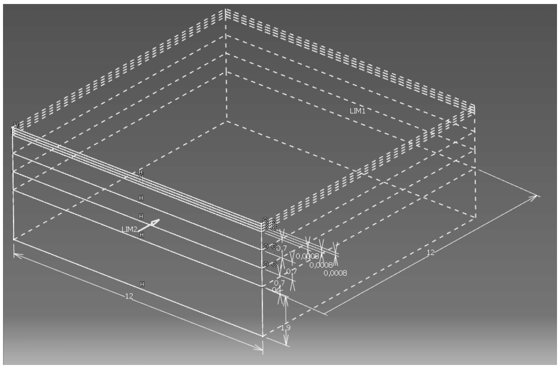

Fig. 2. Dimensioning model in SD section

Table 1.
Arrangement of individual zones in models

| | 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 7 (0.8µm) | TiC | (0.3 Ti, 0.7 Al)N | TiC | (0.3 Ti, 0.7 Al)N |
| Zone 6 (0.8µm) | Ti(C,N) | (0.7 Ti, 0.3 Al)N | Ti(C,N) | (0.7 Ti, 0.3 Al)N |
| Zone 5 (0.8µm) | TiN | TiN | TiN | TiN |
| Zone 4 (0.7mm) | HS 6-5-2 + 12%WC | HS 6-5-2 + 12%WC | HS 6-5-2 + 12%TiC | HS 6-5-2 + 12%TiC |
| Zone 3 (0.7mm) | HS 6-5-2 + 8%WC | HS 6-5-2 + 8%WC | HS 6-5-2 + 8%TiC | HS 6-5-2 + 8%TiC |
| Zone 2 (0.7mm) | HS 6-5-2 + 4%WC | HS 6-5-2 + 4%WC | HS 6-5-2 + 4%TiC | HS 6-5-2 + 4%TiC |
| Zone 1 (1.9mm) | HS 6-5-2 | HS 6-5-2 | HS 6-5-2 | HS 6-5-2 |

Table 2.
Material's data of individual models

| | MODEL 1 HS+WC/Ti(C,N) | MODEL 2 HS+WC/(Ti,Al)N | MODEL 3 HS+TiC/Ti(C,N) | MODEL 4 HS+TiC/(Ti,Al)N |
|---|---|---|---|---|
| $\lambda_x$ [W/m*K] | 36.316 | 36.273 | 34.018 | 33.981 |
| $\lambda_y$ [W/m*K] | 37.108 | 37.103 | 34.581 | 34.576 |
| $\rho$ [kg/m$^3$] | 7752.179 | 7756.032 | 7395.515 | 7399.368 |
| c [J/kg*K] | 656.654 | 657.018 | 657.45 | 657.605 |

Table 3.
Properties of individual layers

| | Poisson ratio | Young's modulus [MPa] | Thermal expansion coefficient [1/K] $10^{-6}$ |
|---|---|---|---|
| TiN | 0.26 | 510 | 9.5 |
| Ti(C,N) | 0.24 | 410 | 9.4 |
| TiC | 0.19 | 390 | 7.8 |
| (0.7 Ti, 0.3 Al)N | 0.23 | 420 | 7.9 |
| (0.3 Ti, 0.7 Al)N | 0.27 | 480 | 8.3 |
| HS 6-5-2 | 0.30 | 215 | 11.5 |
| HS 6-5-2 + 4%WC | 0.30 | 195 | 11.3 |
| HS 6-5-2 + 8%WC | 0.30 | 183 | 10.9 |
| HS 6-5-2 + 12%WC | 0.31 | 172 | 10.5 |
| HS 6-5-2 + 4%TiC | 0.30 | 225 | 11.2 |
| HS 6-5-2 + 8%TiC | 0.30 | 233 | 10.7 |
| HS 6-5-2 + 12%TiC | 0.29 | 241 | 10.1 |

Table 4.
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 7 (0.8µm) | (-) 316-821 | (-) 340-820 | (-) 320-815 | (-) 300-869 |
| Zone 6 (0.8µm) | (-) 220-660 | (-) 220-750 | (-) 210-660 | (-) 270-839 |
| Zone 5 (0.8µm) | (-) 100-540 | (-) 260-700 | (-) 100-550 | (-) 100-654 |
| Zone 4 (0.7mm) | (-) 100-368 | (-) 100-363 | (-) 100-368 | (-) 100-334 |
| Zone 3 (0.7mm) | (-) 100-473 | (-) 100-470 | (-) 100-460 | (-) 100-400 |
| Zone 2 (0.7mm) | (-) 150-752 | (-) 100-620 | (-) 100-680 | (-) 100-750 |
| Zone 1 (1.9mm) | (-) 230-998 | (-) 150-998 | (-) 180-950 | (-) 190-1000 |

