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FEM CODE FOR THE MULTISCALE SIMULATION OF THE STRESS – STRAIN STATE OF THE BLOOD CHAMBER COMPOSED OF POLYURETHANE AND TiN NANOCOATING

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Abstract

The ventricle sometimes cannot work efficiently and therefore, must be outfitted with prosthesis-pulsatile ventricular assist device (VAD) often made of polyurethane (PU) and biocompatible TiN deposited by pulsed laser deposition (PLD) method. The values of compressive residual stresses are the biggest of all measured, when TiN nanocoating is deposited by applying the PLD method.

The purpose of the present paper is development of the computer finite element method (FEM) code for the multi-scale simulation of the stress - strain state for the PU/TiN blood chamber of VAD, which will be used to determine the most dangerous places at surface of the chamber under predicted loadings.

The algorithms of finite elements mesh processing, implementation of boundary conditions and obtaining numerical solution are presented in this paper.

The developed FEM code is based on the new approach to the simulation of multilayer materials obtained by using PLD method. The model in microscale includes two components - model of the initial stresses caused by deposition process and simulation of active loadings observed in the blood chamber of VAD.

Predicted distributions of stresses and strains are helpful to define precisely the regions of blood chamber, which can be defined as the failure-source areas.

Key words: pulsed laser deposition (PLD), representative volume element (RVE), finite element method (FEM), ventricular assist device (VAD), polyurethane (PU)

1. INTRODUCTION

A ventricular assist device is a mechanical circulatory device that is used to partially or completely replace the function of a failing heart. The titanium nitride is deposited on the whole outer surface of the VAD's blood chamber made of polyurethane. Using temperature-sensitive polymers, especially substrates in VADs, demands low-temperature coating techniques to deposit biocompatible coatings like TiN (Lackner, 2005), but there is a lack of industrially scaled vacuum coating techniques at temperatures below 50°C. The PLD technique (Lackner, 2005) is an alternative for overcoming this problem. The comparison between literature studies and results reached for biocompatible TiN nanocoating deposited on PU by using PLD method is shown in (Kopernik et al., 2011) and leads to a conclusion that values of compressive residual stresses are bigger, when TiN nanocoating is deposited by using PLD method. Thus, knowledge about the real mechanical properties of nanomaterials, which are used in the VADs, is crucial. The thickness of biomaterial coatings could be changed from submicron to several hundred micrometers, and therefore, a nanoindentation test was selected to determine mechanical properties of coatings, as well as applying the Stoney's

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equation and observations of TEM images to obtain residual stress for coatings (Pauleau, 2006).

The FEM solid structure problem solved in own computer program is focused on strain and stress analysis for macromodel of VAD's blood chamber with option of local strain and stress analysis in micromodel by applying RVE. The RVE micromodel also includes residual stress distribution and modelling unloading in micromodel of wall of VAD's blood chamber.

The purpose of proposed approach can be formulated as development of the multiscale FEM model for the PU/TiN blood chamber, which is performed to determinate the most dangerous places at surface of the chamber under predicted loadings.

The scheme of proposed macroscale solution is composed of two stages:

– residual stresses modelling and
– active loadings modelling.

In the first stage the residual stress is reached by applying experimental results and inverse method (Kopernik et al. 2011) in microscale. In the second step, the computed stress and strain states are used as initial values for analysis the influence of working loadings on material of blood chamber. In this stage boundary conditions are moved from solution in microscale to macroscale.

2. FINITE ELEMENT SOLUTION

2.1. Macroscale

The shape of the blood chamber during filling phase and its main parts are described in figure 1 (Litwiński et al., 2005). The geometry of VAD created in CAD program is used in the FEM model. The full model of VAD is composed of two connectors (inlet and outlet), the biggest part – blood bowl, the large but also very thin pneumatic bowl and two valves (inlet and outlet – mechanical valves: commercial Medtronic, Moll or three leaflet polyurethane valve). The presented geometry of VAD is a little bit simplified. The final model of geometry of chamber performed by the Authors is composed of two main parts: the top pneumatic bowl and the bottom blood bowl, as well as two channels: reduced connectors.

