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# The computer simulation of stresses in the Ti+TiC coatings obtained in the PVD process

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**Analysis and modelling**

## ABSTRACT

**Purpose:** The aim of the research is the computer simulation of the internal stresses in bilayer coatings Ti+TiC obtained in the magnetron PVD process on the ASP 30 sintered high-speed steel.

**Design/methodology/approach:** Computer simulation of stresses was carried out in ANSYS environment, using the FEM method and the experimental values of stresses were determined basing on the X-ray diffraction patterns.

**Findings:** The computer simulation results correlate with the experimental results. 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.

**Research limitations/implications:** In order 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:** 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. 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:** Computer materials science; Finite Element Method; Stresses; Coatings PVD

## 1. Introduction

Specification of contemporary production of tools are subject to essential changes in comparison to the situation observed few years ago. Then , in relation to material tools and technology of their production, it is expected an assurance of the best functional and using qualities which are the most possible to achieve and it especially concerned tool life and the time of its using. Such approach however needs huge financial amounts and much time, because it is connected with carrying out complex basic research of material tools, technology of their producing, technology which improving their properties and applied research, consists in complex technological tests which allows to estimate the functional qualities of tools.

Surface treatment as a new branch of science plays a key role and has a particular meaning in development of material tools. Advanced technique of surface treatment and particularly among them PVD and CVD techniques which allows to improve functional qualities of tools made with conventional material tools when they are not under such treatment they don't come up to users expectations in many cases. Specification of PVD coating production process causes that it is necessary to carry out the analysis of parameters influence on base material in temporarily zone. It should be specified here the effect of creating internal stresses in coating as the result of thermodynamic processes proceeding during deposition of coating.

The fundamental matter is a skill to correct interpretation of appearing effects through thermal, mechanical analysis and also through analysis of transformation phase. Contemporary, such as analysis are often made by using of advanced computational techniques , among others the finite elements methods MES. These methods allows to carry out complex analysis of effects appearing during processes of coatings deposition. It should be underline that such analysis needs knowledge of many quantities which are parameters of this analysis and consist of physical and mechanical properties in base and coating and also the parameters of coating deposition process. As a result of this MES program allows to create model describing mechanical and usage properties of coating depending on parameters of process and also on type of coating and base [1-3].

The paper presents 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 Ti+TiC 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 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 [4-6].

The real specimen's dimensions were used for development of its model needed for determining the stresses in the Ti+TiC 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 [7-9]. In order to avoid a mistake in calculation of internal stresses in coatings the finite elements variable was used. At spots ,where higher stresses values were expected, the mesh is more thickened than at spots where stresses should have similar values. That is why in the coatings were used minor elements, better imaging of bigger stresses values and the elements in high speed steel increase together with going away from the coatings [10].

The geometrical model of tested coating with an applied mesh of finite elements was presented in fig.1 and 2. Conditions of spreading in those samples and their mechanical properties, which were determined in experimental way and used in computer simulation and then were presented in tables 1 and 2 [11].

In order to carry out the simulation of internal stresses in Ti + TiC coatings, the following boundary conditions were applied:

- symmetry axis of sample is fixed on the whole length by taking away the all degrees of freedom from nodes which are on this axis.
- change of temperature in PVD process presents the cooling process of specimen from 540, 500 and 460°C to ambient temperature of 20°C,
- for TiC 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.

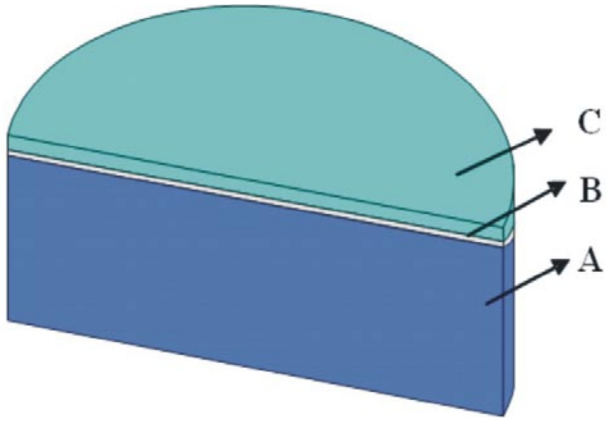


Fig. 1. Test piece from the ASP 30 sintered high speed steel with the deposited Ti+TiC coatings: A – Substrate (ASP 30), B – Interface (Ti), C – Outer coating (TiC)

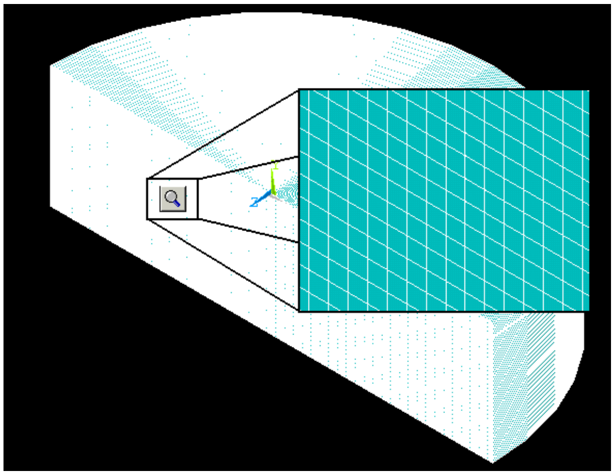

Fig. 2. Specimens model of sintered high-speed steel covered with coatings after meshing.