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 $2\theta$ 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 $\psi$ of samples towards primary beam was changed in range 0° - 70°

## 3. Investigations results

Using experimental results and assumpted datas given in Table 4 internal stresses were modelled using PATRAN 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 x-ray diffraction pattern on the basis of which were calculated internal stresses in the coatings, interlayers and in substrate materials. Example of stresses measurements in investigated gradient PVD coatings obtained with use of $sin^2\psi$ method on X'Pert Stress software on the basis of XRD results is presented in Fig. 12.

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 4 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 differ insignificantly 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), on the flank face the stresses show medium value, while edges of the zone are characterized by little stresses values.

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. 6).

The maximum stresses value ascends while changing of analyzed zone towards the surface of the sample (Zone 5-7) (Figures 7-9) and reach the level over 800 MPa in Zone 7, in area near to edges (Fig. 9). 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.

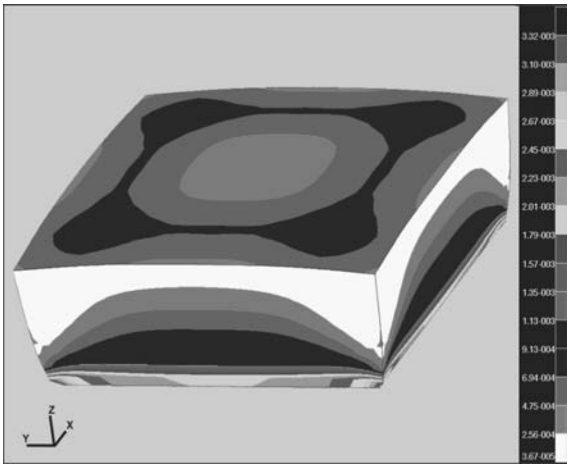

Fig. 3. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) gradient coating. [TPa]

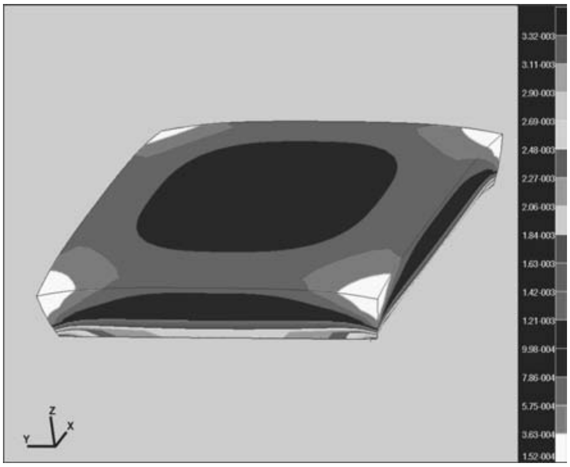

Fig. 4. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) gradient coating (Zone 1) [TPa]

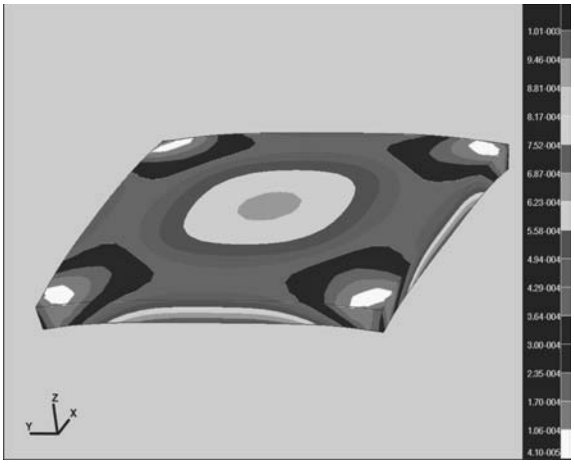

Fig. 5. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) gradient coating (Zone 2) [TPa]

