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The computer simulation of internal stresses on the PVD coatings

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ABSTRACT

Purpose: The general topic of this paper is the computer simulation with the use of finite element method for determining the internal stresses in coatings Ti+TiN, Ti+Ti(CxN1-x) i Ti+TiC obtained in the magnetron PVD process on the sintered high-speed steel of the ASP 30 in different temperatures of 460, 500 and 540°C

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.

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 ANSYS 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: 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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METHODS OF ANALYSIS AND MODELLING

1. Introduction

The main purpose of this paper is formulate prognosis model of distribution of internal stresses in PVD coatings obtained on tools material with the use of finite element method. Formulated model allows in considerable range limit the necessity of making expensive and time- consuming experimental researches thanks to computer simulation. Specific processes way of PVD production causes that it is necessary to make interacting analysis of parameters on coatings' and substrate materials' interaction in transitory zone. It should be presented formation phenomena of inner stresses in a coating as a result of thermodynamic processes which proceeds during their spreading [1, 8, 20]. Very important thing is the skill of correct interpretation of proceeding phenomena by thermal and mechanical analysis. The material of spread coating the most frequently differs from substrate material, both in respect of chemical and phase constitution and in respect of microstructure, moreover temperature of coatings spread causes that within occurs high inner stresses which determine lot of properties, such as adhesion, microhardness and what is the most important; toll life and capacity of cut tools. Fast development of computer technique caused that finite element method is at the present one of the most meaningful method of numerical analysis [2, 9, 10, 15, 17-19]. 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 [11].

The paper shows a model enabling the user to evaluate overall stresses in the examined specimens and to evaluate the computer simulation results of the deposition conditions effect on stresses on the PVD coatings. The comparative analysis was carried out of the results of computer simulation of stresses with the experimental results.

2. Investigation methodology

The tests were carried out on the samples made of high-speed sintered steel of the ASP30 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 [3].

The evaluation of the phase composition of the obtained Ti+TiN coatings was carried out employing the SEIFERT-FPM XRD7 Advance X-ray diffractometer, using the filtered radiation of the cobalt Kα anode lamp, powered with 40 kV voltage, at 40 mA heater current. The measurements were made in the 2Θ angle range from 30 to 120°. Internal stresses value was calculated on the basis of reflexes extension deriving from crystallographic lattices planes of phases which are part of coatings composition and this internal stresses value was calculated on the basis of Young modulus value which was determined experimentally [4].

Internal stresses calculated using formula 1:

$$NW = -\frac{E}{2\nu} \cdot \frac{d - d_0}{d_0} \qquad (1)$$

where:
ν – Poisson ratio,
E – Young's modulus,
d – net's parameter with internal stresses described on the basis of X-ray diffractometer (Fig. 1.),
d_0 – net's parameter without internal stresses (table value).

Parameter d is calculated using Bragga's formula 2:

$$2d \sin \Theta = \lambda \qquad (2)$$

where:
λ– wavelength.

The micro hardness 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 3:

$$\frac{1}{E_r} = \frac{1 - v_i^2}{E_i} + \frac{1 - v_s^2}{E_s} \qquad (3)$$

where:
E_i – Young's modulus of the indenter, kN/mm^2,
E_s – Young's modulus of the specimen, kN/mm^2,
v_i - Poisson ratio of the indenter,
v_s - Poisson ratio of the specimen.

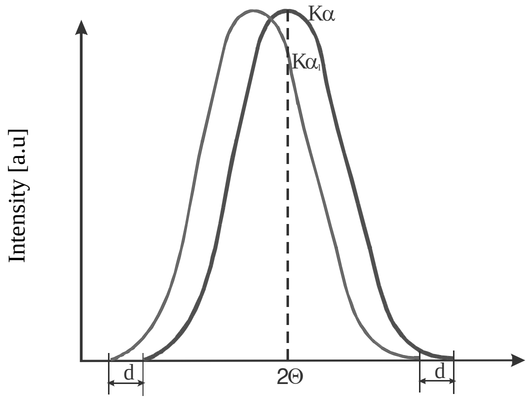

Fig. 1. Displacement of reflex $K\alpha_1$ in relation to standard reflex Kα

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.

