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Simulation of the microhardness and internal stresses measurement of PVD coatings by use of FEM

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ABSTRACT

Purpose: The goal of this work is to determine microhardness of coats and stresses obtained in PVD process with the use of finite elements method and comparative analysis with results obtained by laboratory investigations.

Design/methodology/approach: Article introduce the usage of finite elements method for simulation of microhardness and stresses measurement process in TiN and TiC coats obtained in magnetron PVD process on high-speed steel ASP 30. Simulation of indenters depression in investigated coat permitted on disclosure of deformation of the layer PVD and allows to create the maps of stresses.

Findings: Basing tensions obtained as a result of indenter depression in investigated surfaces we obtained the maps of stresses, deformations analyzed of coats, and then we calculated the microhardness.

Research limitations/implications: On the basis of tensions in investigated coat obtained in result of computer simulation effected in ANSYS software environment was possible to compute the microhardness of the coating, and the results was compared with the microhardness data of coats received by physical examination with use of the Vickers method.

Originality/value: From results of the simulation based on the finite element method is possible to compute the mechanical properties of coatings obtained in PVD process.

Keywords: Numerical techniques; Microhardness; Stresses; Computer simulation; Finite Element Method

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METHODS OF ANALYSIS AND MODELLING

1. Introduction

Sintered high-speed steels are important group of engineer materials. They are in use in production of cutting off tools for hard treatment materials tooling. They work with large efficiency at required enlarged coefficients of work reliability. Numerous scientific investigations showed, that influence on considerable improvement of tools exploitation persistence has the covering of tools with thin layer hard-melting compounds of carbon, nitrogen, boron with interim metals and some oxides with use of physical of-settling from gas- phases PVD (physical vapour deposition) techniques. Increasing of persistence of tools covered with PVD coats binds with considerable increase of coat hardness with reference to base material. Hardness of coat material depends on bonds out in coat. Materials with ionic bonds (eg. oxides) have high hardness but simultaneously are brittle, metal materials assure very good adhesion to substrate. Proprieties that provide the most universal materials with metallic bond (borons, carbides and nitrogen's of interim metals) and therefore these materials have the widest practical use [1-6].

Finite elements method is at present one of most widely used practical methods of dissolving of all engineering problems. It finds use eg in such spheres of science as: solid mechanics fluid mechanics, biomechanics, material engineering, thermal analysis and magnetical and electrical analysis. Finite elements method permits on time shortening of projecting and gives possibility to research the influence of each factors on the whole mathematical model. Usage of this method from economic point of view is well-founded because more than once it permits to avoid expensive laboratory investigations, and results obtained during simulation are reliable and approximate to real values [7-11].

Model presented in the work makes possible fixing of microhardness and stresses of TiN and TiC coats obtained with PVD techniques in examined samples in dependencies of deposition circumstances.

2. Materials

Thin films were deposited by reactive magnetron sputtering onto polished high-speed steel ASP 30 substrates containing 1.28% C, 4.2% Cr, 5.0% Mo, 6.4% W, 3.1% V and 8.5% Co. Before the process of deposition, the substrates were heat treated in the salt bath furnaces with austenitising at the temperature of 1180°C and three-stage tempering at the temperature of 540°C and next specimens were mechanically polished. Depositions were carried out using the single chamber vacuum furnace with the magnetron built in for ion sputtering and the target to substrate distance were 125, 95 and 70 mm. The magnetron target was made from the titanium alloy containing 90% Ti, 5.7% Al, 1.4% Cr and 2.0% Mo. The coating deposition process was carried out at temperatures of 460, 500 and 540°C. The TiN layer was put down in 60 minutes at the temperature relevant for this process [12-14].

3. Methodology

The chemical composition of the films (Table 1) was determined by Glow Discharge Optical Spectroscopy GDOS.

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 [1,3-7].

The microhardness 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 [1,3-7]:

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

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.

X-rays studies for the analyzed coatings are carried out on X´Pert PRO system made by Panalytical Company using filter radiation of a cobalt anode lamp. A phase analysis of the analysed materials is carried out in Bragg-Brentano geometry using a Xcelerator strip detector.

In order to estimate privileged increase direction of analyzed surfaces, analyse of texture was performed. Not less than three pole figures were measured for each analysed sample made by a reflection method employing Euler's circle of diameter 187 mm in a range of samples inclination angle from zero to 75°.