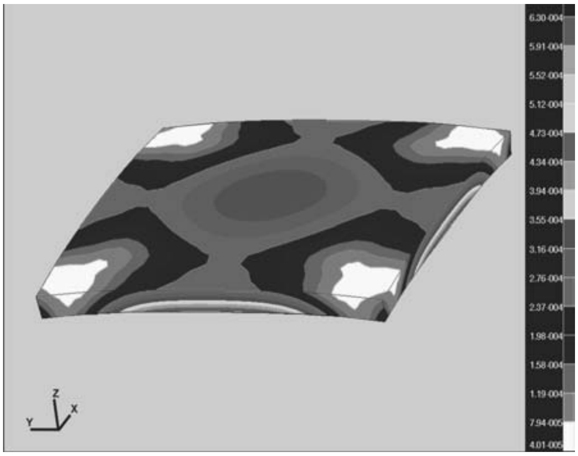

Fig. 6. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) gradient coating (Zone 3) [TPa]

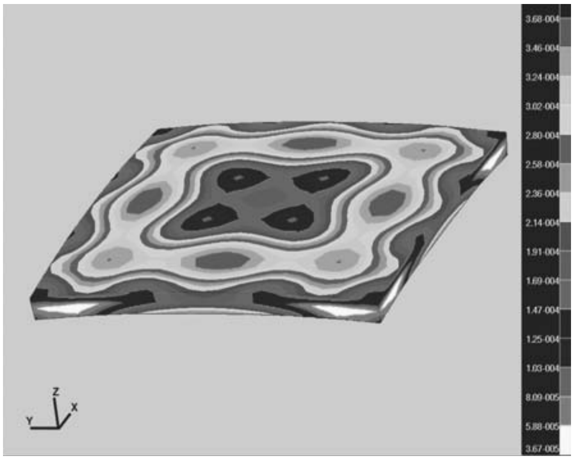

Fig. 7. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) gradient coating (Zone 4) [TPa]

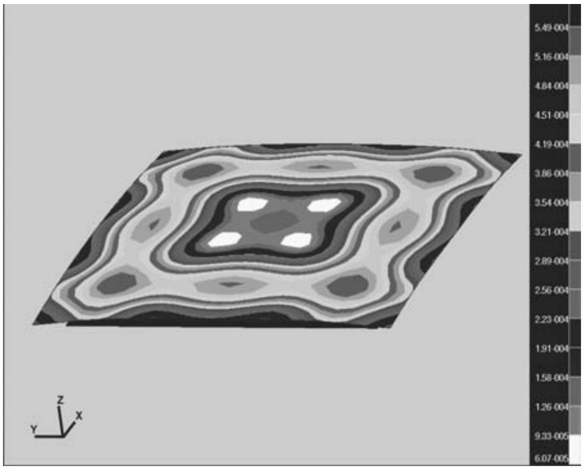

Fig. 8. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) gradient coating (Zone 5) [TPa]

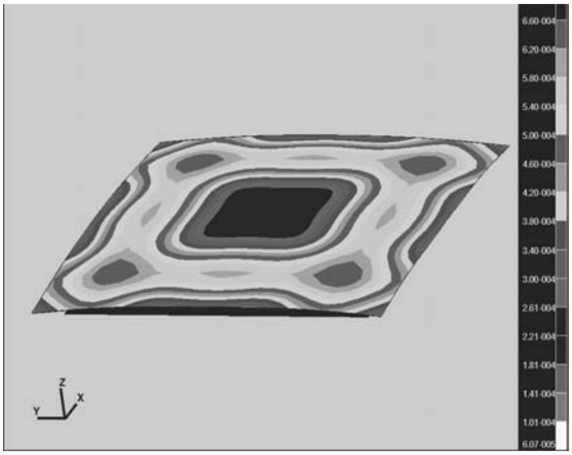

Fig. 9. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) gradient coating (Zone 6) [TPa]

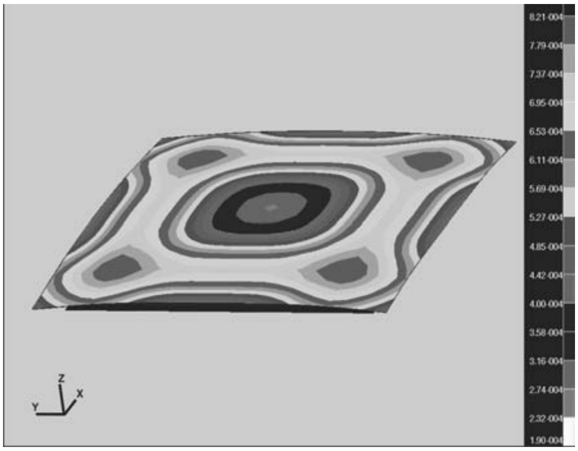

Fig. 10. Distribution of the simulated compression stresses in the HS+TiC/Ti(C,N) gradient coating (Zone 7) [TPa]