The following macroscale model of VAD's blood chamber is proposed by the Authors. Theory of nonlinear elasticity gives basis to formulation the boundary problem, whose goal is determination the distribution of displacement vector U_i. This state corresponds to deformation of VAD's chamber under blood pressure, if:

– proportion between stress and strain is observed;
– strain disappears in unloading conditions.

The nonlinearity in elastic deformation process of blood chamber is a result of:

– nonlinear mechanical properties of polyurethane;
– deposition of the nanocoatings, which causes the additional stress (initial residual stress).

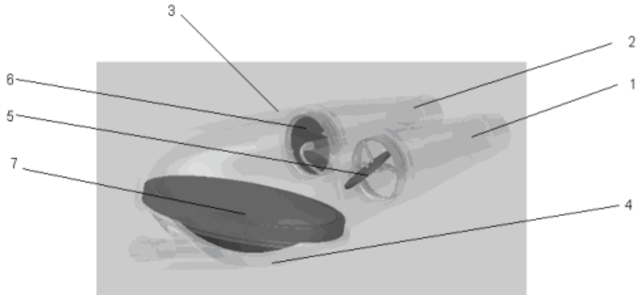

Fig. 1. *The detailed scheme of the ventricular assist device POLVAD: 1 – inlet connector, 2 – outlet connector, 3 – blood bowl, 4 – pneumatic bowl, 5 – inlet valve, 6 – outlet valve, 7 – membrane in filling phase (Litwiński et al., 2005).*

The problem of the blood chamber deformation in macroscale is considered as 3D solution. Thus, the defined boundary problem of theory of nonlinear elasticity is composed of the groups of equations described in (Milenin, 2010). In the case of small nonlinearity of material the Young's modulus is assumed as a constant value. In the plastic zone of deformation the effective stress is equal to yield stress σ_p and the plasticity modulus is used instead of Young's modulus. The plasticity modulus is:

$$E' = \frac{\sigma_p}{\varepsilon_i} \tag{1}$$

The components of stiffness matrix $[K]$ and complete load vector $\{F\}$ are written according to forms:

$$[K_e] = \int_{V_e} [B]^T [D][B]\, dV \tag{2}$$

$$\{F_e\} = -\int_{S_e} \left[\bar{N}\right]^T \{p\}\, dS \tag{3}$$

where: S – contact surface, $\{p\}$ – pressure inside VAD, $[B]$ – matrix containing derivatives of shape functions, $[D]$ – matrix containing the appropriate material properties (E, ν), $\left[\bar{N}\right]$ – matrix of shape functions of finite element, V – volume, V_e – volume of current finite element e, S_e – contact surface between current element and tool. The tetrahedron element was proposed in the FEM modelling in macroscale. The five-point scheme of integration was used.

The boundary conditions in macromodel are given as follows (figure 2):
– distribution of blood pressure p = 16 kPa on the inner surface of blood chamber;
– fixed inlets of both connectors of blood chamber (no displacement, no loading);
– no fixed surfaces in outer upper part of blood chamber (no fixed surfaces, no loading).

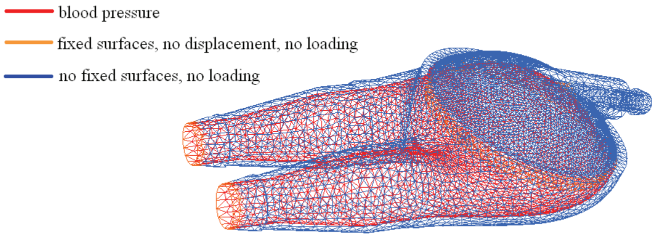

***Fig. 2.** Set boundary conditions.*

2.2. Microscale

The analysis of strain distributions at inner surface of the heart chamber in the macroscale FEM model is helpful to determine correctly the areas with the biggest tendency to failure. Therefore, only these places are further taken into account and investigated in microscale model, which is not available in commercial FE program. Subsequently, the strain state reached during loading in macromodel is introduced into FEM micromodel. The following microscale model of wall of VAD's is proposed by the Authors.