Measurements of stresses for the analyzed coatings were made by $\sin^2\psi$ on the basis of X'Pert Stress Plus company's programme, which contains, in a form of a database indispensable to calculate, values of material constants. In the method of $\sin^2\psi$based on diffraction lines displacement effect for different ψ angles, appearing in the conditions of stress of materials with crystalline structure, a silicon strip detector was used at the side of diffracted beam. Samples inclination angle towards the primary beam was changed in the range of 0°-75°.

Model created in the program consists from surface that represents penetrator side, investigated PVD layers and steel - substrate. Taking under attention, that real model is symmetrical, the other model created in Ansys has a quarter of the real model size (Fig. 1). At maintenance of suitable margin conditions in the symmetry surfaces of such simplification does not have an influence on simulation result, but in considerable shortening of time necessary for calculations program.

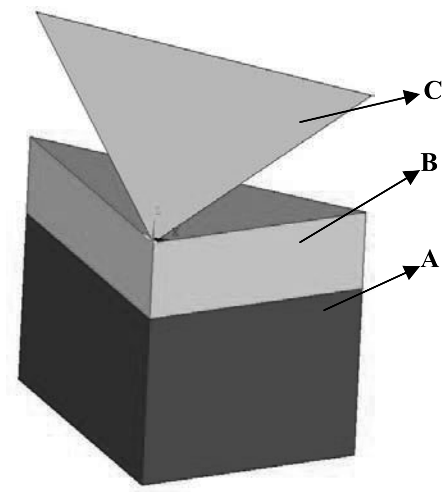

Fig. 1. Model of the sample: A - Substrate (ASP 30), B - Coating (TiN, TiC), C - Indenter Model Surface

Surface, that represents the penetrator side has been modeled as unmemorable by use for the purpose of MESH200 library unit. This unit is a "net unit" and is not a subject of any calculations. Significantly unit MESH200 is linea and possesses two hitches. In the work square unit described on four hitches (QUAD 4-NODE) was used. Model of the investigated sample with inserted net of finite elements is showed in Fig. 2.

Selection of elements on PVD layer and steel substrate should assure the ability to deformations and occurrence of tensions. That's why the unit SOLD185 was chosen. This unit is used for three-dimensional modeling of block structures. The model is defined by eight hitches, each has three translate degrees freedoms in every direction (UX, UY, UZ) and also defined by the use of material properties (eg Young module, Poisson coefficient, thickness, thermal conduction). Significantly unit accepts global system of coordinates.

Mechanical properties of PVD coats are qualified according to Tables 1 and 2. However steel materials used as substrate remain consistent for invariable each simulations and carry out:

- Poisson coefficient: $\nu = 0.28$,
- Thermal expansion coefficient, 11.88 [1/K] 10^{-6},
- Young module: $E = 2.05 \times 10^5$ MPa.

To assure the univocal position model in space the bottom surface of the model was fixed as not movable (Fig. 2) All degrees freedoms was taken. The edge conditions in this surface of symmetry are given on axis Y on surface XZ, and on axis X on surface YZ (Fig. 2).

Table 1.
Influence of deposition conditions on chemical bonds and mechanical properties of analyzed TiN coatings

Number of sample	Process temperature, [°C]	Coating thickness, [µm]	Young's modulus, [MPa]	Poisson ratio	Thermal expansion coefficient [1/K] 10^{-6}	$HV_{0,05N}$	Computer simulation of stresses produced by the penetrator [MPa]	Computer simulation of microhardness, [HV]
1	460	4.7	440000	0.26	9.35	3300	15440	2918
2		6.7	415000			2500	10195	1926
3		10.0	350000			1400	9774	1847
4	500	2.2	380000			1750	9131	1725
5		3.7	355000			1450	10125	1913
6		5.0	355000			1450	10218	1931
7	540	2.3	380000			1750	9385	1773
8		3.8	400000			2200	10216	1930
9		6.1	365000			1600	9804	1852

Table 2.
Influence of deposition conditions on chemical bonds and mechanical properties of analyzed TiC coatings

Number of sample	Process temperature, [°C]	Coating thickness, [µm]	Young's modulus, [GPa]	Poisson ratio	Thermal expansion coefficient [1/K] 10^{-6}	$HV_{0,05N}$	Computer simulation of stresses produced by the penetrator [MPa]	Computer simulation of microhardness, [HV]
1	460	2.5	370	0.19	7.8	1900	9656	1824
2		3.9	400			2200	10195	1926
3		6.4	370			1900	9651	1824
4	500	2.6	350			1750	9458	1787
5		4.2	420			2350	10417	1968
6		6.6	400			2200	10246	1936
7	540	2.6	385			2050	9687	1811
8		4.6	440			2650	12532	2369
9		6.9	400			2200	9928	1876

