International Exhibition of Innovation
IEI 2023

Innovative method of properties determination in PVD coatings using FEM

Tomasz Tański, Agata Śliwa, Marek Sroka, Mirosław Bonek, Waldemar Kwaśny

Silesian University of Technology, Institute of Engineering Materials and Biomaterials,
Konarskiego St. 18a, 44-100 Gliwice, Poland
Corresponding author:agata.sliwa@polsl.pl

Introduction

The aim of the research is the computer simulation of the internal stresses in PVD process. The experimental values of stresses were determined basing on the X-ray diffraction patterns using method sin2Ψ and computer simulation of stresses was carried out in MARC environment, with the help of finite elements method. 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. It was confirmed that using of finite element method for estimating stresses in PVD coatings can be a way for reducing the investigation costs Results reached in this way are satisfying and in slight degree differ from results reached by experimental method. However for achieving better calculation accuracy in further researches it should be developed given model which was presented in this paper, Presently the computer simulation is very popular, what 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

Results and discussion

As a result of the factographic investigations performed on a scanning electron microscope, it was found that the deposited coatings determine column structure and particular layers are uniformly deposited and tightly adhere to each other as well as to the substrate's material (Fig.1). The results of X-ray qualitative phase analysis confirmed occurrence of adequate phases in tested substrate and in coating material. (Fig.2). On the basis of performed pole figures (Fig.3, 4) it was found that apart from temperature process of analyzed coating shows privileged <110> increase direction. Above-mentioned coatings are characterized by very good adhesion to substrate material what is indicated by high values Lc obtained during the time of parameter's measurement by "scratch- test" method. The results of carried out researches concerning internal stresses of analyzed coatings indicates the interdependence between stresses' value and their adhesion to substrate material.

Using experimental and table data, internal stresses in coatings in environment ANSYS were modeled by the use of the finite elements method. Figure 5 and 6 presents obtained results of numerical analyze shown as stresses deposition maps in coatings Ti+Ti(C,N)). Numerical analyze showed existence of compress stresses in analyzed coatings, which don't exceed -1430 MPa. Table 1 presents results of stresses experimental determined and by the use of computer simulation and also results of thickness, and microhardness.

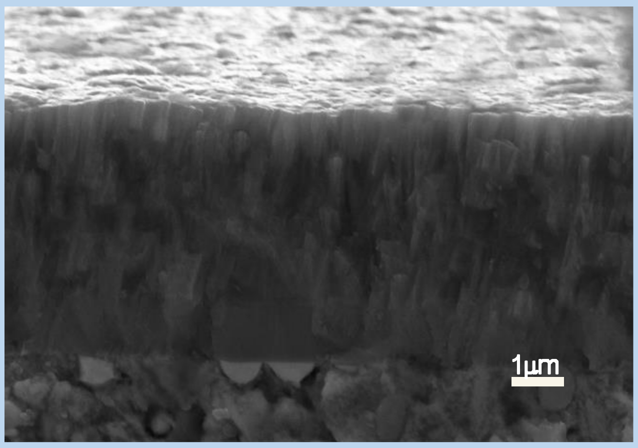

Fig. 1. Brittle fracture of a coating Ti+Ti(C,N) obtained in the magnetron PVD process, (the process temperature 500ºC).

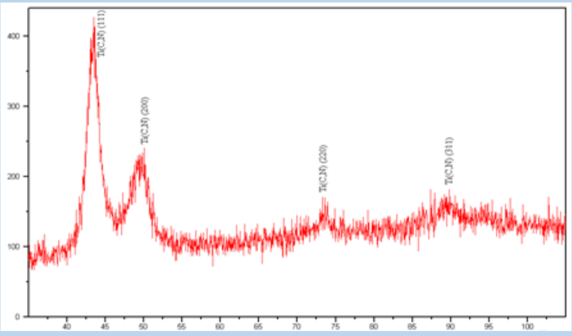

Fig. 2. X-rays diffraction patterns of the sintered high-speed steel PM HS6-5-3-8with the Ti+Ti(C,N) coatings, (the process temperature 500ºC). Geometry of constant angle of incidence.

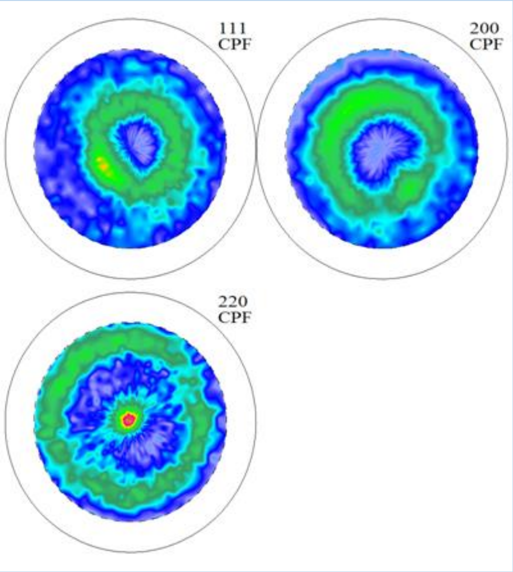

Fig. 3. Experimantal pole figures (111), (200) and (220) of Ti+TiN coating, (the process temperature 500ºC).

