Stress-strain Analysis In Mechanical Micro-model Of TiN Nano-coating Deposited On Polymer With Respect To Au Nano-interlayer

Magdalena Kopernik[1] and Andrzej Milenin[2)] AGH University of Science and Technology, Mickiewicza 30, 30-059 Kraków, Poland

ABSTRACT

The Polish pneumatic heart prosthesis will be made of Bionate II with deposited nano-coating of titanium nitride. The multi-scale analysis in the authors' finite element code confirmed possibility of fracture. The residual stress cannot be identified by X-ray technique for amorphous polymer and layer with domains of crystalline TiN. The buffer biocompatible thin film of Au in the TiN/Bionate II material system alters the evolution of residual stress and allows to determine the residual stress in profilometry studies, and helps to improve toughness of the connection between TiN and Bionate II.

EXPERIMENTS

Deposition process

The parameters of PLD process are (50 nm TiN): 100 mJ energy of laser beam, 266 nm wavelength, 4.2 J/cm^2 fluence, 25 ºC temperature of substrate, 12 ns pulse duration at a repetition rate of 10 Hz and 5000 laser shots. The parameters of magnetron sputtering method (5 nm Au) were: discharge current 10 mA and deposition time 5 min.

AFM studies

For the TiN coating an antinode and a wavelength are equal to 12.5 nm and 100 nm, respectively. These values are calculated for a surface wave approximated by a sinusoidal wave, the examples of AFM's results are shown in **FIGURE 1**.

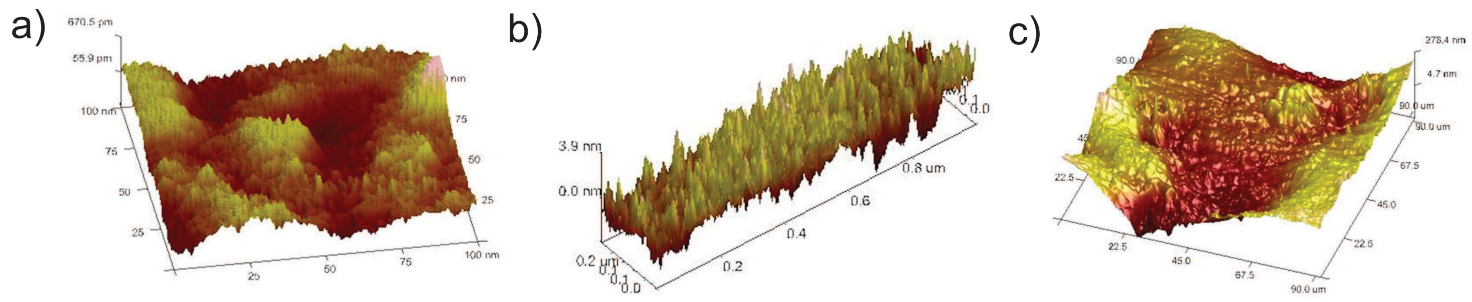

FIGURE 1. The AFM images showing coatings' topography on the selected line of areas in 3D: a) 100 nm x 100 nm, b) 1 µm x 1 µm and c) 100 µm x 100 µm.

In situ SEM micro-tension test

During micro-tensile tests the samples are elongated by steps, and tensile force in the range from 0 to 40 N and elongation from 0 to 132 µm are applied. After each step of elongation the surface of deformed thin film was observed using SEM in order to detect cracks appearance, the examples of SEM's results are presented in **FIGURE 2**.

