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Simulation of the microhardness measurement of PVD coatings by use of FEM

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Analysis and modelling

ABSTRACT

Purpose: The purpose of the presented work is describing the numerical determination of coatingss microhardness obtained in PVD process with use of finite elements method and comparative analysis with results obtained by laboratory investigations.
Design/methodology/approach: Article introduce the usage of finite elements method for simulation of the TiN coatings microhardess measurement. Coatings was obtained in magnetron PVD process on high-speed steel ASP 30 substrate. Simulation of indenters pit in investigated coat permitts in deformation disclosure of the PVD layer and allows to create the stresses maps.
Findings: Basing on tensions acquired in result of the depression caused in investigated surfaces by the intenter the maps of stresses, the deformations of analyzed coats, and the microhardness was calculated.
Research limitations/implications: On the tensions basis obtained in result of computer simulation effected in ANSYS software environment was possible to compute the microhardness of the coating. The results was compared with the microhardness of the coatings acquired by physical examination with use of the Vickers method.
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: Numerical techniques; Microhardness; Computer simulation; Finite Element Method

1. Introduction

Sintered high-speed steels are important group of ingineur materials. They are applied in production of machinning tools for tooling of hard treatment materials. They work with large efficiency at required enlarged coefficients of work reliability. Numerous scientific investigations has shown, that influence on considerable improvement of tools exploitation persistence has the covering process of tools with thin hard-melting compounds layer of carbon, boron nitrogen, interim metals and some oxides The covering technique is physical of-settling from gas- phases PVD (physical vapour deposition). Increasing covered tools persistence with PVD coatings is binded with the considerable increase of coat hardness with the reference to the base material. Hardness of coaing material depends on bondings in coat. Materials with ionic bondings (eg oxides) have high hardness but simultaneously are brittle, metal materials having very good adhesion to substrate. Proprieties, that provide the most universal usage are materials with metallic bonings (borons, carbides and nitrogens of interim metals) and therefore these materials have the widest practical use [1, 2].

Finite elements method is at present one from most widely used practical methods for dissolving of all ingineur problems. They are in use eg in such spheres of science as: solid mechanics, fluid mechanics, biomechanics, material engineering, thermal analysis and magnetically and electrically analysis. Finite elements method permits in considerable time shortening for projecting processes and gives the possibility to research the influence of each factors on the whole mathematical model. Usage of this method from the economic point of view is well-granted, because, more than once, it permits to avoid the expensive laboratory investigations, and results obtained during this simulation are reliable and well approximate to real values [3-8].

Model presented in this work makes possible to determine the TiN coatings microhardness of the examined samples obtained in PVD process in various deposition circumstances.

2. Materials

Thin films of the coatings was deposited by reactive magnetron sputtering onto polished high-speed steel ASP 30 substrates, that contains 1.28% C, 4.2% Cr, 5.0% Mo, 6.4% W, 3.1% V and 8.5% Co. Before deposition the substrates were heat treated in the salt bath furnaces with austenitising at the temperature of 1180°C and three-stage tempering at the temperature of 540°C After that, all specimens were mechanically polished. Depositions were lead using the single chamber vacuum furnace with the built in magnetron for ion sputtering. The distance between target and substrate were 125, 95 and 70 mm. The magnetron target was made from the titanium alloy containing 90%Ti, 5.7%Al, 1.4%Cr and 2.0%Mo. The coating deposition process was take place at temperatures of 460, 500 and 540°C. The TiN layer was deposited by 60 minutes at the temperature relevant for this kind of process [1,3-7].

3. Methodology

The chemical composition of the coated films (table 1) was determined by Glow Discharge Optical Spectroscopy GDOS.

Examinations of the coating thickness were made with use of the ”kalotest” method. The measurement process took place by the characteristic parameters of the crater developed as a result of the wear on the specimen surface caused by the steel ball with the diameter of 20 mm [1,3-7].

The microhardness tests of the coatings were done on the SHIMADZU DUH 202 ultra-microhardness tester. Young's modulus was calculated using the HARDNESS 4.2 program, that is a part of the ultra-microhardness tester system, according to the formula [1,3-7]:

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

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

Mathematical model created in the program is created by surfaces, that are representations of indenter surface, investigated PVD layers and steel substrate. By taking under consideration, that the real model is symmetrical, the other model created in Ansys is a quarter of the real model size (fig. 1). At maintenance of suitable margin conditions in the symmetry surfaces, such simplification doesn't have any influences on simulation results, but produce considerable shortening of time necessary for calculations in the program.