The evaluation of the phase composition of the obtained Ti+TiC 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 [12-13].

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 1:

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

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.

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.

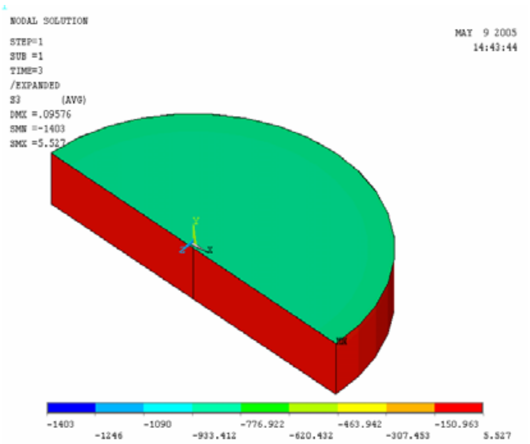


Fig. 3. Distribution of the simulated compression stresses in spicemen covered with the Ti+TiC coatings (coating thickness g=2,6 µm, process temperature 540°C )

## 3. Investigations results

Using experimental and table data (table 1 and 2) internal stresses were modeled in coatings in ANSYS, by using the finite element method. Figures 3-4 presents obtained results of numerical analysis with the help of the finite element method gathered as distribution maps of stresses in Ti + TiC coatings. 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, what was showed in table 3.

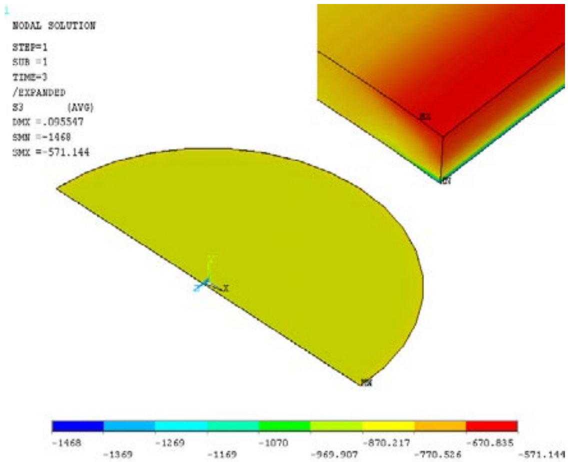


Fig. 4 Distribution of the simulated compression stresses in the Ti+TiC coating (coating thickness g=2,6 µm, process temperature 540°C)

Table 1.
The summary data of the substrate and interface material used for computer simulation of stresses in the 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 | 113 | 8,6 | 0,34 |
| | 0,9 | | | |
| | 0,7 | | | |

Table 2.
The summary data of the coating material used for computer simulation of stresses in the TiC coatings

| Process temperature, [°C] | Coating thickness TiN, [µm] | Young's modulus, [GPa] | Thermal expansion coefficient, [1/K] $10^{-6}$ | Poisson ratio |
|---|---|---|---|---|
| 540 | 2,6 | 370 | 7,8 | 0,19 |
| | 4,6 | 400 | | |
| | 6,9 | 370 | | |
| 500 | 2,6 | 350 | | |
| | 4,2 | 420 | | |
| | 6,6 | 400 | | |
| 460 | 2,5 | 385 | | |
| | 3,9 | 440 | | |
| | 6,4 | 400 | | |

Table 3
Effect of the deposition conditions on chemical composition and mechanical properties of the analysed coatings

| Process temperature [°C] | Specimen distance from the magnetron disk, [mm] | Coating thickness [µm] | Atomic fractions of the elements, [%] | | | Experimental results of overall stress [MPa] | Computer simulation results of overall stress [MPa] | Error [MPa] |
|---|---|---|---|---|---|---|---|---|
| | | | Ti | N | Al | | | |
| 460 | 125 | 2,5 | 55,7 | 34 | 8,1 | (-) 1138 | (-) 1140 | 2 |
| | 95 | 3,9 | 56,8 | 33,9 | 7,9 | (-) 919 | (-) 913 | 6 |
| | 70 | 6,4 | 57,9 | 33,3 | 7,6 | (-)993 | (-)921 | 72 |
| 500 | 125 | 2,6 | 54,7 | 32,4 | 8,3 | (-) 1015 | (-)1020 | 5 |
| | 95 | 4,2 | 56,9 | 34,6 | 7,5 | (-) 1035 | (-) 1008 | 27 |
| | 70 | 6,6 | 57,1 | 35,2 | 6,7 | (-) 1091 | (-) 1100 | 9 |
| 540 | 125 | 2.6 | 55,9 | 34,8 | 7,7 | (-) 1007 | (-)1015 | 8 |
| | 95 | 4,6 | 57,2 | 34,6 | 7,3 | (-) 1259 | (-)1251 | 8 |
| | 70 | 6,9 | 56,9 | 34,9 | 7,1 | (-) 1083 | (-) 1100 | 17 |

## 4. Conclusions

The finite element method is currently commonly used in such branches of science, like: mechanics, biomechanics, mechatronics, materials engineering, and thermodynamics. 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 [14-15].

Basing on 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 gives 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+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 ensure the rise of strength properties.

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