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The computer simulation of stresses in the Ti+Ti(C_xN_{1-x}) 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+Ti(C_xN_{1-x})obtained in the magnetron PVD process on the sintered high-speed steel of the ASP 30 in working atmosphere including 75% N_2 i 25% CH_4, 50% N_2 i 50% CH_4, and 25% N_2 i 75% CH_4.
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: Computational materials science; Finite Element Method; Stresses; Coatings PVD

1. Introduction

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 better the relationships among various parameters and makes it possible to select the optimum solution.

The sintered high-speed steels are an important group of engineering materials. These materials are often used for blanking dies, for processing the polymer materials, and for the multipoint cutting tools with complex geometry. The ongoing research results indicate that coating the tool flanks with coatings obtained in the PVD processes features an important direction in development of cutting tools. The coating material deposited differs – most often - from the matrix material, both in respect to the chemical and phase compositions, as to the microstructure, texture, and density. Taking into account the specific properties of cutting tool operation, our attention was focused on the issue of stresses occurring in coatings. The coatings deposited in vacuum reveal overall stresses, which are composed of thermal and internal stresses. Thermal stresses result from the difference of the thermal coefficients of expansion of the coating and substrate material, whereas the internal stresses are closely connected with the deposition method and conditions [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 $Ti+Ti(C_xN_{1-x})$ 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 [4-6].

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 [7-8].

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 simulation and then were presented in tables 1 and 3 [9-11].

In order to carry out the simulation of internal stresses in $Ti+Ti(C_xN_{1-x})$ 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 $Ti(C_xN_{1-x})$ 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 3.

The evaluation of the phase composition of the obtained $Ti+Ti(C_xN_{1-x})$ 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 [9-10].

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

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.

3. Investigation results

Using experimental and table data (table 1,3) internal stresses were modeled in coatings in ANSYS, by using the finite element method. Figures 1-2 present obtained results of numerical analysis with the help of the finite element method gathered as distribution maps of stresses in $Ti+Ti(C_xN_{1-x})$ coatings. Numerical analysis showed occurrence of compress stresses on the surface of analyzed coatings, which don't exceed 1700 MPa. Value stress error in the simulated model do not exceed 5%. The comparative analysis was carried out of the results of computer simulation of stresses with the experimental results, what was presented in table 2.

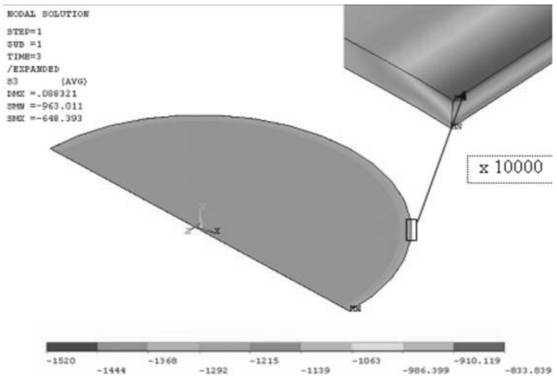

Fig. 1. Distribution of the simulated compression stresses in the $Ti+Ti(C_xN_{1-x})$ coatings in working atmosphere including 75% N_2 i 25% CH_4. (coating thickness g=6,4 μm, process temperature 460°C)

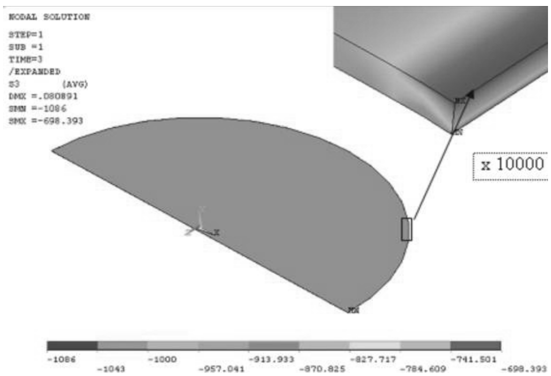

Fig. 2. Distribution of the simulated compression stresses in the $Ti+Ti(C_xN_{1-x})$ coatings in working atmosphere including 25% N_2 i % 75CH_4. (coating thickness g=4,7 μm, process temperature 500°C)

Process temperature, [°C]	Coating thickness, [μm]	Young's modulus, [GPa]	Poisson ratio
540	1,9	640	0,24
	3,5	550	
	5,5	520	
500	3,5	580	
	6	480	
	9,1	400	
460	4	440	
	6,4	400	
	10,1	400	

a.

Process temperature, [°C]	Coating thickness, [μm]	Young's modulus, [GPa]	Poisson ratio
540	2,9	500	0,20
	4,7	460	
	6,6	460	
500	3,1	480	
	4,7	460	
	9,1	440	
460	3,3	420	
	6	400	
	9,1	380	

c.

Process temperature, [°C]	Coating thickness, [μm]	Young's modulus, [GPa]	Poisson ratio
540	4,4	380	0,22
	7,4	420	
	11	365	
500	4,4	380	
	7,5	355	
	11	355	
460	4,1	540	
	6,7	500	
	4,4	380	

b.

Table 1.
The summary data of the coating material used for computer simulation of stresses in the Ti+Ti(C_xN_{1-x})

a. Ti+Ti(C_xN_{1-x}) coatings in working atmosphere including 75% N_2 i 25% CH_4
b. Ti+Ti(C_xN_{1-x}) coatings in working atmosphere including 50% N_2 i 50% CH_4
c. Ti+Ti(C_xN_{1-x}) coatings in working atmosphere including 25% N_2 i 75% CH_4

Where thermal expansion coefficient for all examined coatings amount to 9,4 [1/K] 10^{-6}

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
Ti+Ti(C_xN_{1-x}) coatings in working atmosphere including 75% N_2 i 25% CH_4									
Computer simulation results of overall stress,[MPa]	1224	1098	1122	1470	1215	1020	1670	1400	1378
Experimental results of overall stress,[MPa]	1237	1091	1126	1476	1215	982	1672	1409	1379
Error, [MPa]	13	7	4	6	0	38	2	9	1
Ti+Ti(C_xN_{1-x}) coatings in working atmosphere including 50% N_2 i 50% CH_4									
Computer simulation results of overall stress,[MPa]	997	1100	900	920	889	850	1076	957	950
Experimental results of overall stress,[MPa]	995	1107	905	917	882	849	1132	948	931
Error, [MPa]	2	7	5	3	7	1	56	9	19
Ti+Ti(C_xN_{1-x}) coatings in working atmosphere including 25% N_2 i 75% CH_4									
Computer simulation results of overall stress,[MPa]	1234	986	1030	998	885	882	835	930	802
Experimental results of overall stress,[MPa]	1233	983	1032	997	911	879	836	928	808
Error, [MPa]	1	3	2	1	26	3	1	2	6

Table 3.
The summary data of the substrate and interface material used for computer simulation of stresses in the Ti+Ti(C_xN_{1-x}) 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

4. Conclusions

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 [14-16].

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 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+Ti(C_xN_{1-x}) 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.

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