The chemical compositions of the coatings were determined using the glow discharge optical emission spectrometer GDOS.

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 [6, 7].

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 [4, 5, 16].

In order to carry out the simulation of internal stresses in Ti+N 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 coating an interface Ti and a substrate (steel ASP 30), materials properties were established on the basis of and Mat Web catalogue, which was presented in Tables 1 and 2.

Table 1.
The summary data of the TiN, $Ti(C_xN_{1-x})$ and TiC coatings used for computer simulation of stresses

Material	Material thickness, [μm]	Young's modulus, [GPa]	Thermal expansion coefficient, [1/K] 10^{-6}	Poisson ratio
Coatings TiN	2.2-10	470-562	9.5	0.26
Coatings $Ti(C_xN_{1-x})$	1.9-10	355-640	9.4	0.24
Coatings TiC	2.5-6.9	350-440	7.8	0.19

Table 2.
The summary data of the substrate ASP 30and interface Ti material used for computer simulation of stresses in the Ti+TiN, $Ti+Ti(C_xN_{1-x})$ i Ti+TiC coatings

Material	Material thickness, [μm]	Young's modulus [GPa]	Thermal expansion coefficient, [1/K] 10^{-6}	Poisson ratio
Substrate (ASP 30)	4000	207	11.88	0.25
Interface (Ti)	1.1 / 0.9 / 0.7	113	8.6	0.34

3. Investigations results

Figure 2 presents the geometrical form of the ASP 30 sintered high speed steel test piece with the deposited Ti+TiN, $Ti+Ti(C_xN_{1-x})$ and Ti+TiC coatings. The geometrical model of the investigated coating overlaid with the finite elements' mesh is presented in Figure 3.

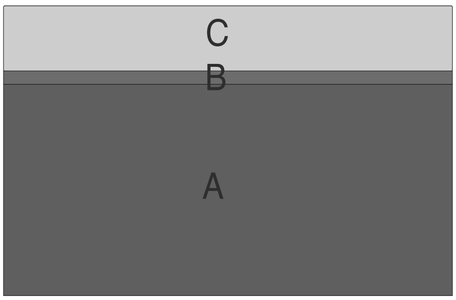

Fig. 2. Test piece from the ASP 30 sintered high speed steel with the deposited TiN, $Ti+Ti(C_xN_{1-x})$ i Ti+TiN coatings: A – Substrate (ASP 30), B – Interface (Ti), C – Outer coating (TiN), $(Ti(C_xN_{1-x}))$, (TiC)

Using experimental and table data (Table 1 and 2) internal stresses were modeled in coatings in ANSYS, by using the finite element method. Figures 4-7 present obtained results of numerical analysis with the help of the finite element method gathered as distribution maps of stresses in Ti+TiN, $Ti+Ti(C_xN_{1-x})$ i Ti+TiC coatings. Figure 8 presents x-ray diffraction pattern on the basis of which were calculated inner stresses in the coating, interlayer and in substrate material. The results of inner stresses are presented in Table 3.

Numerical analysis showed occurrence of compress stresses on the surface of analyzed coatings, which don't exceeds 1700 MPa. 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.

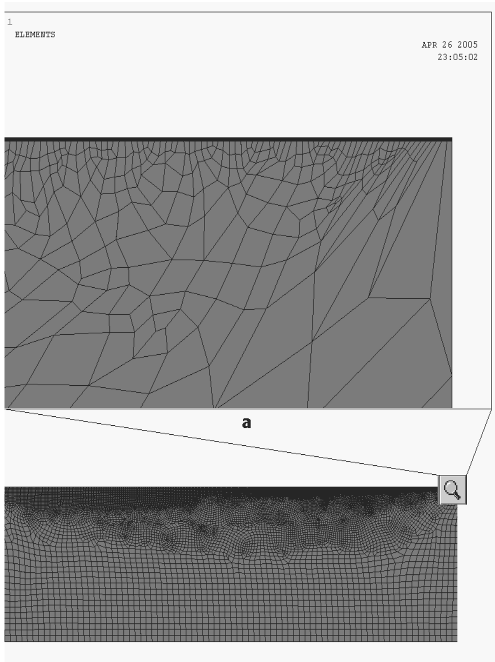

Fig. 3. Specimens model of sintered high-speed steel covered with coatings after meshing