The representative volume element is composed of substrate (polyurethane) material layer and deposited very thin TiN coating, whose thickness is expressed in nanometers. The $2\frac{1}{2}$D FEM micromodel has 4-node finite elements, which are used to solve the boundary problem. The material model of TiN was identified in the previous works (Kopernik at al., 2011). Inverse analysis was applied for determination of the mechanical properties of TiN coating. It is observed that the nonlinearity of mechanical properties between TiN coating and polyurethane exists. Thus, assuming the elastic-plastic or nonlinear elastic material model is justified. Considering the phenomena: elastic as well as elastic-plastic deformation and unloading process (in elastic-plastic case), the boundary problem in the FEM micromodel is solved. The initial stress $\{\sigma_{0res}\}$ in TiN nanocoating is taken into account in formulation of boundary problem. The relation between stresses and strains (Zienkiewicz and Taylor, 2000) is written using the matrix (vector) definition:

$$\{\sigma\} = [D]\{\varepsilon\} - [D]\{\varepsilon_{0\,\text{res}}\} \tag{4}$$

where: $\{\varepsilon_{0res}\}$ – residual strains; $\{\sigma\}$ and $\{\varepsilon\}$ – stress and strain tensors in the cylindrical coordinate system.

The variational principle of the non-linear elastic and elastic-plastic theory leads to the following functional form for finite element e:

$$W_e = \int_{V_e} \frac{1}{2}\{U\}^T [B]^T [D][B]\{U\} dV -,$$
$$\int_{V_e} \{U\}^T [B]^T [D]\{\varepsilon_{0\,\text{res}}\} dV - \int_{S_e} \{U\}^T [\overline{N}]^T \{p\} dS \tag{5}$$

where: $\{U\}$ – displacement vector in nodes of elements.

For linearization of this functional for nonlinear problem, the value of E is written as $E = E'$, where: E' (eq.1) – effective Young's modulus, which is equal to Young's modulus in elastic zone.

The stiffness matrix $[K]$ is as in eq. (2) and load vector $\{F\}$ is written according to form:

$$\{F\} = -\int_V [B]^T [D]\{\varepsilon_{0\,\text{res}}\} dV - \int_S [\overline{N}]^T \{p\} dS \tag{6}$$

The comparison between literature studies and results reached for biocompatible TiN nanocoating deposited on PU by using PLD method shown in (Kopernik et al. 2011; Milenin and Kopernik, 2009) leads to conclusion that values of compressive residual stresses are bigger, when TiN nanocoating is deposited by using PLD method. The big values of compressive residual stresses were observed in many studies of this type of materials and are attributed to the influence of surface tension and may be due to the influence of the conditions for the formation of a layer. Summarizing, the initial stresses (residual stresses) in polyurethane and TiN nanocoating are results of technology of deposition (PLD) and must be evaluated before simulation of loading.

The initial stresses (residual stress) distribution has to be specified for each element of FEM mesh in the beginning stage of solution process. This stage of solution is based on the inverse idea. The collocated distribution of $\varepsilon_{0\,\mathrm{res}}$ is determinated on the basis of minimization of the following function:

$$R = \sum_{e=1}^{N_e} \int_{V_e} \left[\sigma_{0\,res}\left(\varepsilon_{0\,\mathrm{res}}\right) - \bar{\sigma}_{0\,res} \right]^2 dV \qquad (7)$$

where: e – number of current finite element, N_e – number of finite elements in zone with initial stress, $\bar{\sigma}_{0\,res}$ – experimental value of initial stress in current finite element e, in the present work $\bar{\sigma}_{0\,res}$ = 0.5 GPa for TiN nanocoating, σ_{0res} $\{\varepsilon_{0res}\}$ – calculated distribution of initial stresses as function of ε_{0res}.

After determination of ε_{0res} distribution, the simulations of loading and unloading stages of blood chamber of VAD in microscale are possible. In the present work the value of experimental residual stress is interpreted as a mean stress and is localized in a thin TiN coating. The proposed solution in multiscale modelling is shown in figure 3 and is formulated as residual stresses modelling, which is reached by applying experimental results and inverse method in microscale (Kopernik et al. 2010).