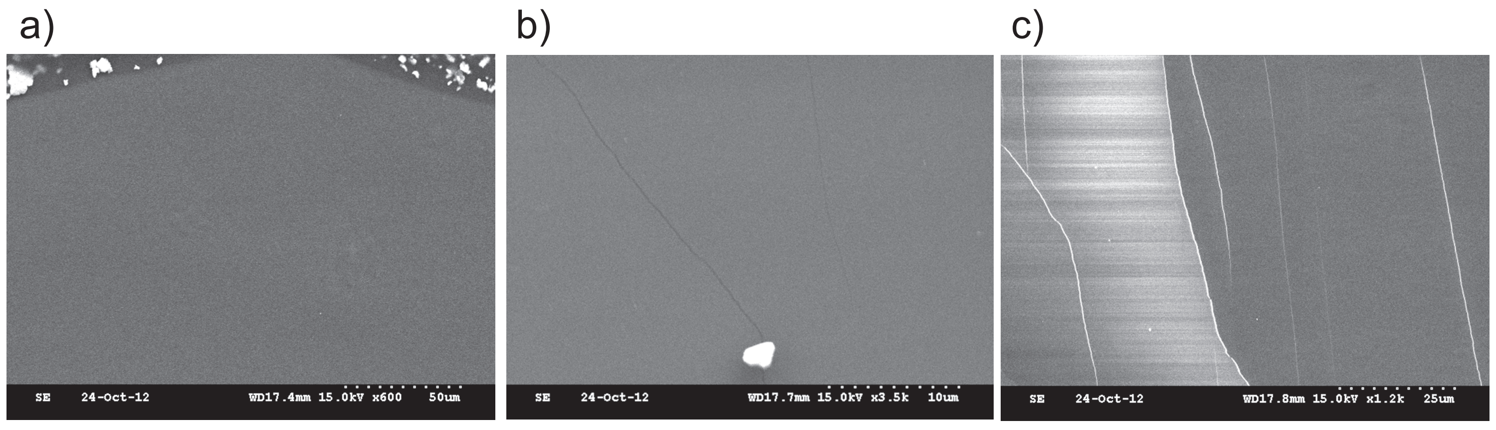

FIGURE 2. The SEM's images of 50 nm of the TiN coating stretched at: a) 8 N, b) 15 N and c) 40 N.

MODELS

Analytical Model of Residual Stress

According to the set of parameters introduced in the analytical model of residual stress proposed in [2] and their values taken from profilometry studies and from literature [2-4] (**FIGURE 3**): E_{PU} = 200 MPa, ν_{Pu} = 0.45, E_{TiN} = 290.4 GPa, ν_{TiN} = 0.25, E_{Au} = 1.3 GPa, ν_{Au} = 0.3, f = 0.976 mm, L = 23 mm; the residual stress and volumetric strain calculated in the analytical model in the TiN is σ_0 = 690 MPa and ε_0 = 0.0012 for the material system TiN/Au/Bionate II.

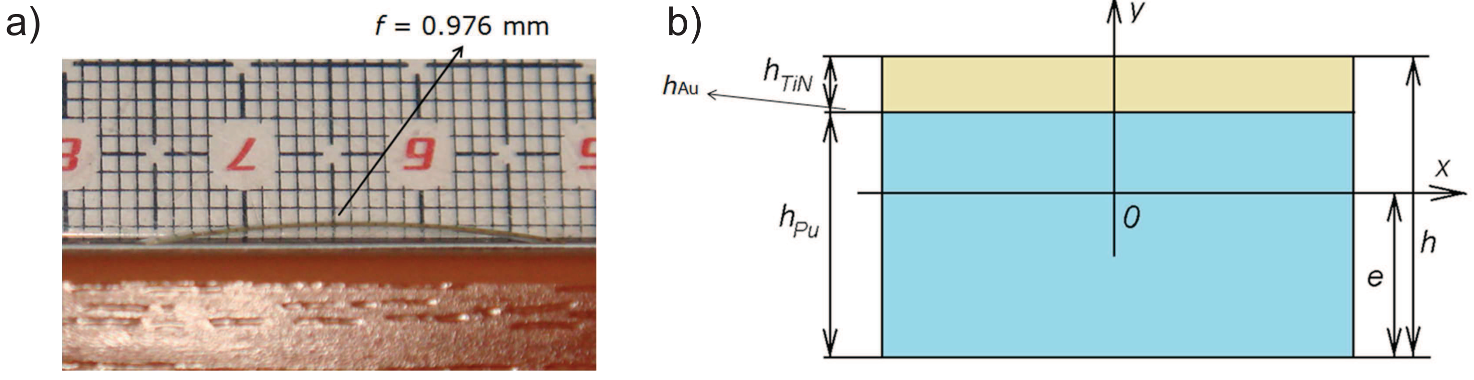

FIGURE 3. a) Camera picture of the material system TiN/Au/Bionate II taken at the side of the specimen. b) Sketch of the sample TiN/Au/Bionate II and parameters used in analytical model of residual stress.

