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Employment of the Finite Element Method for determining stresses in coatings obtained on high speed steel with the PVD process

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Abstract: The paper presents the possibility to employ the Finite Element Method for evaluation of stresses in the Ti+TiN coating obtained in the magnetron PVD process on the sintered high-speed steel of the ASP 30 type, taking into account their deposition conditions. Computer simulation results were compared with the experimental results of stress measurement in the analysed coatings.

Keywords: Coatings PVD, Computer Simulation, Stresses.

1. INTRODUCTION

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. Taking into account the specific properties of cutting tool operation, our attention was focused on the issue of stresses occurring in coatings.

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 the relationships among various parameters better and makes it possible to select the optimum solution [1-2].

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+TiN coatings. The comparative analysis was carried out of the results of computer simulation of stresses with the experimental results.

2. MATERIALS

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, 5.0% 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 [3,4].

3. METHODOLOGY

The evaluation of the phase composition of the obtained Ti+TiN coatings was carried out employing the SEIFERT-FPM XRD7 Advance X-ray diffractometer, using the filtered radiation of the cobalt K α anode lamp, powered with 40 kV voltage, at 40 mA heater current. The measurements were made in the 2 Θ angle range from 30 to 120°. The macro-stresses values were evaluated basing on spacing of reflections coming from the crystallographic lattices' planes of phases constituting the coatings and basing on the Young's modulus values determined experimentally [9-14]. The internal macro-stresses were determined using the formula:

$$\sigma = -\frac{E}{2\nu} \cdot \frac{d - d_0}{d_0} \quad (1)$$

ν - Poisson ratio,

E – Young's modulus,

d - lattice parameter with internal stresses, determined basing on the X-ray diffraction pattern,

d_0 - lattice parameter without internal stresses (obtained from tables).

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 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 [5].

The real specimen's dimensions were used for development of its model needed for determining the stresses in the Ti+TiN 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 [6].

Figure 1 presents the geometrical form of the ASP 30 sintered high speed steel test piece with the deposited Ti+TiN coatings. The geometrical model of the investigated coating overlaid with the finite elements' mesh is presented in Figure 2.

Table 1.

The summary data of the substrate, interface, and outer coating material used for computer simulation of stresses in the Ti+TiN coatings

Material	Thermal expansion coefficient, [1/K] 10 ⁻⁶	Young's modulus, [MPa] 10 ³	Poisson ratio
Substrate (ASP 30)	11.88	207	0.25
Interface (Ti)	8.6	113	0.34
Outer coating (TiN)	9.35	350-440	0.26

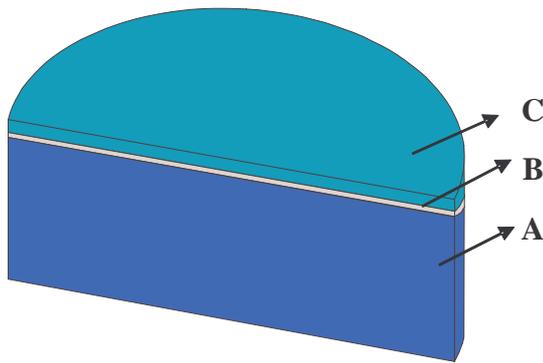


Figure 1. Test piece from the ASP 30 sintered high speed steel with the deposited Ti+TiN coatings: A – Substrate (ASP 30), B – Interface (Ti), C – Outer coating (TiN)

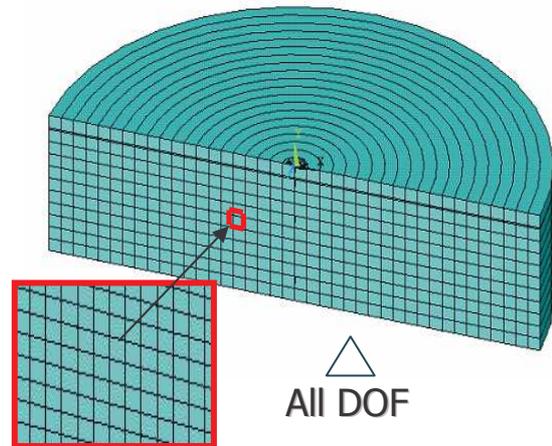


Figure 2. Analysed geometrical model with the overlaid finite elements mesh.