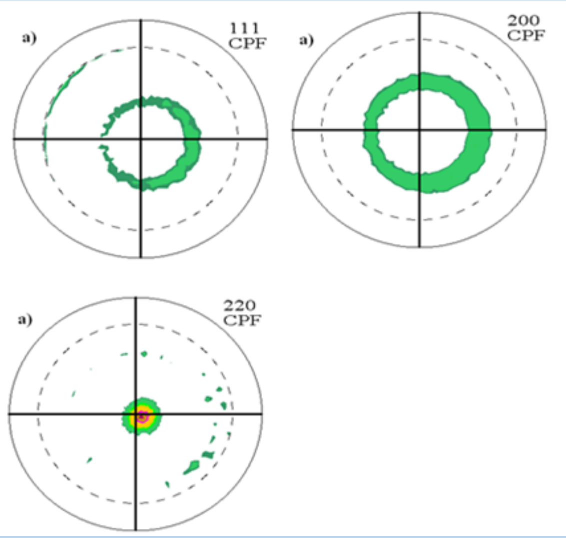

Fig. 4.. Experimantal pole figures (111), (200) and (220) of Ti+Ti(C,N) coating, (the process temperature 500ºC

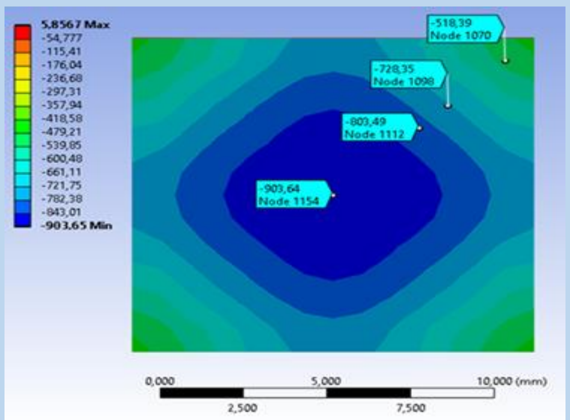

Fig. 5. Distribution of the simulated compression stresses in specimen covered with the Ti+Ti(C,N) coatings, (process temperature 540°C).

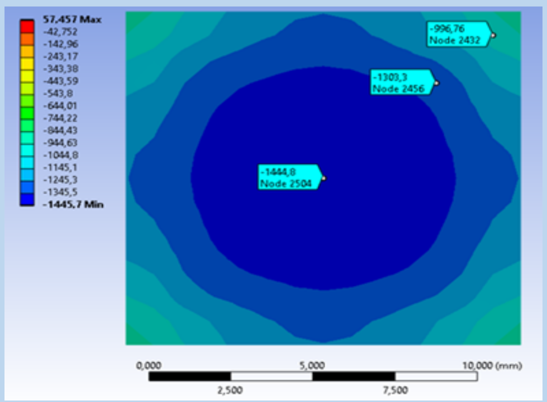

Fig. 6. Distribution of the simulated compression stresses in specimen covered with the Ti+Ti(C,N) coatings, (process temperature 460°C).

Table 1. Results mechanical properties of Ti(C,N) coatings at sintered high-speed steel PM HS6-5-3

Process temp. [°C]	Thickness [μm]	Microhardness [HV0,07]	Experimental stress results, [MPa]	Computer simulation stress results, [MPa]
460^0	4,6	2650	-1400	-1444
500^0	4,2	2590	-1215	-1200
540^0	3,9	2420	-1060	-903

Summary

I In the result of analyzed texture it was found that tested coasting shows privileged <110> increase direction apart from conditions of their obtaining.

On the basis of performed researches it was found that the coatings shows higher values of compression stresses and shows better adhesion to substrate material and also higher microhardness.

The model presented in the project was developed by the use of the finite element method, using ANSYS program what makes possible to estimate internal stresses occurring in coatings Ti+Ti(C,N) obtained in magnetron process PVD. On the basis of the data concerning properties of material's substrate and coatings (Young's modulus, Poisson ratio, Thermal expansion coefficient) it is possible to estimate internal stresses in tested samples. The results of computer simulation correlate with results obtained in experimantal way.