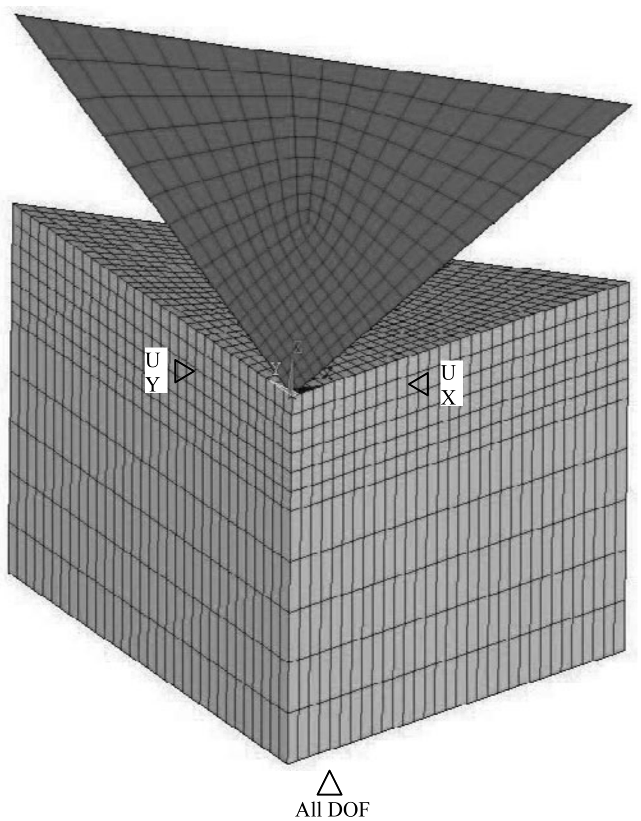

Fig. 2. Analyzed model with the overlaid finite elements mesh

To define contact among penetrator surface and frontal surface of PVD layers unit CONTA174 was used. This unit is placed on block surface and is defined across eight hitches.
Geometry of unit and bearings of hitches are showed in Fig. 3.

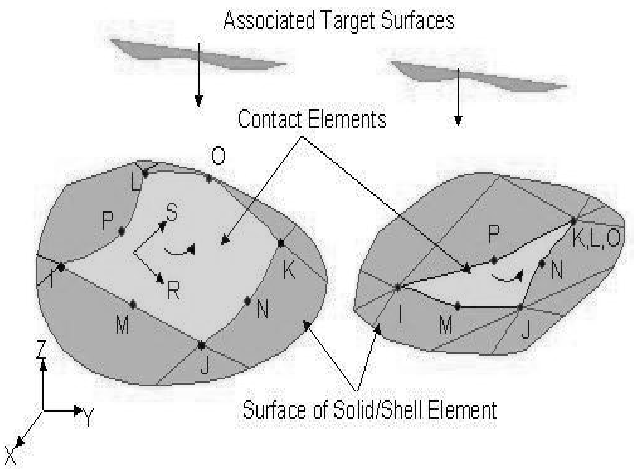

Fig. 3. Geometry and position of CONTA174 elements

Taking into account, that used contact - model with friction is strongly non-linear we added an encumbrance through dislocation to obtain better numeric stability.

The encumbrance during microhardness tests with use of Vickers method was precisely chosen, so that penetrator engrossment was not greater than 1/10 thicknesses of deposited coatings. Therefore, to behave the nearest to real conditions through whole simulation the given engrossment of surface, that represents the penetrator side was set on 0.1 of thicknesses of examined layers.

4. Results

Results of mechanical property show, that examined coatings posses high hardness, dependent on parameters of deposition process. On the basis of dependence of encumbrance and relief in function of penetrator engrossment in the examined material during microhardness measurements the module of analyzed coatings longitudinal elasticity was calculated (Tables 1, 2).

Using experimental data in the modeling process of tensions in examined coatings was obtained in the result of penetrator engrossment in investigated coat. In the result of deformation simulation of the model and contour- maps of tensions were obtained (Figs. 4, 5), and then the microhardness of analyzed coatings was calculated.

