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Simulation of internal stresses coatings deposited onto magnesium alloys by use of FEM

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ABSTRACT

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

Design/methodology/approach: Article introduces the usage of finite elements method for simulation of stresses measurement process in Ti/Ti(C,N)/CrN, Ti/Ti(C,N)/(Ti,Al)N, Ti/(Ti,Si)N/(Ti,Si) N, Cr/CrN /CrN, Cr/CrN/TiN and Ti/DLC/DLC coatings of the physical vapour deposition and chemical vapour deposition surface treatment performed on samples of heat treated cast magnesium alloy

Modeling of stresses was performed with the help of finite element method in ANSYS environment, and the experimental values of stresses were determined basing on the $\sin^2\psi$.

Findings: 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: The computer simulation results correlate with the experimental results. However for achieving better calculation accuracy in further researches it should be developed given model which was presented in this paper.

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: Magnesium alloys; Residual stress; Computer simulation; PVD, CVD, MES

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METHODOLOGY OF RESEARCH, ANALYSIS AND MODELLING

1. Introduction

Finite elements method is at present one of most widely used practical methods of dissolving of all engineer problems and permits on time shortening of projecting and gives possibility to research the influence of each factors on the whole mathematical model [1-8, 27,28]. 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 [9-12].

Internal stresses occurred in analysed materials 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 [13-15, 29,30].

The general topic of this paper is very important surface engineering issue, namely, surface treatment of selected magnesium cast alloys using vacuum techniques [16-24]. These alloys are currently recognised by materials science experts as future materials combining low density and high strength. This improves their functional properties and makes it possible to employ the FEM for evaluation of stresses in the investigated coatings. The key question here seems to be how to promote the simultaneous development of both the production technology and processing of these light construction materials and the technology of forming and protecting their surface. This will, in consequence, enable a balance to be maintained between the modern substructure material and new generation coating.

2. Methodology and computer simulation

2.1. Investigation methodology

The tests were carried out on the samples made of magnesium alloy on which were deposited Ti/Ti(C,N)/CrN, Ti/Ti(C,N)/(Ti,Al)N, Ti/(Ti,Si)N/(Ti,Si)N, Cr/CrN/CrN, Cr/CrN/TiN and Ti/DLC/DLC coatings in PVD and CVD process. Conditions for the deposition of the individual coatings are shown in Table 1.

In the plasma assisted CVD process, a relatively low surface treatment temperature was used to produce a carbon DLC coating at a specified pressure and in a C2H2 acetylene atmosphere. The gradient of the resulting coating was achieved by a variable concentration of silicon (Me) in the middle layer. Silicon was supplied to the furnace chamber in the gas phase: Ti/a-C:H-Me/a-C:H. The second method was implemented using the DREVA device ARC400, supplied by Vakuumtechnik, using the electric arc cathodic evaporation method. The device is equipped with three independent sources of metal vapours. Discs of 65 mm optical density were used for PVD coatings, cooled with water, containing pure metals (Cr, Ti) and alloys TiAl and TiSi. The coatings were deposited in an inert atmosphere of Ar and reactive N2 atmosphere in order to obtain a mixture of nitrides, as well as N2 and C2H2 mixture in order to obtain layers of carbonitrides. The gradient concentration change of the chemical composition of the coating cross-section was obtained by changing the proportion of reactive gas or by changing the evaporation current on the arc sources. The set coating process conditions are presented in a previous in Table 1.

Measurements of stresses for the analysed 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 ψ towards the primary beam was changed in the range of 0° - 75° (Fig. 1) [25,26].

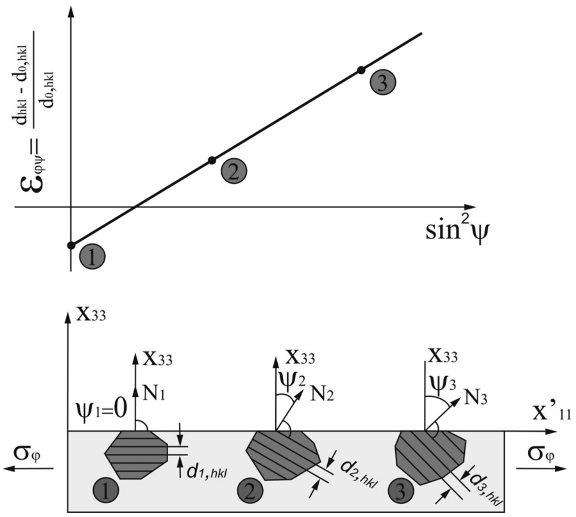

Fig. 1. Linear dependence in a classical method of $\sin^2\psi$ valid for assumptions of homogenous and plain stress state at points 1, 2, 3 correspond to measurements of values for interplanar distance at suitably - oriented grains of microstructure in different directions at y angle

2.2. Numerical simulation model

Computer simulation of the stresses occurring in the PVD and CVD coating was performed using the finite element program ANSYS.