3. RESULTS

The mechanical properties tests carried out revealed that the analysed coatings are characteristic of the high microhardness, whose values depend on their deposition parameters. Young's modulus, was determined basing on the logged relationship of the load and unload values versus the indenter's penetration into the investigated material, during the microhardness tests of the analysed coatings. Stresses in the analysed specimens were modelled in the ANSYS environment using the finite element method, employing the experimental data and data obtained (Table1). The spatial stress distribution maps were obtained from the simulation (Figs.3, 4). Computer simulation results comparison with the experimental results of stress measurement in the analysed Ti+TiN coatings shown in Figures 5.

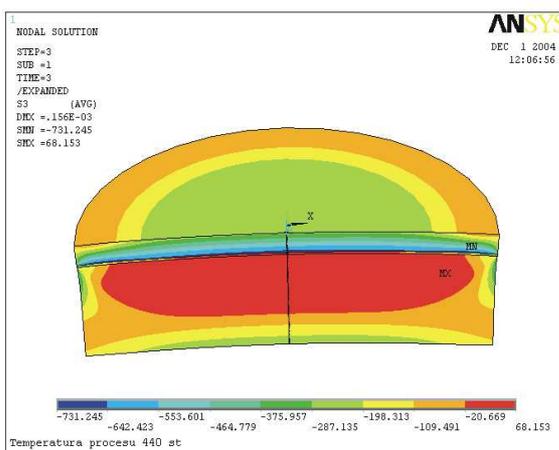


Figure 3. Distribution of the simulated compression stresses in the specimen (coating thickness $g=6,1 \mu\text{m}$, process temperature 460°C)

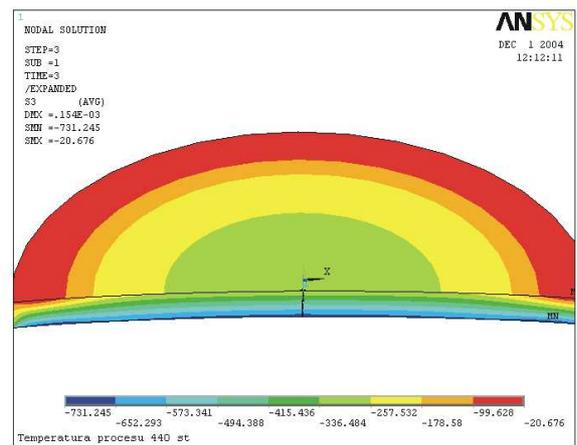


Figure. 4. Distribution of the simulated compression stresses in the Ti+TiN coating. (coating thickness $g=6,1 \mu\text{m}$, process temperature 460°C)

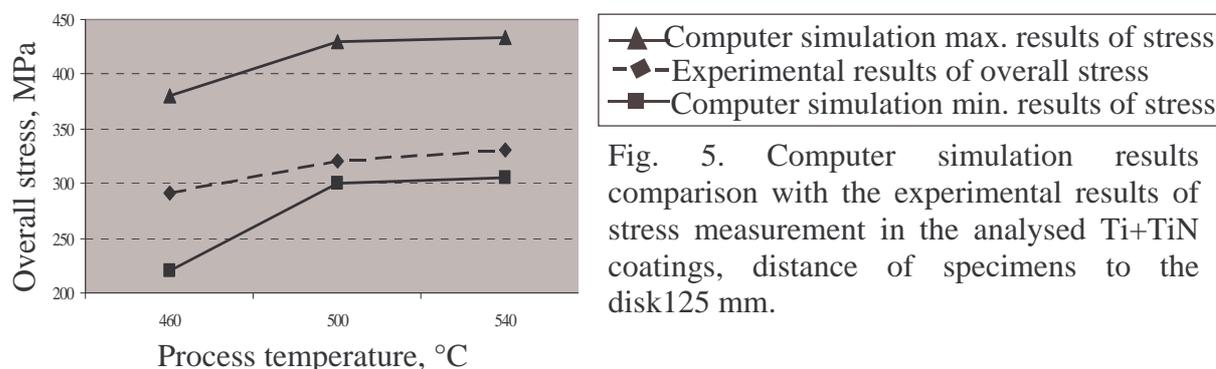


Fig. 5. Computer simulation results comparison with the experimental results of stress measurement in the analysed Ti+TiN coatings, distance of specimens to the disk 125 mm.

4. CONCLUSION

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. 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 gives ground to the assumption about its usability for determining the stresses in coatings, employing the finite element method using the ANSYS program.

Basing on the experimental results and computer simulation of stresses developed in the Ti+TiN coatings put down onto the substrate from the ASP 30 high-speed steel in the PVD process, the compression stresses were revealed.

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