Surface, that represents the indenters surface is modeled as unmemorable by use of the MESH200 library unit. This unit is a "mesh unit” and is not a subject of any calculations. Significantly unit MESH200 is lineal and possesses two hitches. In work was used a square unit described on four hitches (QUAD 4-NODE). The model of the investigated sample with inserted mesh of finite elements is showed on fig. 2.

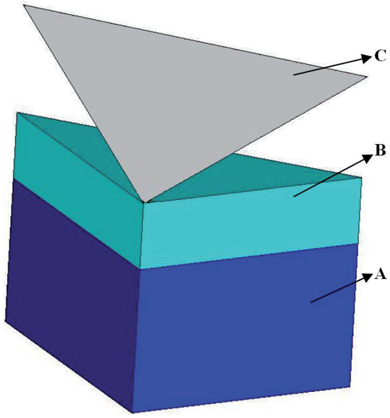

Fig. 1. Model of the sample: A – Substrate (ASP 30), B – Coating (TiN), C – Indenter Model Surface

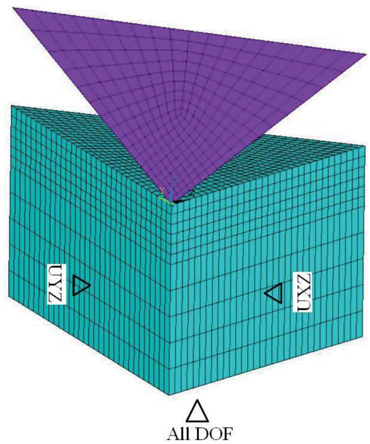

Fig. 2. Analyzed model with the overlaid finite elements mesh

Selection of the PVD layer elements and steel substrate elements should assure the ability to deformations and stresses occurrence. That's why the unit SOLD185 was chosen. This unit is used for three-dimensional modeling of block structures. Defined across eight hitches, have three translate freedom degrees in every direction (UX, UY, UZ) and material properties (eg Young modulus, Poisson ratio, thickness, thermal conduction). Significantly, unit describes the global system of coordinates.

Mechanical properties of PVD coats are described according to table 1. However steel materials used as substrates remains consistent for numerous simulations and carry out:

- Young modulus,: E = 2.05 × 10^5 MPa,
- Poisson ratio: ν = 0,28.

Table 1.
Influence of deposition conditions on chemical bonds and mechanical properties of analyzed coatings

Number of the sample	Process temperature, [°C]	Coating thickness, [µm]	Young's modulus, [MPa]	Poisson ratio	$HV_{0,05N}$	Computer simulation of stresses, [MPa]	Computer simulation of microhardness, [HV]
1	460	4.7	440000	0.26	3300	15440	2918
2		6.7	415000		2500	10195	1926
3		10.0	350000		1400	9774	1847
4	500	2.2	380000		1750	9131	1725
5		3.7	355000		1450	10125	1913
6		5.0	355000		1450	10218	1931
7	540	2.3	380000		1750	9385	1773
8		3.8	400000		2200	10216	1930
9		6.1	365000		1600	9804	1852

To assure the univocal position of the model in space the bottom surface of the model was fixed as unmovable (fig. 2) All freedom degrees was taken. The edge conditions in symmetry surfaces are given on axis Y on surface XZ, and on axis X on surface YZ (fig. 2).

For description of the contact the indenter surface and frontal surface of PVD layer the CONTA174 unit was used. This unit is placed on block surface and is defined across eight hitches. Geometry of the unit and bearings of hitches one showed on fig. 3.

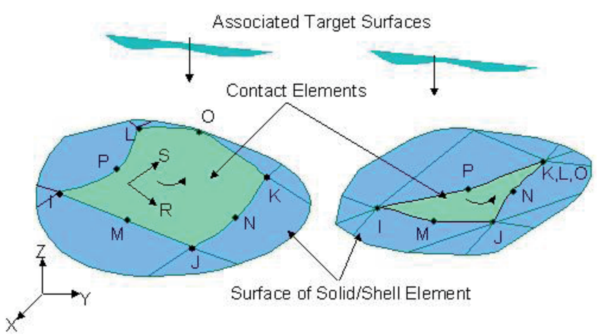

Fig. 3. Geometry and position of CONTA174 elements

In attention, that the used friction contact model is strongly non-linear the addiction of an encumbrance through dislocation was performed in aim of better numeric stability obtainment.

The encumbrance during microhardness tests with use of Vickers method was precisely chosen, that penetrator engrossment was not greater than 1/10 of the deposited coatings thicknesses. Therefore, to hold the conditions so near to the real conditions as possible across the whole simulation, the given surface engrossment, that represents the indenter surface was set on 10% of the examined layers thicknesses.