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.

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.

In order to carry out the simulation of internal stresses in Ti/Ti(C,N)/CrN, Ti/Ti(C,N)/(Ti,Al)N, Ti/(Ti,Si)N/(Ti,Si)N, Cr/CrN/CrN, Cr/CrN/TiN and Ti/DLC/DLC 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 and CVD process presents the cooling process of specimen from 150°C to ambient temperature of 20°C, for Ti/Ti(C,N)/CrN, Ti/Ti(C,N)/(Ti,Al)N, Ti/(Ti,Si)N/(Ti,Si)N, Cr/CrN/CrN, Cr/CrN/TiN Ti/DLC/DLC and a substrate (magnesium alloy),

materials properties were established on the basis of and Mat Web catalogue, which was presented in Table 2.

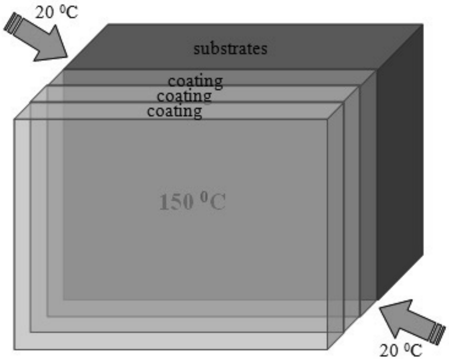

Fig. 2. Real model of coatings

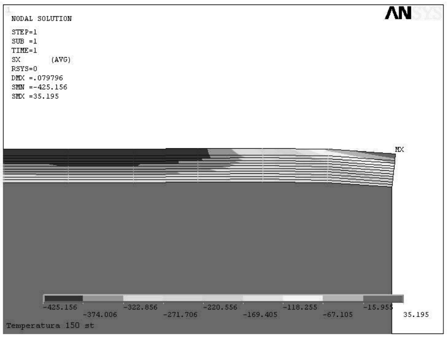

Fig. 3. Distribution of the simulated compression stresses in the Ti/DLC/DLC coating: stress distribution of the edge

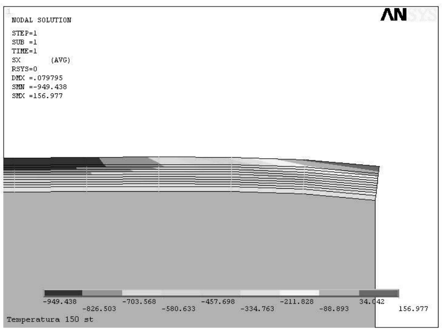

Fig. 5. Distribution of the simulated compression stresses in the Ti/(Ti,Si)N/(Ti,Si)N coating: stress distribution of the edge

Fig. 2 presents the geometrical form of magnesium alloy with the deposited Ti/Ti(C,N)/CrN, Ti/Ti(C,N)/(Ti,Al)N, Ti/(Ti,Si)N/(Ti,Si)N, Cr/CrN/CrN, Cr/CrN/TiN and Ti/DLC/DLC coatings.

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.

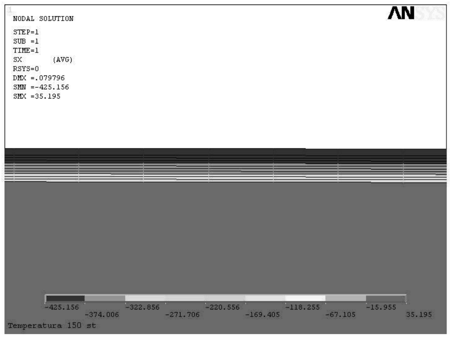

Fig. 4. Distribution of the simulated compression stresses in the Ti/DLC/DLC coating: stress distribution of the centre

