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The computer simulation of internal stresses in coatings obtained by 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+TiN, Ti+Ti(CxN1-x), Ti+TiC obtained in the magnetron PVD process on the sintered high-speed steel of the ASP 30.
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: Artificial intelligence methods; Coatings PVD; Finite Element Method; Stresses

1. Introduction

Internal 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. However, the excessive compression stresses occurring in the coating may cause its buckling. 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 softwears make possibile the creation of more precise models and more adequate ones to reality [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+TiN, Ti+Ti(C_xN_{1-x}), Ti+TiC coatings. The comparative analysis was carried out 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 [4-6].

The evaluation of the phase composition of the obtained Ti+TiN, Ti+Ti(C_xN_{1-x}), 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. [7-8] 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.

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 Ti+TiN, Ti+Ti(C_xN_{1-x}), 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 [9-12].

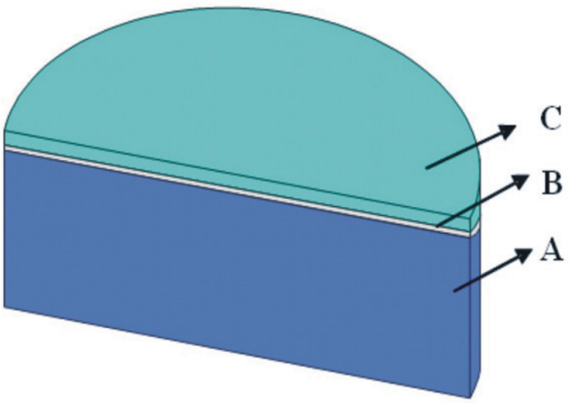

Fig. 1. Test piece from the ASP 30 sintered high speed steel with the deposited Ti+TiN, Ti+Ti(C_xN_{1-x}), Ti+TiC coatings: A–Substrate (ASP 30), B–Interface (Ti), C–Outer coating (TiN, Ti(C_xN_{1-x}), TiC)

The geometrical model of tested coating with an applied mesh of finite elements was presented in fig.1. The calculation model consists of 86880 nods and 86241 elements, of which TiN coating includes 61938 nods and 63000 finite elements, and the interface Ti includes 4004 nods and 3000 of finite elements, and the substrate consists of 21813 nods and 20241 finite elements [13].

3. Investigations results

Fig. 2 presents the X-ray diffraction patterns of the sintered high-speed steel with the Ti+TiN coatings deposited at 440, 500 and 560 °C process temperatures. It was found out using the X-ray phase quantitative analysis that according to the initial assumptions the Ti+TiN coatings were developed on the surface of the investigated ASP 30 high speed steel. Moreover, occurrences of reflections coming from the TiN, Ti and Feα were observed in the X-ray diffraction patterns.

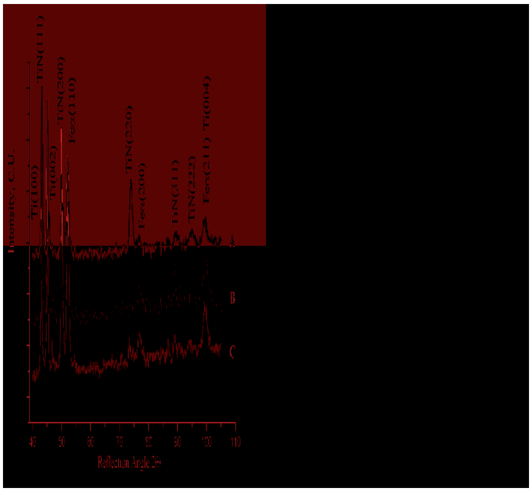

Fig. 2. Diffraction patterns of the sintered high-speed steel with the Ti+TiN coatings obtained at the distance of 125 mm of the specimens from the magnetron disk: A – Process temperature 440°C, B – Process temperature 500°C, C – Process temperature 560°C

Fig. 3 presents obtained results of numerical analysis with the help of the finite element method gathered as distribution maps of stresses in PVD coatings. Tables 1-3 present comparison of computer simulation results with the experimental results of internal stresses in the analysed PVD coatings.

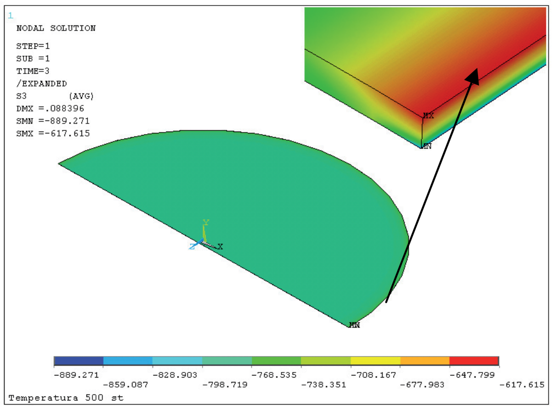

Fig. 3. Distribution of the simulated compression stresses in the Ti+TiC coating. (coating thickness g=10 µm, process temperature 500°C, sspecimen distance from the magnetron disk 95 mm)

Table 1.
Comparison of computer simulation results with the experimental results of internal stresses in the analysed PVD coatings Ti+TiN

Process temperature, [°C]		540			500			460	
Specimen distance from the magnetron disk, [mm]	125	95	70	125	95	70	125	95	70
Computer simulation results of overall stress, [MPa]	822	792	778	880	818	895	930	860	882
Experimental results of overall stress, [MPa]	837	763	785	879	823	884	925	840	874
Terror, [MPa]	15	29	7	1	5	11	5	20	8

Table 2.
Comparison of computer simulation results with the experimental results of internal stresses in the analysed PVD coatings $Ti+Ti(C_xN_{1-x})$

Process temperature, [°C]		540			500			460	
Specimen distance from the magnetron disk, [mm]	125	95	70	125	95	70	125	95	70
Computer simulation results of overall stress, [MPa]	822	792	778	880	818	895	930	860	882
Experimental results of overall stress, [MPa]	837	763	785	879	823	884	925	840	874
Terror, [MPa]	15	29	7	1	5	11	5	20	8

Table 3.
Comparison of computer simulation results with the experimental results of internal stresses in the analysed PVD coatings Ti+TiC

Process temperature, [°C]		540			500			460	
Specimen distance from the magnetron disk, [mm]	125	95	70	125	95	70	125	95	70
Computer simulation results of overall stress, [MPa]	822	792	778	880	818	895	930	860	882
Experimental results of overall stress, [MPa]	837	763	785	879	823	884	925	840	874
Terror, [MPa]	15	29	7	1	5	11	5	20	8

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.

Basing on the experimental results and computer simulation of stresses developed in the Ti+TiN, Ti+Ti(C_xN_{1-x}), Ti+TiC coatings put down onto the substrate from the ASP 30 high-speed steel in the PVD process, the compression stresses were revealed.

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