FE Model Of Micro-Tension Test

The FE models of micro-tension test corresponding to two types of samples TiN/Bionate II and TiN/Au/Bionate are developed. The following compositions of material layers are applied in the models: 1) 50 nm of TiN, 5 nm of Au and 1000 nm of Bionate II, and 2) 55 nm of TiN and 1000 nm of Bionate II. The FE models are used to solve the boundary problem and are composed of 13320 nodes. The boundary conditions, materials' layers, a normal strain ε_{xx} and a mesh applied in the FE models are shown in **FIGURE 4**.

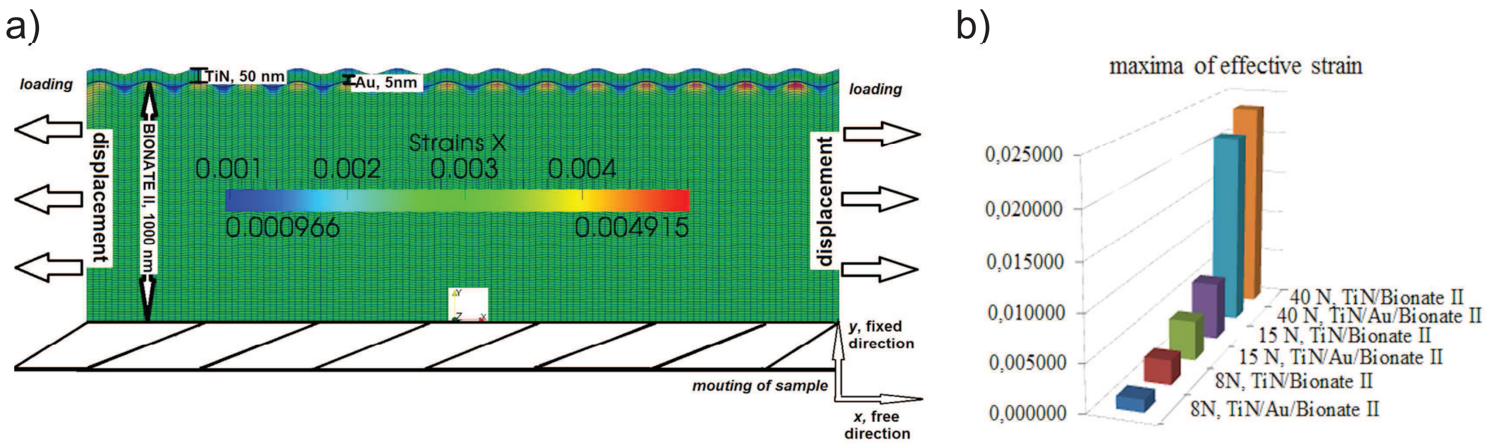

FIGURE 4. a) The Boundary conditions, a normal strain ε_{xx} and a mesh used in the FE models of micro-tension test. b) The values of maxima of effective strain ε_i for the FE model of micro-tension test of samples TiN/Au/PU and TiN/PU stretched at 8 N, 15 N and 40 N.

Basing on settings of the experimental micro-tension tests, the corresponding numerical models of the tests are prepared in a micro scale. The simulations are performed for the initial, middle and final stages of the test, which corresponds to the forces 8 N (ε_{xTiN} = 0.0011903), 15 N (ε_{xTiN} = 0.0028368) and 40 N (ε_{xTiN} = 0.0109978). These stages are selected because significant changes on the surface of samples are observed in relation to the previous steps of deformation. The maximum and minimum values of effective strain, normal stress and shear stress computed in the FE models of micro-tension test for samples: TiN/Au/Bionate II and TiN/Bionate II are plotted in **FIGURE 4a** and **FIGURE 5**.