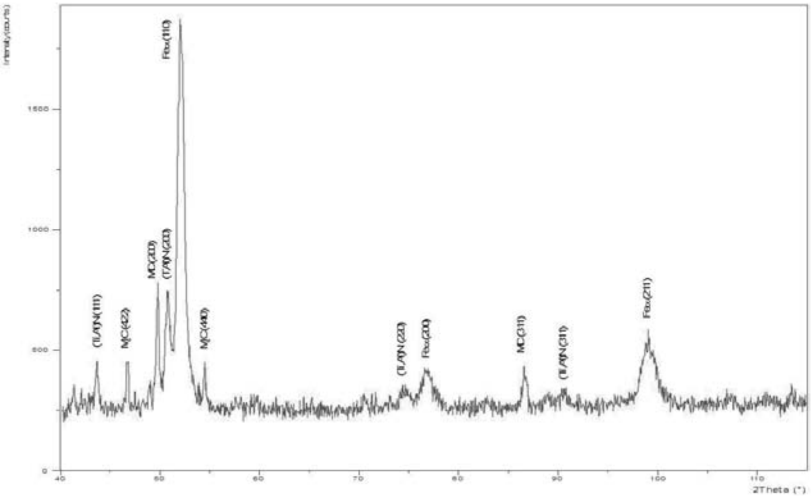

Fig. 11. Diffraction patterns of the HS+TiC/(Ti,Al)N variant of PVD coated high-speed steel matrix composite

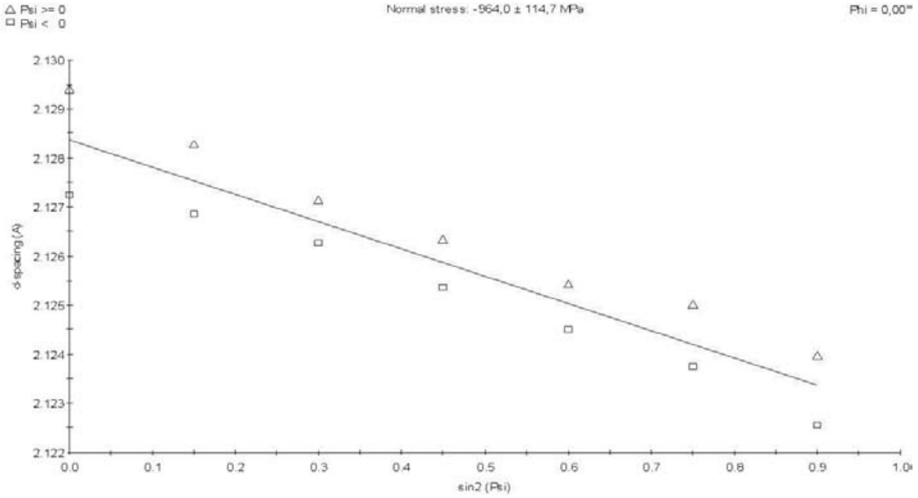

Fig. 12. Change of interplanar distance *d* for (200) reflection of Ti(C,N) coating in function of $\sin^2 \psi$

## 4. Conclusions

New generation of the composite gradient 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 gradients of the chemical composition and properties, cutting simultaneously 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 gradient (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 PATRAN software. It was confirmed that using of finite element method in stresses modelling occurring in gradient- structured 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 gradient-structured 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 charaterise 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 gradient substrates and also gradient 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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## References

[1] J. Mikuła G. Matula, K. Gołombek, L.A. Dobrzański, Sintered composite gradient tool materials, Archives of Materials Science and Engineering 32/1 (2008) 25-28.

[2] G. Matula, K. Gołombek, J. Mikuła, L.A. Dobrzański, Structure of sintered gradient tool materials, Journal of Achievements in Materials and Manufacturing Engineering 32/1 (2009) 23-28.