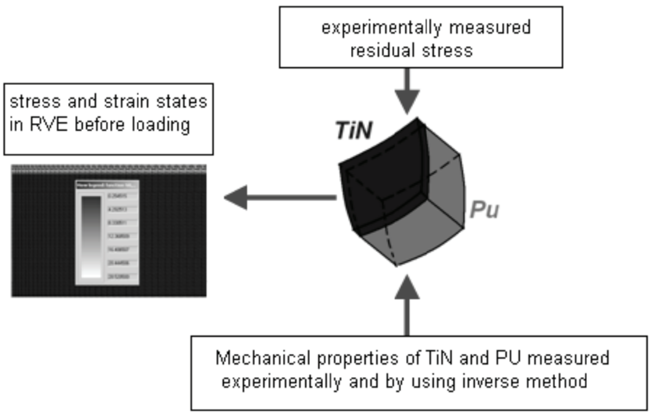

Fig. 3. General conception of micromodel of blood chamber for residual stress modelling.

The boundary conditions for the RVE are modeled according to the following principles. The deformation tensor is obtained from the macromodel. The value of the strain ε_2 (second principal strain) is introduced into the micromodel as a constant. Therefore, the 3D boundary problem of the RVE deformation is transformed to the 2D plane strain problem with the present value of ε_2. The principle strain ε_1 and work pressure p are also used in the micromodel of the RVE. Periodic boundary conditions are applied according to conclusions reached by (Thibaux at al., 2000).

Concluding, in the second stage of multiscale modelling (figure 4) the computed stress and strain states are used as initial values for analysis the influence of working loadings on material of blood chamber. In this stage boundary conditions are moved from solution in microscale to macroscale.

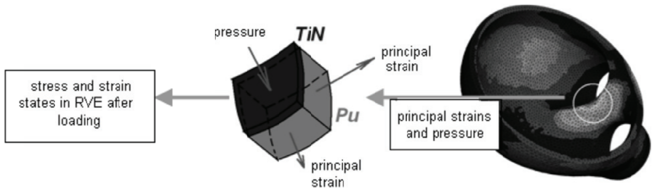

Fig. 4. General conception of multiscale model of blood chamber for active loading modelling.

3. FEM MESH PROCESSING

The majority of the known commercial FE programs, allows to generate mesh, but does not provide information on the mesh which allows to distinguish whether the node is an external or internal (lack of documentation to the generated files, which contain detailed information about the mesh). Therefore, it was necessary to develop an algorithm of separating from the whole FE mesh of the surface of the mesh elements that come into contact only with the surroundings. It is prepared basing on the fact that each mesh contains data about the coordinates of nodes and their connections in the finite elements. The example of mesh generated in commercial program ABAQUS is shown in figure 5.

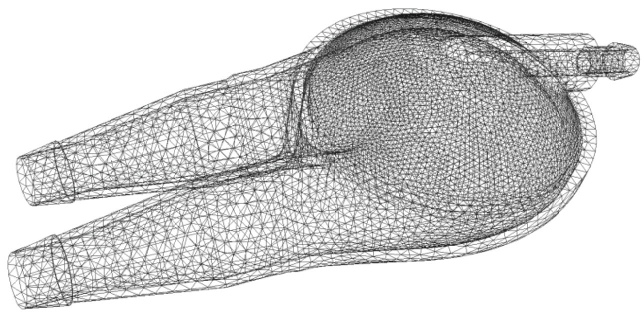

Fig. 5. Mesh generated in ABAQUS code and available in text file.

Methodology for determining nodes on the surface and surfaces is implemented through the algorithm described below:

– Four surfaces are analyzed for each element of FE mesh. In the rest of the FE mesh a surface is searched, which contains the same nodes. If such a surface exists, the both surfaces are considered as internal finite elements of the area. However, in the opposite case, the outer surface is considered.

– The solution assumes that all external nodes belong to the external surface, while the remaining nodes are internal.

Graphical representation of the result of the separation of the external surface is given in figure 6 and is prepared by using developed interface.