In the ANSYS system was computed the median value of tensions with use of the equation [9]:

$$SMX = \max_n \left\{\sigma_n^a\right\} = \frac{\sum_{i=1}^{N_e^n} \left\{\sigma_n^i\right\}}{N_e^n} \qquad (2)$$

where:

N_e^n - number of units adjoining with hitch *n*,

σ_n^i - tensions in hitch n counted for i- unit.

In ANSYS program the SMX signature is used in printouts and on maps of tensions.

Microhardness of examined coatings was computed from the equation:

$$HV_{simulation} = 0.189 \times SMX \qquad (3)$$

Microhardness results obtained with the use of computer simulation was compared with results appointed by experiment what was presented in Figs. 10 and 11.

Figures 6-9 present obtained results of numerical analysis with the help of the finite element method gathered as distribution maps of stresses in TiN and TiC coatings. Stresses' error in the simulated model doesn't exceed 5%. The comparative analysis of the results of computer simulation of stresses with the experimental results was carried out, and was presented in Figures 12 and 13.

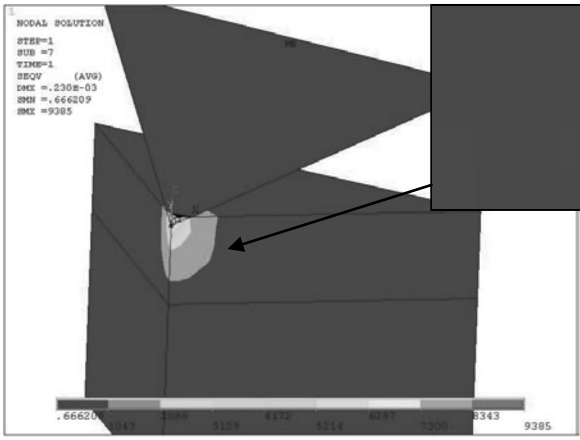

Fig. 4. Deformation and distribution of tensions in TiN coat (thickness of coat g=2.2 μm, temperature of process 540°C)

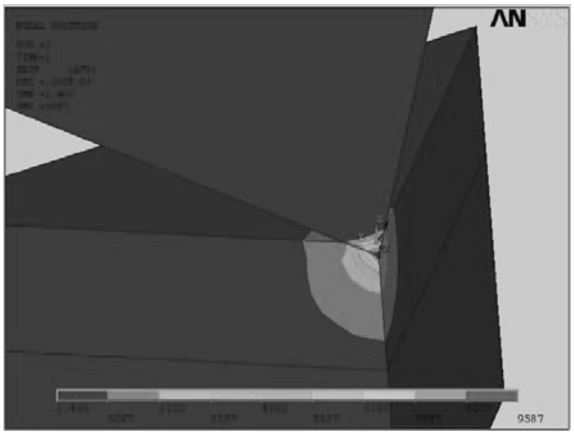

Fig. 5. Distribution of tensions in TiC coat (thickness of coat g=2.6 μm, temperature of process 540ºC)

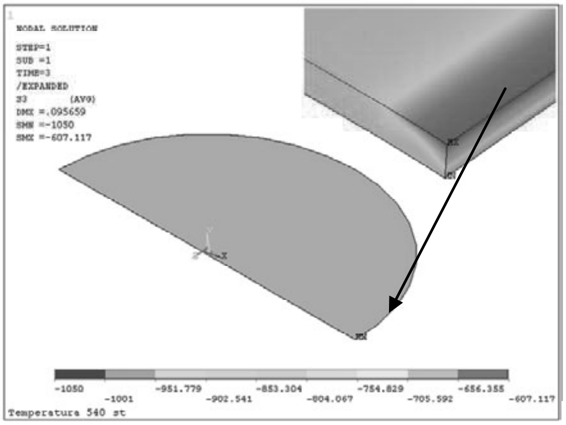

Fig. 6. Distribution of the simulated compression stresses in the TiN coating (coating thickness g=4.6 μm, process temperature 540°C, specimen distance from the magnetron disk 95 mm)

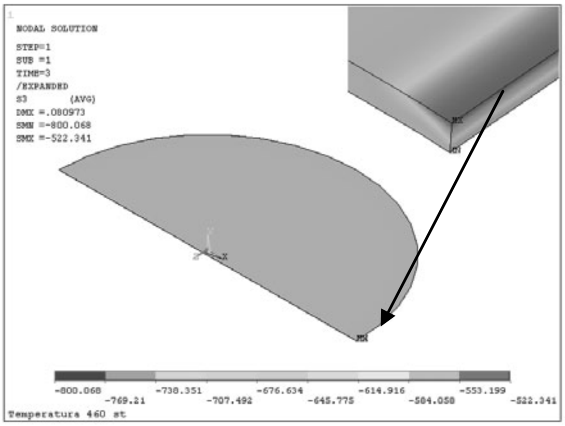

Fig. 7. Distribution of the simulated compression stresses in the TiN coating (coating thickness g=3.9 μm, process temperature 460°C, specimen distance from the magnetron disk 125 mm)