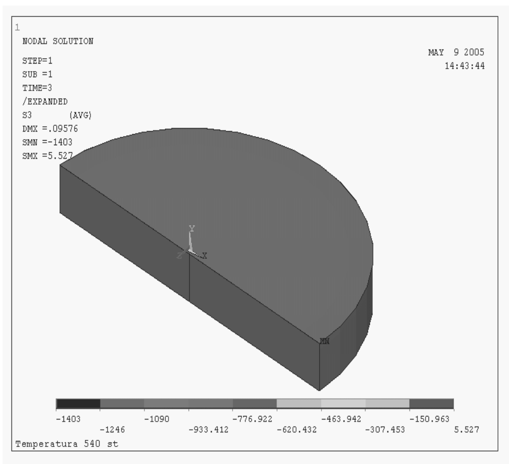

Fig. 4. Distribution of the simulated compression stresses in the Ti+TiN coating. (coating thickness g=10 μm, process temperature 540°C)

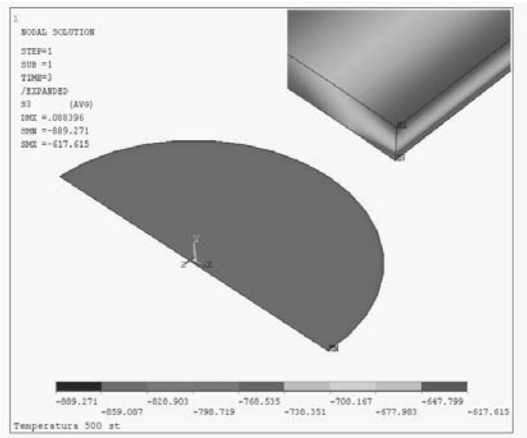

Fig. 5. Distribution of the simulated compression stresses in the Ti+TiN coating. (coating thickness g=10 µm, process temperature 540°)

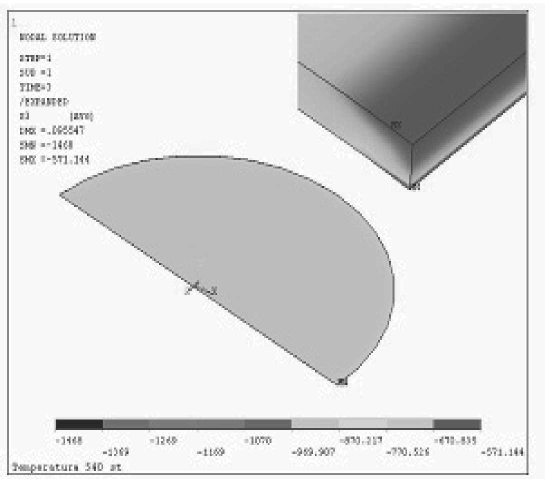

Fig. 6. Distribution of the simulated compression stresses in the Ti+TiN coating. (coating thickness g=10 µm, process temperature 540°C)

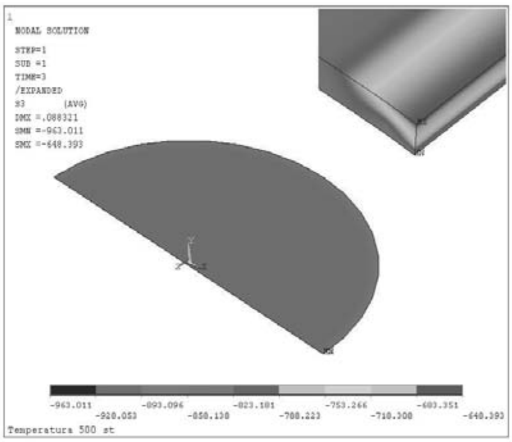

Fig. 7. Distribution of the simulated compression stresses in the Ti+Ti(C_xN_{1-x}) coatings in working atmosphere including 75% N_2 i 25% CH_4. (coating thickness g=6,4 µm, process temperature 460°C)