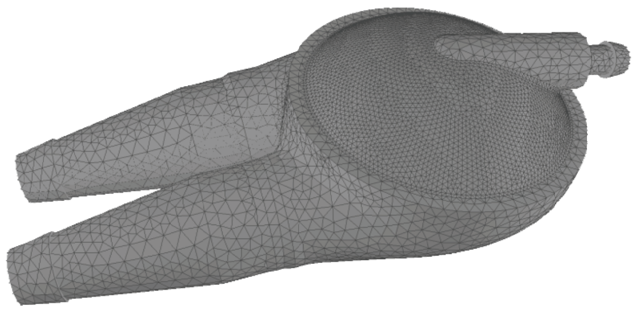

Fig. 6. *Mesh after separation the elements which are in contact with surroundings.*

decoupled from the finite element type and specificity of the commercial FEM program. The various steps of this algorithm lead to separation of the inner surfaces of the all surfaces basing on the directional cosine of the surfaces of elements while reducing the distance to the closest surroundings of the central point and applying algorithm of current surface.

In the first stage of the calculation the boundary conditions were used according to figure 2 and the result of the separation the external surface from the internal was also visible in figure 2. The separation of fixed nodes was carried out on the basis of the analysis of slope of surface. According to presented result, the proposed procedure and algorithm applied to separation the nodes of FE mesh allow setting the boundary conditions in any location of the analyzed blood chamber of VAD.