3. Results

Based on data referring to the substrate, and coating material properties (Young's modulus, Poisson's ratio, and thermal expansion coefficient), the stresses in the investigated specimens can be determined (Table 2). Analysis of the obtained simulation results shows that, in each case, the stress has a compressive nature, a negative value, causing 'compression' of the achieved coatings to the substrate surface, with the average value σ=425/1377 MPa (Table 3). The occurrence of compressive stress in the surface layer can prevent the formation of cracks under operating conditions, when the element is subjected to stresses coming from outside forces. However, compressive stresses that are too great can lead to adhesive wear and excessively high tensile stresses in the coating, so reducing the fatigue resistance of the element. It was found out from the performed simulation that either the use of magnesium substrate and the application of the CVD method results in a significant decrease in the absolute value of the residual stresses that occur. Reduction of the residual stresses in the deposited coatings also influences the adhesion to the substrate; this was confirmed using the scratch test and could be one of the main factors to improve functional properties such as wear resistance.

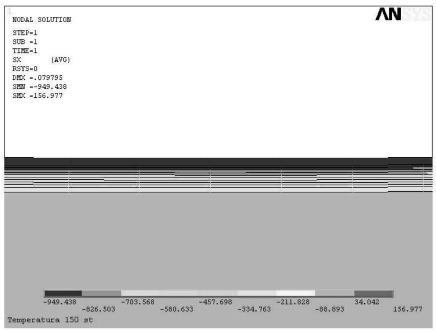

Fig. 6. Distribution of the simulated compression stresses in the Ti/(Ti,Si)N/(Ti,Si)N coating: stress distribution of the centre

Table 1.
Conditions of coatings deposition

Process parameters	Type of produced coatings and used technique of coating application					
	PVD					PACVD
	Ti/TiCN-gradient/CrN	Ti/TiCN-gradient/TiAlN	Cr/CrN-gradient/CrN	Cr/CrN-gradient/TiN	Ti/TiSiN-gradient/TiSiN	Ti/DLC/DLC
Base pressure, Pa	$5x10^{-3}$	5×10^{-3}	5×10^{-3}	$5x10^{-3}$	$5x10^{-3}$	$1x10^{-3}$
Working pressure, Pa	$9.0x10^{-1}$ /1.1-1.9/2.2	$9.0x10^{-1}$ /1.1-1.9/2.8	1.0/1.4-2.3/2.2	1.0/1.4-2.3/2.2	$8.9x10^{-1}$ /1.5-2.9/2.9	2
Argon flow, cm^3/min	80*	80*	80*	80*	80*	80*
	10**	10**	80**	80**	20**	-
	10***	10***	20***	20***	20***	-
Nitrogen flow, cm^3/min	225→0**	0→225**	0→250**	0→250**	0→300**	-
	250***	350***	250***	250***		
Acetylene flow cm^3/min	0→170**	140→0**	-	-		230
Substrat voltage, V	70*	70*	60*	60*	70*	500
	70**	70**	60**	60**	100**	
	60***	70***	60***	100***	100***	
Current intensity in cathode, A	60	60	60	60	60	-
Proses temperature, ºC	<150	<150	<150	<150	<150	<180

* during deposition of metallic coating, ** during deposition of gradient coating, *** during deposition of ceramic coating

Table 2.
Parameters used in computer simulation of stresses occurring in analysed coatings and substrate material

Material	Young's modulus, [GPa]	Thermal expansion coefficient, [1/K] 10^{-6}	Poisson ratio
Substrate (magnesium alloy AZ91)	45	7.0	0,35
Couting DLC	140	8.6	0.22
Couting (Ti,Si)N	450	13	0.25
Couting CrN	360	2.3	0.28
Couting Ti(C,N)	460	9.4	0.2
Couting Cr	140	6.2	0.31
Couting Ti	113	8.5	0.34
Couting (Ti,Al)N	460	9.35	0.25

Table 3.
Reduced stress values occurring in analysed coatings and thickness

Substrate	Coatings type					
	Ti/Ti(C,N)/CrN	Ti/Ti(C,N)/(Ti,Al)N	Cr/CrN /CrN	Cr/CrN/TiN	Ti/(Ti,Si)N/(Ti,Si)N	Ti/DLC/DLC
	Thickness/μm					
AZ91	< 3.3	< 3.2	< 1.8	< 1.8	< 1.5	< 2.5
	Stress values achieved / MPa					
	-1325	-1210	-1377	-1329	-949	-425

