DOI: 10.1515/amm-2016-0084

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COMPUTER SIMULATION OF THE RELATIONSHIP BETWEEN SELECTED PROPERTIES OF PVD COATINGS

The possibility to apply the Finite Element Method to calculate internal stresses which occur in Ti+TiN, Ti+Ti(C_xN_{1-x}) and Ti+TiC coatings obtained in the magnetron PVD process on the sintered high-speed steel of the PM HS6-5-3-8 type. For the purpose of computer simulation of internal stresses in coatings with the use of MES, the correct model of analyzed specimens was worked out and then it was experimentally verified by comparison of calculation results with the results of computer simulation. Accurate analysis of correlations indicated especially strong dependence between internal stresses and microhardness and between microhardness and erosion resistance what created conditions for establishing the dependence between internal stresses obtained in the result of computer simulation and erosion resistance as basic functional quality of coating. It has essential practical meaning because it allows to estimate predictable erosion resistance of coating exclusively on the base of the results of computer simulation for used parameters in the process of coating manufacturing.

Keyword: Numerical techniques; Stresses; Microhardness, Computer simulation; Finite Element Method.

1. Introduction

Finite elements method is at present one of most widely used practical methods of solving of various engineering problems and it permits on time shortening of projecting and gives possibility to research the influence of each factors in the mathematical model [1-6]. 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 [7-10]. Sintered high-speed steels are important group of engineer materials. They are in use in production of cutting tools for hard-treatment materials [11-15].These steels work with large efficiency at required high working coefficients of reliability. Numerous scientific investigations showed, that influence on considerable improvement of tools exploitation persistence has the covering of tools with thin layer with the help of physical of-settling from gas- phases PVD (physical vapor deposition) techniques [16-18].

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.

In the paper mathematical model was presented which describes dependence between functional properties of two layers coatings Ti+TiN, Ti+Ti(C_xN_{1-x}) and Ti+Tin, in this case erosion resistance, with process parameters of its production. Elaborated model of the tool covered with coatings in the PVD process was verified by comparison of results obtained in calculation with experimental results.

2. Materials and methodology

The investigations were carried out on the samples made of sintered high-speed steel PM HS6-5-3-8 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 formig 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 forming in 6 minutes at the temperature relevant for this process, after which the next coating was forming within 60 minutes.

Measurements of stresses for the analyzed coatings were made by $\sin^2\psi$ rule 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 ψ towards the primary beam was changed in the range of 0° ÷ 75°

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 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):

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

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

Conditions deposition of analyzed coatings and their mechanical conditions which were experimentally determined and used in computer simulation were presented in table 1.

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 [13-15].

To avoid the error in the calculation of internal stresses in coatings applied variable size of finite elements, in places where the larger value of stresses was expected the mesh is more concentrated than in the area where the stresses should take similar values, so smaller elements are used in the coatings.

3. Results

Using experimental and table data , the internal stresses in coatings were simulated with the help of MES method using ANSYS. In the figures 1-2 were presented results of numerical analysis obtained by the finite element method gathered as maps of stresses distribution in Ti+TiN, Ti+Ti(C_xN_{1-x}), Ti+TiC coatings. Numerical analysis demontrated occurence of compress stresses on the surface of analysed coatings, which do not exceed 1700 MPa. On the basis of numerical analysis of the sample model with deposited coatings, it was found that value of the stresses on the surface of coatings depend on the coatings type and conditions of their deposition.

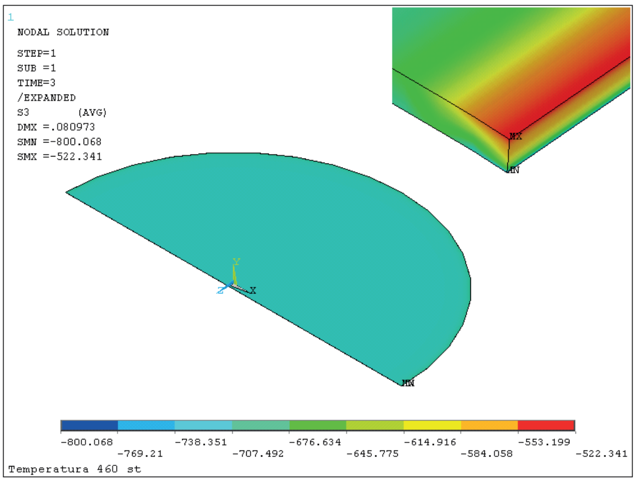

Fig. 1. Distribution of the simulated compression stresses in the TiN coating (coating thickness g=3.9 μm, process temperature 460°C)