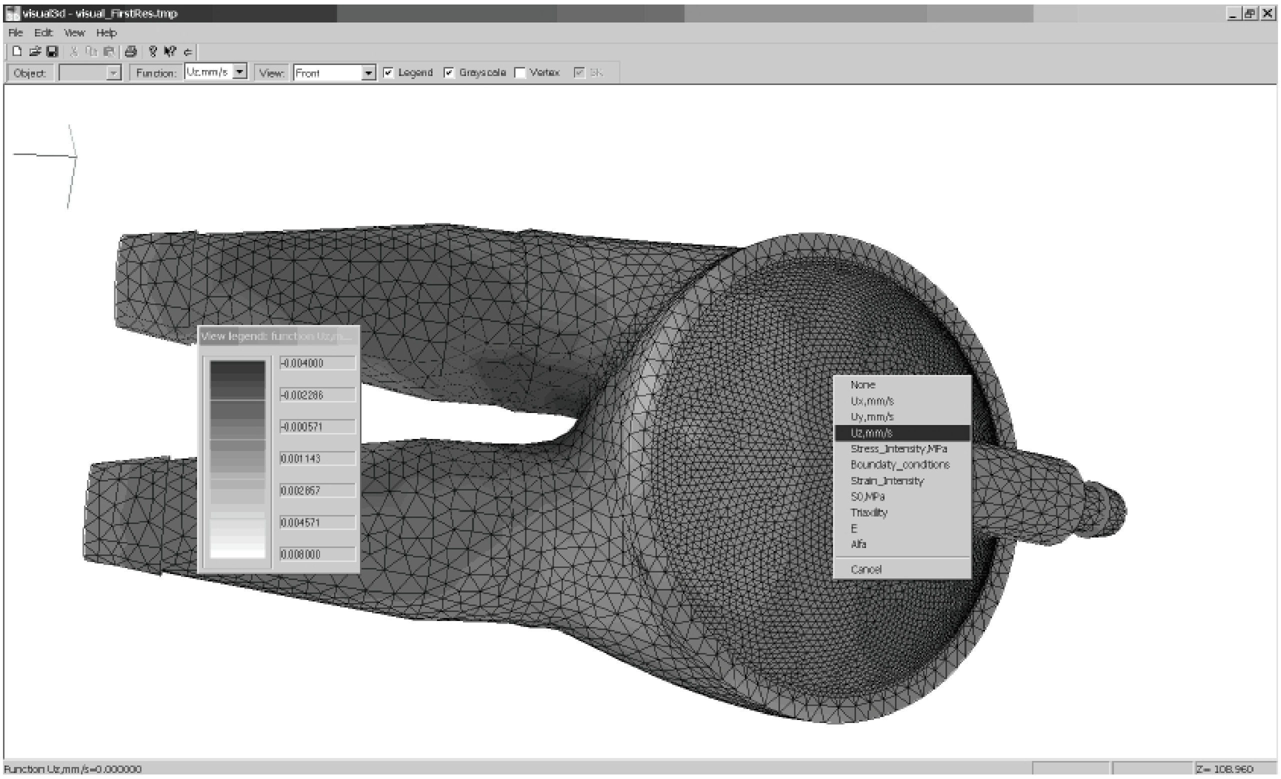

Fig. 7. *Result of visualization for distribution of displacement in X direction with set of available parameters.*

It was also developed a second method of separation the internal from the external surface of VAD, in which the cloud of points is generated around FE mesh and around center point of blood chamber. The center point inside the FE mesh is located exactly inside the blood chamber, and more specifically coincides with its center of gravity the mass. Each node, which is the closest to the central point of blood chamber, is recognized as an internal node. This approach is proposed to verify additionally the eligibility of the node (external or internal). It is also

4. NUMERICAL SOLUTION AND VISUALIZATION OF 3D RESULTS

The solver was implemented in the developed computer FE program. Basing on Irons algorithm (Irons, 1975) the frontal method was applied to solve equations. The procedure of minimization the front and program to solve the system of equations were used in previous work (Milenin, 1998). The stiffness matrixes and load vectors were also computed in the developed program.

Using the Direct X library the program to visualization the result was built. The text file generated in FE program is loaded to present the results. Thus, the developed tool for visualization is universal and the array of output data is defined in a special text file, which is listed below: displacements μm in *X*, *Y* and *Z* directions; effective strain x 100 and stress kPa; average stress kPa, triaxility factor and Young's modulus.

The FE results were obtained with the mesh in macroscale and are shown in figure 7 as distributions of displacement in *X* direction. Additionally, the whole parameters computed and available to visualization are also presented in figure 7.

6. EXAMPLES OF SIMULATION

The developed program was used to perform the tested simulation of deformation process for material of blood chamber of VAD. The tested loading was equal to physiological value of blood pressure (16 kPa). The following elastic properties were accepted for polyurethane of blood chamber (Chronothane 55D): $E = 423$ MPa i $\upsilon = 0.4$.

The selected results are shown in figures 8-10. The distributions of effective strain (figure 8), average stress (figure 9) and effective stress (figure 10) in wall of blood chamber under working loading are observed on inner surface of bottom part of blood chamber in side view of cross-section between two connectors. The results of simulations show values of stress equal tens of kPa on wall of blood chamber, what in comparison with applied outer working loadings and material properties of chamber can be assumed as correct. The values of computed strain are very small. The most dangerous to maintain the continuity of the material are the locations of compressive and tensile stresses. The maximum values of tensile stresses (positive) and compressive stresses (negative) are placed very close to each other, what is clearly visible in figure 9 and this fact can lead to material failure in the distinguished regions - inner surface of bottom part of blood chamber in side view of cross-section between two connectors. The obtained results at this stage of project should be considered more qualitatively than quantitatively, because of lack of adequate number of experimental results dedicated to residual stress and distribution of strain in material of blood chamber (extensometer studies).

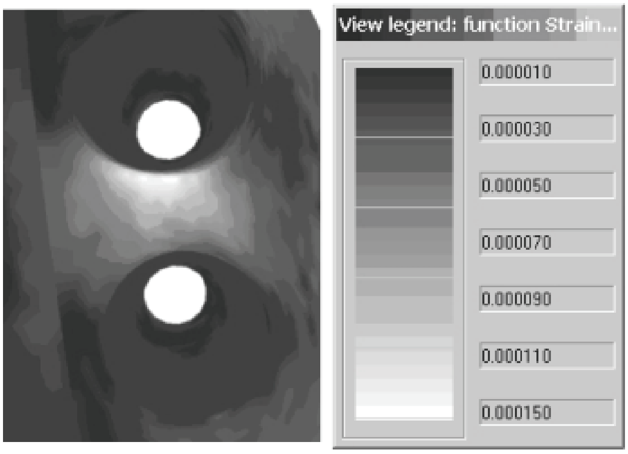

Fig. 8. Effective strain inside blood chamber of VAD between two connectors.

