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IDENTIFICATION OF MECHANICAL PROPERTIES OF TIN BASING ON EXPERIMENTAL AND NUMERICAL NANOINDENTATION TEST AND *in situ* SEM MICROTENSION TEST

M. Kopernik[1*], A. Milenin[2]

[1]AGH University of Science and Technology, 30-059 Kraków, kopernik@agh.edu.pl,
[2]AGH University of Science and Technology, 30-059 Kraków, milenin@agh.edu.pl

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The Polish left ventricular assist device [1] will be made of thermoplastic polycarbonate-urethane Bionate II with deposited biocompatible nanocoating of titanium nitride by pulsed laser deposition (PLD) method. The two scale model [2] developed in the authors' finite element code was composed of a macro model of blood chamber and a micro model of wall of TiN/Bionate II. The numerical analysis [3] confirmed the possibility of fracture [4], because of the big values of residual stress observed in the deposited TiN, and the significantly different mechanical properties of coating and substrate. Thus, the complete design of multilayer wall of the medical device requires the knowledge of the real mechanical properties of the TiN: residual stress, material model and fracture model.

The titanium-based thin coatings deposited by physical vapor deposition techniques exhibit big values of residual stress [5], especially if the coating is deposited on polymer by applying the PLD method in a room temperature. However, there are no works which present residual stresses measured for the TiN nanocoatings deposited on the polyurethane due to nano scale of the problem (the experimental and numerical studies are burdened with certain errors) and amorphous character of the coating and the substrate.

The mechanical properties of the TiN are needed to anticipate the stress - strain state of the VAD construction. Thus, the nanoindentation test is used for this purpose in the present work. The interpretation of the results of nanoindentation test to obtain elastic-plastic material model of the TiN nanocoating is realized by applying the inverse analysis [6] and finite element method in the authors' code [7]. The theory of elastic-plastic deformations is used in the finite element model, which simulates both loading and unloading phases, accounting for the real geometry of the indent. The nanoindentation test will be also used as an alternative method [8] to determine the residual stress in the TiN as a macro stress basing on results of the nanoindentation test.

The experimental *in situ* SEM microtension test provides detailed data for fracture analysis in a micro scale, especially for materials in which the crystal plasticity problems arose [9]. The same trend is observed in numerical research (for example by applying FEM) of the tests inspired by the *in situ* SEM microtension/microcompression tests [10]. The tensile test in a micro chamber of the SEM was performed to calibrate the fracture parameters of the TiN/Bionate II in the present work. Basing on experimental boundary conditions, the micro model of tension test was developed in the authors' finite element code. The defined fracture parameters depend on critical deformation. The critical deformation was calculated at the stage of the test, in which the initiation of fracture occurred. The micro-model includes the surface roughness (AFM results) and critical deformation under tension for different thicknesses of coatings.

Concluding, the FEM model of multilayer wall of VAD enriched with residual stress, material model and fracture model of TiN developed in authors' finite element code in the present work is able to predict the real states of stress and strain. The developed model of wall of VAD can be applied in optimization with respect to minimum of stress in the selected material system. The choice of the best construction of wall of VAD will be realized by selection of material layers, substrates, thickness of material layers and selection of parameters of deposition process to obtain high quality coatings without fracture occurrence.

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REFERENCES

[1] M. Kopernik, Shape optimisation of a ventricular assist device using a VADFEM computer program. *Acta Biomech Bioeng*, Vol. **15**, pp. 81-87, 2013.
[2] M. Kopernik, A. Milenin, Two-scale finite element model of multilayer blood chamber of POLVAD_EXT, *Arch Civ Mech Eng*, Vol. **12**, pp. 178-185, 2012.
[3] A. Milenin, M. Kopernik, Microscale analysis of strain-stress state for TiN nanocoating of POLVAD and POLVAD_EXT, *Acta Biomech Bioeng*, Vol. **13**, pp.11-19, 2011.
[4] J.M. Lackner, W. Waldhauser, P. Hartmann, O. Miskovics, F. Schmied, C. Teichert, T. Schöber, Self-assembling (nano-)wrinkling topography formation in low-temperature vacuum deposition on soft polymer surfaces, *Thin Solid Films*, Vol. **520**, pp. 2833-2840, 2012.
[5] R. Machunze, G.C.A.M. Janssen, Stress and strain in titanium nitride thin films, *Thin Solid Films*, Vol. **517**, pp. 5888-5893, 2009.
[6] M. Kopernik, A. Milenin, R. Major, J.M. Lackner, Identification of material model of TiN using numerical simulation of nanoindentation test, *Mater Sci Tech*, Vol. **27,** pp. 604-616, 2011.
[7] M. Kopernik, A. Milenin, Numerical modeling of substrate effect on determination of elastic and plastic properties of TiN nanocoating in nanoindentation test, *Arch Civ Mech Eng*, Vol. **14**, pp. 269-277, 2014.
[8] A. Rydin, P.-L. Larsson, On the Correlation Between Residual Stresses and Global Indentation Quantities: Equi-Biaxial Stress Field, *Tribol Lett*, Vol. **47,** pp. 31-42, 2012.
[9] S. Kumar, D.E. Wolfe, M.A. Haque, Dislocation shielding and flaw tolerance in titanium nitride, *Int J Plasticity*, Vol. **27**, pp. 739-747, 2011.
[10] P.A. Shade, R. Wheeler, Y.S. Choi, M.D. Uchic, D.M. Dimiduk, H.L. Fraser, A combined experimental and simulation study to examine lateral constraint effects on microcompression of single-slip oriented single crystals, *Acta Mater*, Vol. **57**, pp. 4580-4587, 2009.