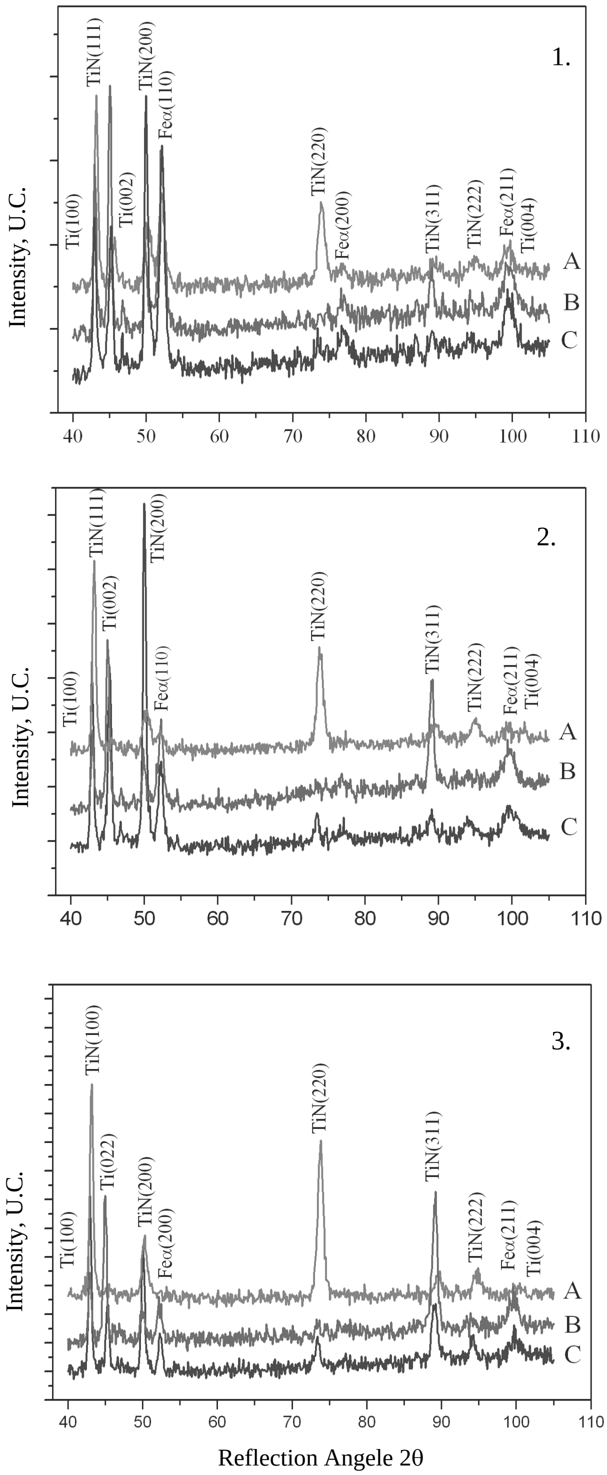

Fig. 8. Diffraction patterns of the sintered high-speed steel with the Ti+TiN coatings obtained at the distance of 1) 125, 2) 90, 3) 75 mm of the specimens from the magnetron disk: A – Process temperature 440°C, B – Process temperature 500°C, C – Process temperature 560°C