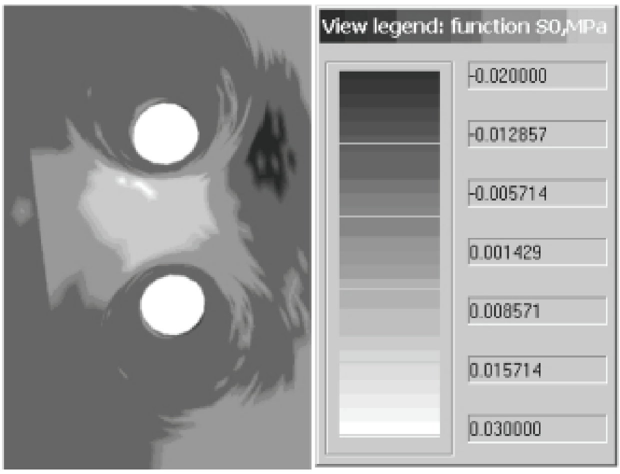

Fig. 9. Average stress inside blood chamber of VAD between two connectors.

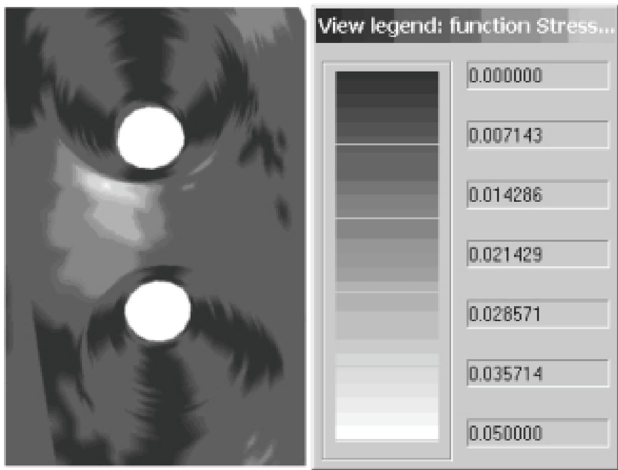

Fig. 10. Effective stress inside blood chamber of VAD between two connectors.

In simulations performed for micromodel of specimen TiN/PU the biggest values of effective strain are located in the very thin zone between two

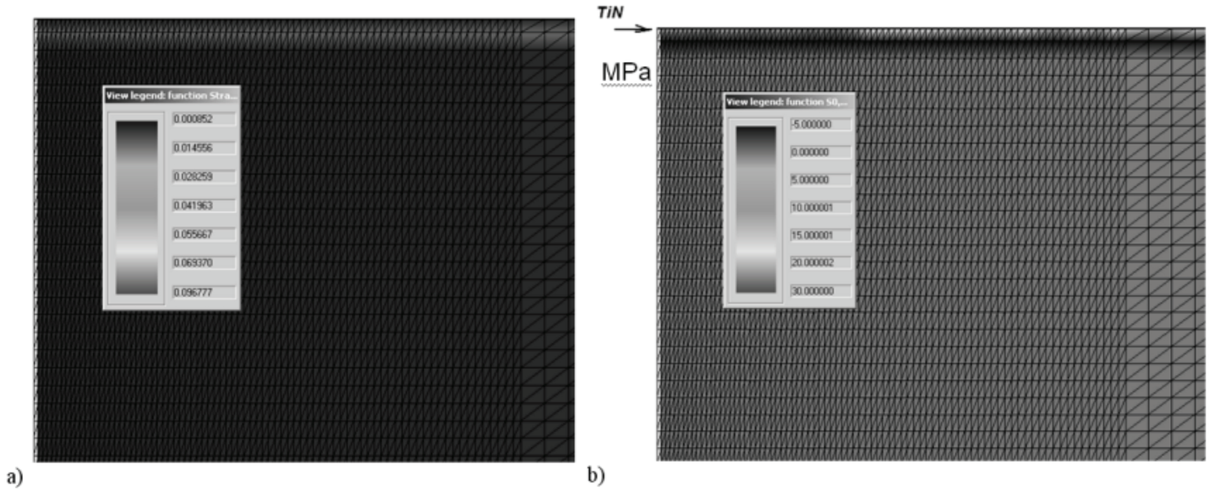

Fig. 11. *Distribution of: a) effective strain and b) average stress in micromodel of specimen PU/TiN.*