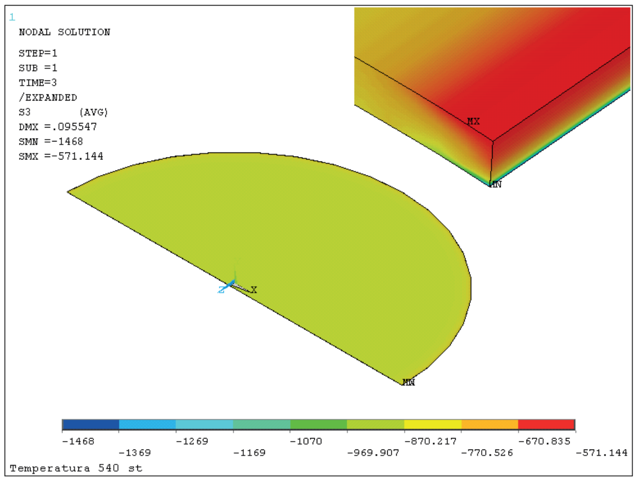

Fig.2. Distribution of the simulated compression stresses in the TiC coating (coating thickness g=2.6 μm, process temperature 540°C)

It was worked out two-dimensional scatter diagram for visual assessment of dependence between two analysed properties. Those diagrams contain value of linear correlation

TABLE1

The summary data of the substrate, interface and outer coatings material used for computer simulation of stresses in the Ti+TiN, Ti+Ti(C_xN_{1-x}) and Ti+TiC coatings

Material	Material thickness, [μm]	Young's modulus, [GPa]	Thermal expansion coefficient, [1/K] 10-6	Poisson ratio
Substrate (PM HS6-3-8)	4000	207	11.88	0.25
Interface (Ti)	1.1 0.9 0.7	113	8.6	0.24
Coatings TiN	2.2-10	470-562	9.5	0.26
Coatings Ti(CxN1-x)	1.9-10	355-640	9.4	0.24
Coatings TiC	2.5-6.9	350-440	7.8	0.19

coefficient, line of linear regression and confidence interval for linear correlation coefficient with established confidence coefficient p=0.95. All calculations were carried out in Statistica programme v.6.0 and total results obtained for all analysed coatings were presented in figures 3-4.

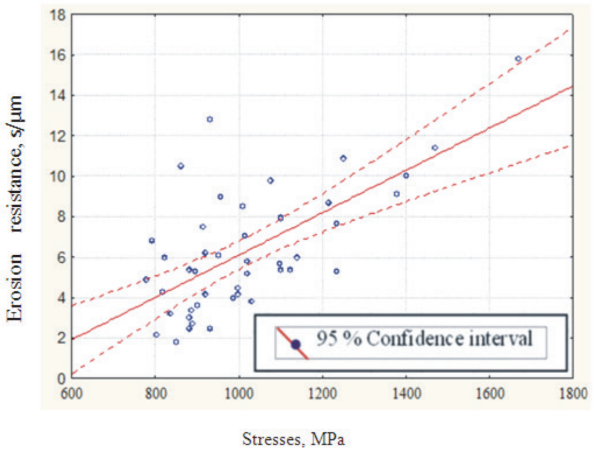

Fig. 3. Erosion resistance as a function of the internal stresses of analyzed coatings