[3] L.A. Dobrzański, L.W. Żukowska, J. Mikuła, K. Gołombek, T. Gawarecki, Hard gradient (Ti,Al,Si)N coating deposited on composite tool materials, Archives of Materials Science and Engineering 36/2 (2009) 69-75.

[4] M. Rosso, Properties of coatings on sintered iron alloys, Journal of Achievements in Materials and Manufacturing Engineering 19/1 (2006) 35-41.

[5] R. Manaila, A. Devenyi, D. Biro, L. David, P.B. Barna, A. Kovacs, Multilayer TiAlN coatings with composition gradient, Surface and Coatings Technology 151-52 (2002) 21-25.

[6] Z. Dyląg, A. Jakubowicz, Z. Orłoś, Strength of materials, WNT, Warsaw, 1996.

[7] S. Łączka, Introduction to the ANSYS Finite element system, Cracow Technical University Press, Cracow, 1999.

[8] T. Burakowski, T. Wierzchon, Engineering of metal surface, WNT, Warsaw, 1995.

[9] O.C. Zienkiewicz, R.L. Taylor, Finite Element Method, Butterworth Heinemann, London, 2000.

[10] W. Walke, Z. Paszenda, Numerical analysis of three-layer vessel stent made from Cr-Ni-Mo steel and tantalum, International Journal of Computational Materials Science and Surface Engineering 1/1 (2007) 129-137.

[11] J. Grum, R. Sturm, Influence of laser surface melt – hardering conditions on residual stress in thin plates, Surface and Coating Technology 100-101 (1998) 455-458.

[12] T. Da Silva Botelho, E. Bayraktar, G. Inglebert, Experimental and finite element analysis of spring back in sheet metal forming, International Journal of Computational Materials Science and Surface Engineering 1/2 (2007) 197-213.

[13] I. Son, G. Jin, J. Lee, Y. Im, Load predictions for non-isothermal ECAE by finite element analyses, International Journal of Computational Materials Science and Surface Engineering 1/2 (2007) 242-258.

[14] S. Ju, C. Fan, G. Wu, Three-dimensional finite element soft steel Boltem connections, Engineering Structures 26 (2004) 403-413.

[15] S. Thipprakmas, M. Jin, K. Tomokazu, Y. Katsuhiro, M. Murakawa, Prediction of Fine blanked surface characteristics using the finite element method (FEM), Journal of Materials Processing Technology 198 (2008) 391-398.

[16] Z. Tong, Y. Zhang, H. Hua, Dynamic behavior and sound transmission analysis of a fluid-structure coupled system using the direct-BEM/FEM, Journal of Sound and Vibration 299 (2007) 645-655.

[17] Y. Kim, S. Yaang, D. Shan, S. Choi, S. Lee, B. You, Three-Dimensional Rigid-Plastic FEM Simulation of Metal Forming Processes, Journal of Materials Engineering and Performance 15/3 (2006) 275-279.

[18] A. Śliwa, L.A. Dobrzański, W. Kwaśny, W. Sitek, Finite Element Method application for modeling of PVD coatings properties, Journal of Achievements in Materials and Manufacturing Engineering 27/2 (2008) 171-175.

[19] L.A. Dobrzański, A. Śliwa, W. Sitek, W. Kwaśny, The computer simulation of critical compressive stresses on the PVD coatings, International Journal of Computational Materials Science and Surface Engineering 1/1 (2007) 28-39.

[20] L.A. Dobrzański, A. Śliwa, T. Tański, Finite Element Method application for modelling of mechanical properties, Archives of Computational Materials Science and Surface Engineering 1/1 (2009) 25-28.

[21] A. Śliwa, L.A. Dobrzański, W. Kwaśny, W. Sitek, The computer simulation of internal stresses on the PVD coatings, Archives of Computational Materials Science and Surface Engineering 1/3 (2009) 183-188.

[22] L.A. Dobrzański, A. Śliwa, T. Tański, Numerical simulation model for the determination of hardness for casting the magnesium alloys MCMgAl6Zn1, Archives of Materials Science 29/3 (2008) 118-124.

[23] M. Kupczyk, Technological and functional quality of cutting tool flanks with the anti wear coatings, Poznan, 1997, (in Polish).

[24] S.J. Skrzypek, New opportunities in measurement of materials internal macrostresses by the use of diffraction of x-ray radiation in glancing angle geometry, Scientifically Didactic College Publishing House, Cracow, 2002.