main material layers TiN and PU (figure 11a). The average stress in TiN layers (figure 11b) is equal 20 MPa (respectively 0.7 MPa for PU blood chamber). The biggest values of average stress and effective strain are concentrated along the boundary between main materials' layers. Thus, it is justified to experimentally investigate the quality of materials' connection during long-time work of blood chamber.

7. CONCLUSIONS

Conclusions focused on details of developed computer program and models:

– The developed model and FEM computer program are applied to analysis the state of stress and strain for macroscale model with the option of a local modelling of stress and strain in microscale using the RVE, in which the model takes into account residual stress and partial or total unloading of the material of blood chamber.
– The developed computer program was used to identification the parameters of material model of the wall of blood chamber on the basis of nanoindentation tests in other works. The program is a basis of a mechanical model for an implantable blood chamber of a ventricular assist device.
– Development the automatic fragmentation of FEM mesh, which provide opportunities to calculation the macro solution for any FEM mesh, which is generated by any commercial program.
– The proposed model was performed in two stages in microscale. The first stage includes residual stress by solving the inverse problem. In the second stage, the resulting states of stress and strain were used as the initial distributions, and the modelling was performed for blood chamber working under loading conditions. At this stage of solution, the boundary conditions were transferred from the problem in microscale to macroscale.
– Due to problems with accurate determination of the residual stress state caused by deposition of TiN, as well as the low accuracy of nanoindentation test, the precise conclusion about the quantitative results of simulation in developed micromodel is difficult. Therefore, the obtained results should be treated qualitatively rather than quantitatively. The quantitative accuracy is expected after numerous measurements and improved methodology of residual stresses and nanoindentation tests.

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KOD MES DO MODELOWANIA WIELOSKALOWEGO STANU ODKSZTAŁCEŃ-NAPRĘŻEŃ W KOMORZE KRWISTEJ ZBUDOWANEJ Z POLIURETANU I AZOTKU TYTANU

Streszczenie

Gdy lewa komora serca nie pracuje prawidłowo, to jest zastępowana protezą – pulsacyjną komorą wspomagania pracy serca (VAD, z ang. ventricular assist device), którą często wykonuje się z poliuretanu (PU) i naniesionej za pomocą metody PLD (osadzenie laserem impulsowym) biokompatybilnej powłoki TiN. Otrzymywane duże wartości ściskających naprężeń własnych, są najwyższe ze wszystkich mierzonych, gdy powłokę TiN nanosi się metodą PLD.

Celem niniejszej pracy jest opracowanie programu komputerowego wykorzystującego metodę elementów skończonych (MES) do wieloskalowego modelowania stanu odkształceń i naprężeń dla komory krwistej zbudowanej z PU/TiN, który to program będzie wykorzystywany do określania najbardziej niebezpiecznych miejsc ze względu na możliwe uszkodzenia materiału powierzchni komory, jakie mogą się pojawiać w warunkach pracy komory.

Algorytmy wykorzystywane do tworzenia siatki elementów skończonych, implementacja warunków brzegowych i otrzymane rozwiązanie numeryczne zaprezentowano w niniejszej pracy.

Opracowany kod MES jest oparty na nowym podejściu do symulowania materiałów wielopowłokowych otrzymywanych metodą PLD. Model w skali mikro zawiera dwa składniki: model naprężeń własnych (naprężeń początkowych) powstałych w procesie nanoszenia powłok i model obciążeń zadawanych w komorze krwistej VAD.

Przewidywane w modelu rozkłady naprężeń i odkształceń pomagają określić dokładnie te strefy komory krwistej, które można zdefiniować, jako obszary będące źródłem jej uszkodzeń

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