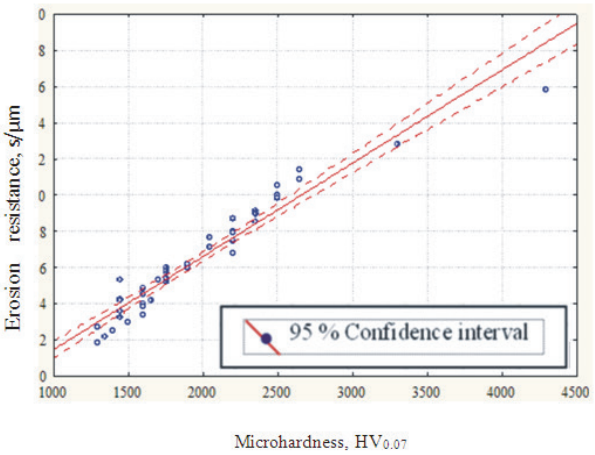

Fig. 4. Resistance to erosion as a function of microhardness analyzed coatings

Precise analysis of correlation research points particularly to strong dependence between internal stresses and microhardness and between microhardness and erosion resistance. It creates conditions for establishing dependence between quantity of internal stresses, obtained as a result of computer simulation, and erosion resistance that is essential usage feature of coatings. It has unusual and essential practical meaning, because after it was found that there is dependence between stresses and erosion resistance, the mathematical model was worked out, which allows to establish predictable erosion resistance of coating exclusively on the base of the results of computer simulation for established parameters in the process of coating production.

It was taken the following equation form (2):

$$ER = b_0 + \sum_{i=1}^{n} b_i x_i + \sum_{i,j=1} b_{i,j} x_i x_j \qquad (1)$$

where:
ER – erosion resistance,
b_i – model coefficient,
x_i – independent variable, in this case microhardness and internal,
n – variable equation number in this case 2.

Analysis of regression was carried out in Statistica programme and obtained values of equation coefficients were presented in table 2.

The formulated model was experimentally verified, which consist in analysis of calculation compatibility with experimental results of research on erosion resistance of coatings. Medium error of erosion resistance estimation for all analysed coatings was assumed as quality criterion of analysed model. Carried out verifying calculations presents that this error is 0.42s/ µm, whereas nominal values of erosion resistance, which were obtained through analyzing the coating, contain in area of 2-16 s/µm. Such value of estimation error one should recognize as sufficient for preliminary quality estimation of obtained coatings. In figure 5 was presented a superficial diagram 3W which shows a graphical formulated mathematical model. Surface generated on the basis of 380 points.

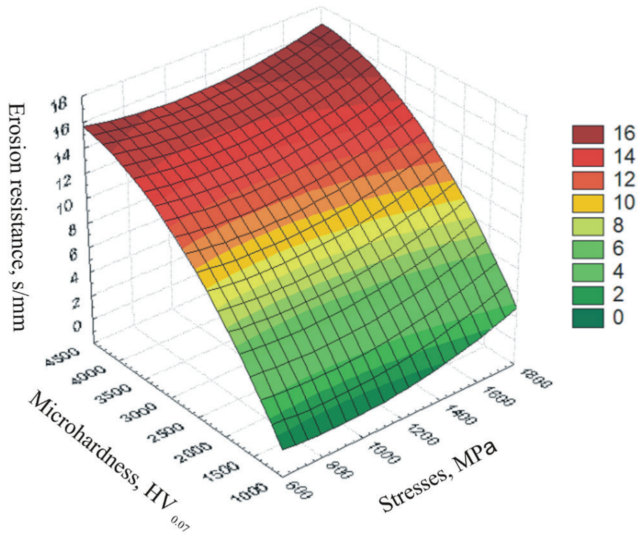

Fig. 5. 3-dimensionalgraph representing the of mathematical model which describes the erosion resistance as a function of internal stresses and microhardness

TABLE 2

Statement of equation coefficients describing the erosion resistance of analyzed coatings

Coefficients	b_0	b_1	b_2	b_{11}	b_{12}	b_{22}
Value	-6.7975	-0.0054	0.0104	3.3E-06	3.77E-07	-1.04E-06

4. Summary

It should be especially emphasized the practical aspect, which is possible thanks to formulated model, because it is able to successfully replace so called a technological test which is very often carried out at present. This technological test consist in single selection of process parameters set needed in coating production, taking for granted required usage properties of coating and next experimental verification of taken properties. In the result of such a test, when a coating demonstrates required properties, the research process and analysis is finished, whereas required properties are not reached by a coating the set of test is carried out for another set of technological parameters. Taking for granted, in the case of technological tests, the complex tests, analysis of process parameters and properties of coating are not carried out in order to avoid time consuming and expensive research. It is dictated by requirements of contemporary process of production, where at regular intervals of period there is a tool rearming of production devices with the purpose of putting in motion a short term production of new products, what creates requirements of competition. Taking into consideration this tendency, presented in this paper the method of stresses simulation and formulated on its base the model, which is used to estimate erosion resistance of coatings, constitutes an alternative for described technological test.

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