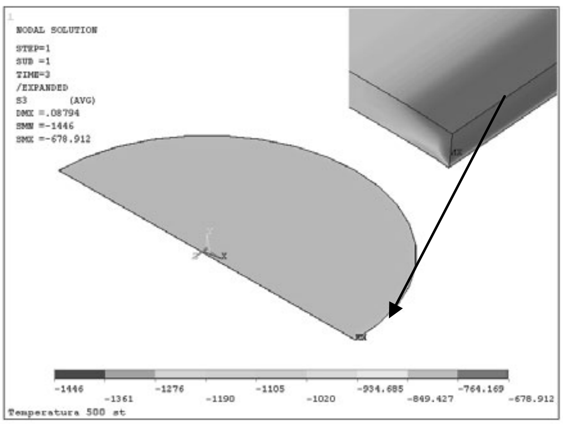

Fig. 8. Distribution of the simulated compression stresses in the TiC coating (coating thickness g=2.6 μm, process temperature 540°C, specimen distance from the magnetron disk 95 mm)

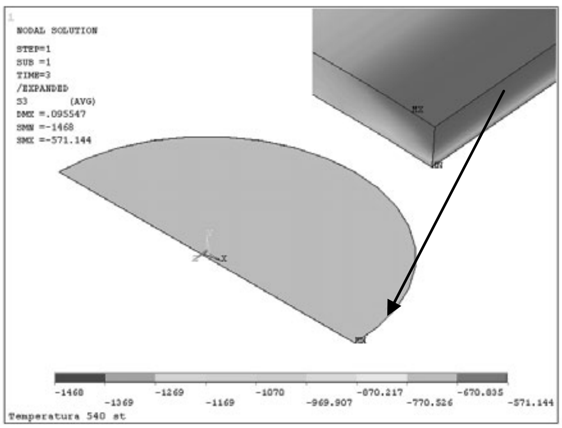

Fig. 9. Distribution of the simulated compression stresses in the TiC coating (coating thickness g=2.6 μm, process temperature 500°C, specimen distance from the magnetron disk 125 mm)

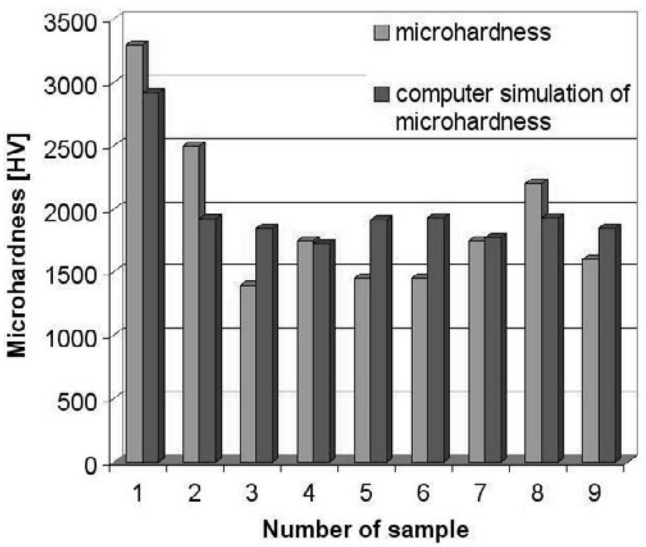

Fig. 10. Comparison of computer simulation with results of experimental investigations for microhardness of TiN coatings

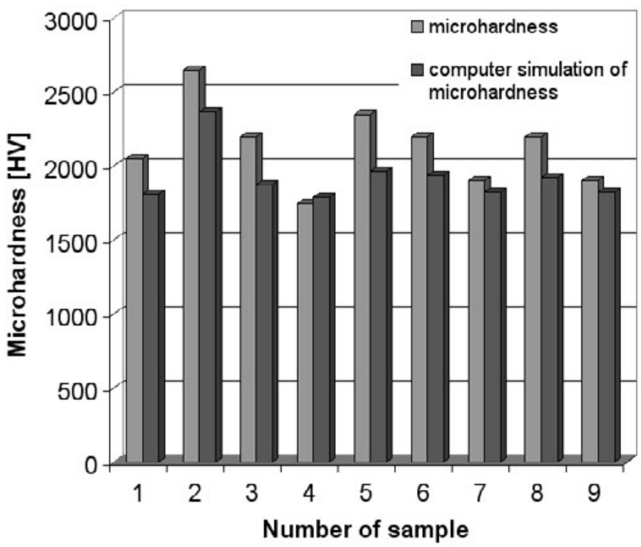

Fig. 11. Comparison of computer simulation with results of experimental investigations for microhardness of TiC coatings