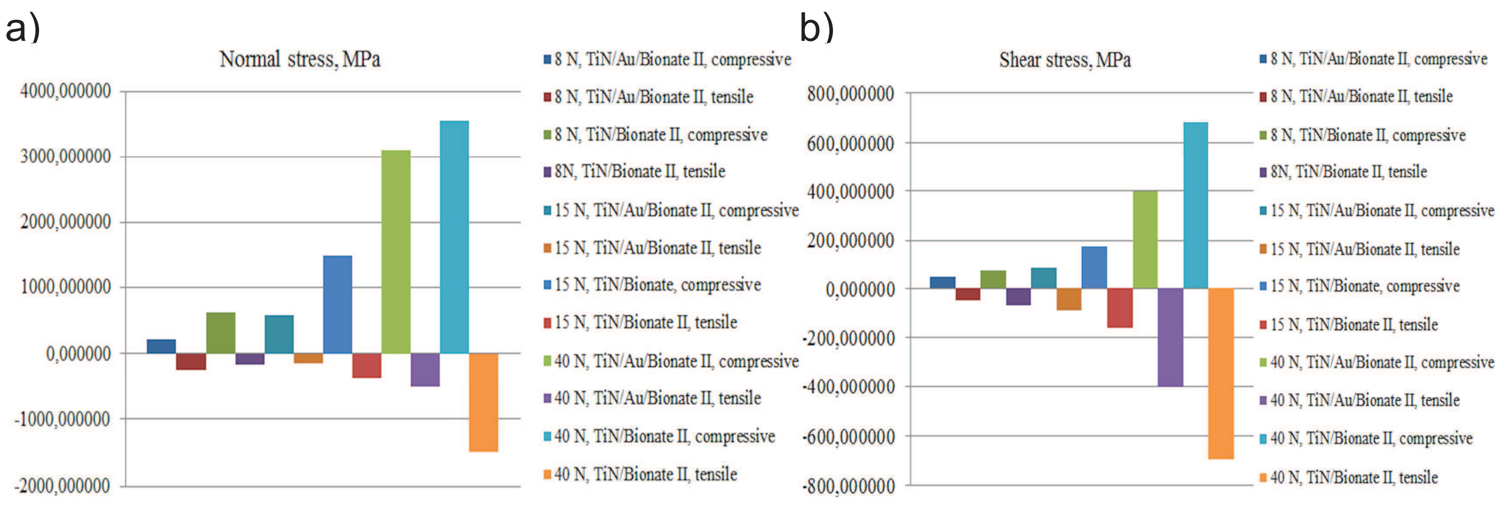

FIGURE 5. The values of a) normal stress σ_{xx} and b) shear stress σ_{xy} in MPa for the FE model of micro-tension test of samples TiN/Au/PU and TiN/PU stretched at 8 N, 15 N and 40 N.

CONCLUSION

The introduction of Au interlayer changes a stress state in each layer of the material system TiN/Au/PU. The particularly important is a change of sign of residual stress in the TiN from tensile to compressive. The presence of compressive stresses increases a toughness of connection what significantly decreases the probability of fracture (it is particularly important for the TiN). Due to character of interatomic bonds the compounds are predisposed to be applied under compressive stress load.

REFERENCES

[1] S. Timoshenko, Strength of Materials, 2-nd edition, D. Van Norstrand Company, Inc., New York, 1940.

[2] M. Kopernik, A. Milenin, R. Major, and J.M. Lackner, Identification of material model of TiN using numerical simulation of nanoindentation test, Materials Science and Technology, vol. 27, no. 3, 2011, pp. 604-616.

[3] M. Kopernik, Failure strain and strain-stress analysis in titanium nitride coatings deposited on Religa Heart Ext ventricular assist device, Archives of Metallurgy and Materials, 2014 (in press).

[4] H. Hirakata, H. Ogiwara, A. Yonezu, and K. Minoshima, Evaluation of incipient plasticity from interfaces between ultra-thin gold films and compliant substrates, Thin Solid Films, vol. 518, no. 18, 2010, pp. 5249-5256.

Corresponding author email: kopernik@agh.edu.pl

NATIONAL SCIENCE CENTRE POLAND
project no. **2011/01/D/ST8/04087**

AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

Foundation of Cardiac Surgery Development