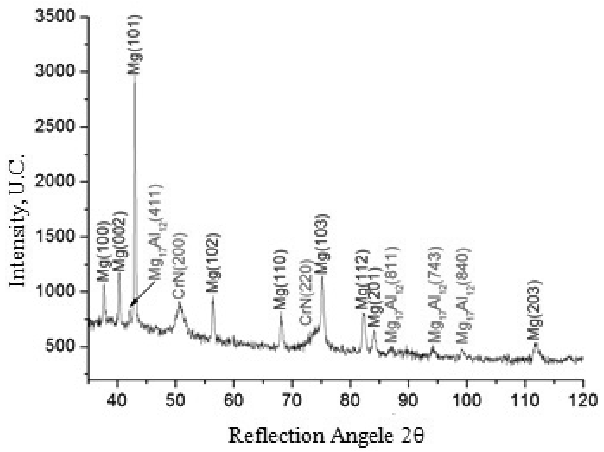

Fig. 7. Diffraction patterns of the magnesium alloy with the Cr/CrN /CrN coatings

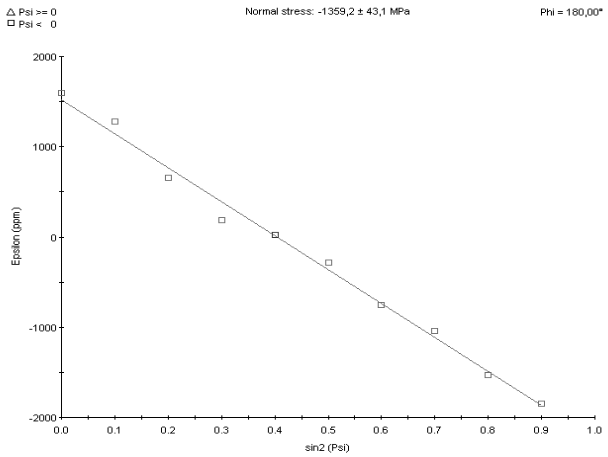

Fig. 8. Change of a_0 value in g-sin$^2\psi$ function for Cr/CrN /CrN coating deposited on cast magnesium alloy substrate

For verification of the computer simulation results, the values of internal stress in selected coatings were calculated using the X-ray technique g-sin^{2}y using the computer software X'Pert Stress Plus. This software contains in the form of a database the necessary data for calculating the values of different material constants.

In the Figs. 3-6 were presented the results of numerical analysis using finite element collected as maps stress distribution on the edge and in the centre of in the Ti/DLC/DLC, Ti/(Ti,Si)N/(Ti,Si)N and Ti/Ti(C,N)/CrN coatings in ANSYS program. Stresses' error in the simulated model doesn't exceed 5%.

Using methods of X-ray qualitative phase analysis found that under the assumptions on the surface of cast magnesium alloy was covered by Cr/CrN /CrN coatings. Diffraction images used for measuring residual stresses of the analysed coatings deposited on sintered high speed steel are shown in Figs. 7 and 8.

Based on the obtained results, using the X-ray g-sin^{2}y method, the applied FEM model assumptions are clearly found to comply with and be fully relevant to the actual measurement data. In each of the cases analysed, the calculation results are consistent with the results of finite element computer analysis and are within the range of error.

All results presented in the work were analysed statistically by calculating average value for each series of measurements, standard deviation, variance and confidence intervals assuming a significance level = 0.05

4. Conclusions

Of the basis of researches results it was found that using advanced technique of calculation among others thing the finite elements method MES, can be exploited as tools using in surface engineering to coatings characterizing. This method allows to realize complex analysis proceeding during processes of coatings spread and also analysis of phenomena occur as an effect of final process. One has to indicate that such analysis need knowledge of many quantities as physical and mechanical properties of substrate material and coating and also its parameters of spread. As a result of this mentioned above method allows to create a model which describes inner stresses in relation to parameters of process and also to kind of substrate material and to coatings.

Taking into consideration the 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 FEM programs.

As a result of experimental researches and computer simulation of formed residual stresses in Ti/Ti(C,N)/CrN, Ti/Ti(C,N)/(Ti,Al)N, Ti/(Ti,Si)N/(Ti,Si)N, Cr/CrN/CrN, Cr/CrN/TiN and Ti/DLC/DLC of the physical vapour deposition and chemical vapour deposition surface treatment performed on samples of heat treated cast magnesium alloy, it was found the occurrence of compressive stresses with the average value of σ=425/1377 MPa, what ensures the rise of strength properties.

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