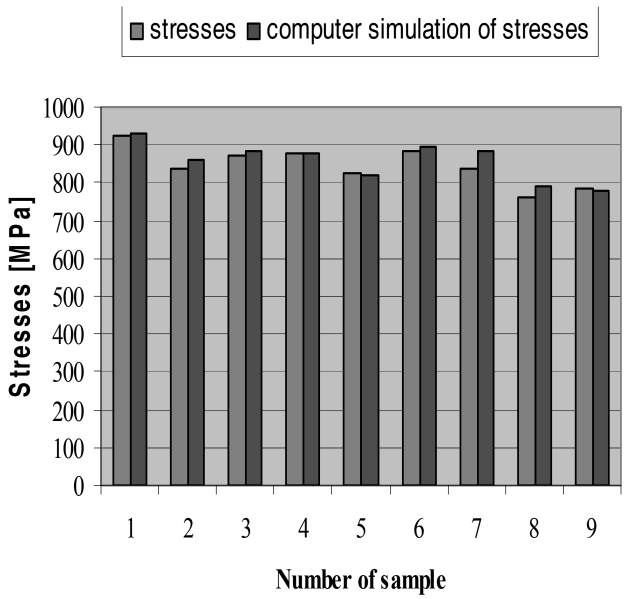

Fig. 12. Comparison of computer simulation with results of experimental investigations for stresses of TiN coatings

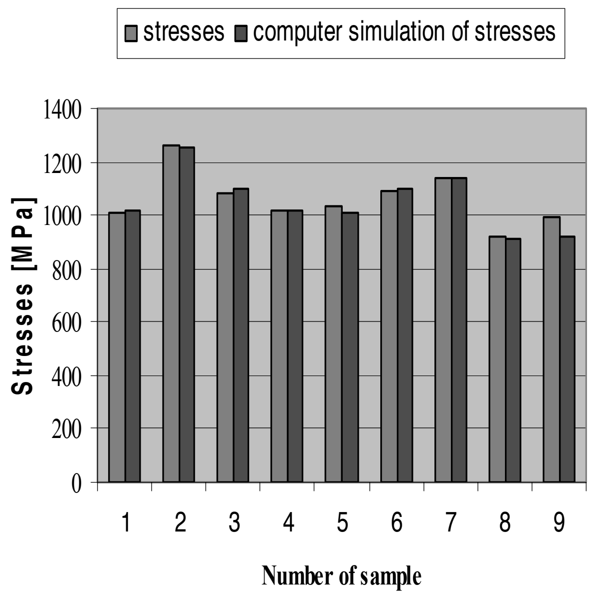

Fig. 13. Comparison of computer simulation with results of experimental investigations for stresses of TiC coatings

5. 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 influencing 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 [15-20].

Microhardness of waste resistant PVD coatings deposited eg. on cutting tools blades is very important material feature.

Superhard coats deposited on sintered steel considerably increase persistence of the tools. Such coatings are characterized by considerably greater resistance on abrasion enlarging persistence of tools several times and make possible the usage of higher machining parameters with maintenance of lower tool temperatures.

This work introduces the model compiled with use of finite elements method, which makes possible to calculate the microhardnees of coats which are obtained in magnetron PVD process. On the material data basis is possible to mark the tensions increase in coatings in result of penetrator engrossment in the examined material, and then, on the basis of these tensions it is possible to calculate the microhardness. Results of computer simulation method are comparable to laboratory results. The ANSYS model programmed with the use of finite elements method permits to analyze the properties of mechanical PVD layers, what makes reliable its application for computation of the anti-waste coatings microhardness, and computer simulation is cheaper than laboratory investigations.

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 [21-23].

As a result of experimental researches and computer simulation of microhardness, stresses in TiN and 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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Additional information

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The paper is published also in the Journal of Achievements in Materials and Manufacturing Engineering.

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