Table 3.
X-ray results of phase analysis

Phase {hkl}	d_0-table, [Å]	d-calculated, [Å]	Stresses determined by I[st] procedure, [MPa]	Stresses determined by II[nd] procedure, [MPa]
X-ray results of phase analysis on the sintered high-speed steel with Ti+TiN coating obtained at the specimen distance of 125mm from the magnetron disk in 460°C temperature				
Feα				
(110)	2.0268	2.0283	(-) 96	(-) 102
(200)	1.4332	1.4347		(-) 86
(211)	1.702	1.7035		(-) 96
Ti				
(100)	2.555	2.755	(-) 426	(-) 438
(002)	2.341	2.541		(-) 442
(101)	2.243	-		-
(102)	1.7262	-		-
(110)	1.4753	-		-
(103)	1.3320	-		-
(200)	1.2776	-		-
(112)	1.2481	-		-
(201)	1.2324	-		-
(004)	1.1707	1.1727		(-)420
TiN				
(111)	2.4491	2.4521	(-)946	(-) 940
(200)	2.1207	2.1236		(-) 901
(220)	1.4996	1,5025		(-) 915
(311)	1.2789	1.2818		(-) 952
(222)	1.2244	1.2273		(-) 922
X-ray results of phase analysis on the sintered high-speed steel with Ti+TiN coating obtained at the specimen distance of 125mm from the magnetron disk in 500°C temperature				
Feα				
(110)	2.0268	2.0286	(-) 101	(-) 112
(200)	1.4332	1.435		(-) 126
(211)	1.702	1.7038		(-) 98
Ti				
(100)	2.555	2.5566	(-) 445	(-) 467
(002)	2.341	2.3426		(-) 482
(101)	2.243	2.2446		(-) 461
(102)	1.7262	-		-
(110)	1.4753	-		-
(103)	1.3320	-		-
(200)	1.2776	-		-
(112)	1.2481	-		-
(201)	1.2324	-		-
(004)	1.1707	1.1721		(-) 453
TiN				
(111)	2.4491	2.4516	(-) 888	(-) 852
(200)	2.1207	2.1232		(-) 886
(220)	1.4996	1.5021		(-) 853
(311)	1.2789	1.2814		(-) 892
(222)	1.2244	1.2269		(-) 873

4. 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 [12-14].

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 ANSYS program.

As a result of experimental researches and computer simulation of formed stresses in Ti+TiN, Ti+Ti(C_xN_{1-x}) i Ti+TiC coatings which were applied on the substrate of high-speed steel ASP 30 in PVD process, it was found the occurrence of compressive stresses what ensures the rise of strength properties.

References

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

[2] T. Da Silva Botelho, E. Bayraktar, 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.

[3] L.A. Dobrzański, W. Kwaśny, Z. Brytan, R. Shishkov, B. Tomov, Structure and properties of the Ti+Ti(C,N) coatings obtained in the PVD process on sintered high speed steel, Journal of Materials Processing Technology 157-158 (2004) 312-316.

[4] L.A. Dobrzański, A. Śliwa, W. Kwaśny, Employment of the Finite Element Method for determining stresses in coatings obtained on high speed steel with the PVD process, Journal of Materials Processing Technology 164-165 (2005) 1192-1196.

[5] L.A. Dobrzański, M. Staszuk, A. Śliwa, Simulation of the microhardness measurement of PVD coatings by use of

FEM, Journal of Achievements in Materials and Manufacturing Engineering 18 (2006) 279-282.
[6] 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.
[7] L.A. Dobrzański, A. Śliwa, W. Kwaśny, The computer simulation of internal stresses in coatings obtained by the PVD process, Journal of Achievements in Materials and Manufacturing Engineering 20 (2007) 355-358.
[8] Z. Dyląg, A. Jakubowicz, Z. Orłoś, Strength of materials, WNT, Warsaw, 1996.
[9] 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.
[10] S. Ju, C. Fan, G. Wu, Three-dimensional finite element soft steel Boltem connections, Engineering Structures 26 (2004) 403-413.
[11] 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.
[12] M. Kupczyk, Technological and functional quality of cutting tool flanks with the anti wear coatings, Technical University Press, Poznan, 1997(in Polish).
[13] S. Łączka, Introduction to the ANSYS Finite element system, Technical University Press, Cracow, 1999.
[14] S.J. Skrzypek, New opportunities in measurement of materials inner macrostresses by the use of diffraction of X-ray radiation in glancing angle geometry, Scientifically Didactic College Publishing House, Cracow, 2002.
[15] 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.
[16] 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.
[17] 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.
[18] Z. Tong, Y. Zhang, 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.
[19] 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.
[20] O.C. Zienkiewicz, Finite elements method, Butterworth-Heinemann Linacre House, Jordan Hill, Oxford, 2000.