4. Results

Accomplished researches of mechanical property demonstrate, that examined coatings having very high hardness, dependenent of deposition process parameters. Basing on relationship between encumbrance and relief in function of indenter engrossment on the examined material during microhardness measurements the longitudinal elasticity module of analyzed coatings was calculated (table 1).

The stresses originate in result of indentent engrossment in the examined coatings was modeled with use of the experimental data. As a result of the simulation the deformation and the contour maps of stresses were determined from the model. (fig. 4).Then, the microhardness of analyzed coatings was calculated.

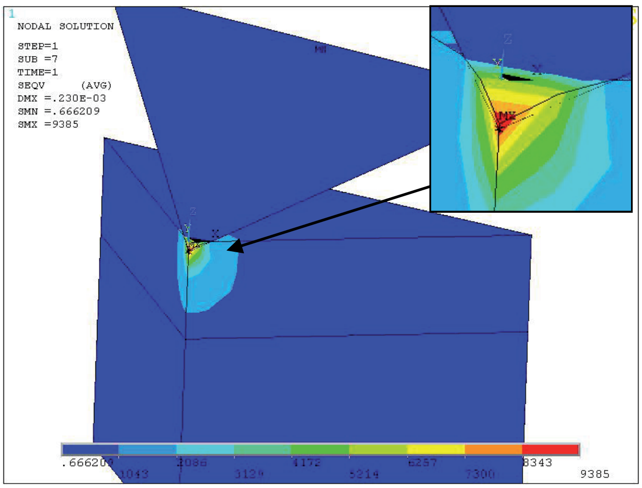

Fig. 4. Deformation and the map of stresses in TiN coat (thickness of coat g=2. 2 µm, temperature of process 540°C)

In the ANSYS system was possible to compute the median value of stresses with use of an equation [9]:

$$SMX = \max_n \{\sigma_n^a\} = \frac{\sum_{i=1}^{N_e^n} \{\sigma_n^i\}}{N_e^n} \tag{2}$$

where:
N_e^n – number of units joining with hitch n,
σ_n^i – stersses in hitch n counted for i- unit.

In ANSYS programme the SMX signature is used for printouts and on maps of stresses.

Microhardness of examined coatings was computed from the equation:

$$HV_{simulation} = 0{,}189 \times SMX \quad (3)$$

Microhardness results obtained with use computer simulation was compared with the experimental results. Results are shown on fig. 5.

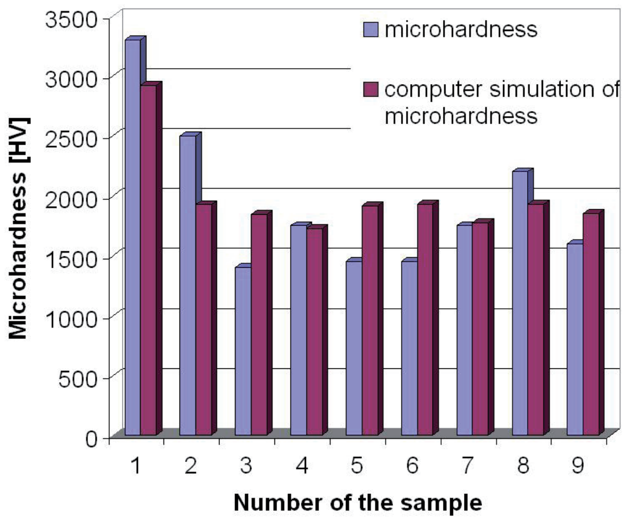

Fig. 5. Comparison between computer simulation results and experimental investigations results for TiN coatings microhardness

5. Conclusions

Microhardness of waste-resistant PVD coatings placed on cutting tools blades is very important material feature. Super hard coatings deposited on sintered steel perform in considerably increase of the tools persistence. Such coatings are characterized by greater abrasion resistance, enlarging the tools persistence and make possible the usage of higher machining parameters with maintenance of lower tool temperatures. This paper describe the model compiled with use of finite elements method, which makes possible the microhardness calculations of coatings obtained in magnetron PVD process. On the material data basis is possible to acquire the arise in coatings stresses in result of indentent engrossment in the examined material, and then, on the basis of these stresses to obtain the microhardness. Results of computer simulation method are comparable with laboratory results. The ANSYS model programmed with use of finite elements method permits to analyze the mechanical properties of PVD coatings, what makes plausible its application for computation of the anti-waste coatings microhardness. The computer simulation is cheaper in comparison with the laboratory investigations.

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