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THE NEW MULTISCALE FINITE ELEMENT MODEL OF MULTILAYER VENTRICULAR ASSIST DEVICE

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Abstract

Ventricular assist device is an artificial organ, which is used to treat heart diseases. In the world, as well as in Poland, efforts are made towards the development of such a device that is biocompatible, durable, low energy consuming, allows monitoring and does not introduce changes to the blood morphology. The review paper discusses the types of ventricular assist devices (VADs), including VADs proposed in Poland. The particular emphasis is put on the numerical modelling and computer aided design of such an artificial organ. The walls of the ventricular assist device are covered with a nanocoating of TiN using modern techniques (Pulsed Laser Deposition) to improve the biocompatibility. The nanocoating modifies the surface properties of the device. Mechanical properties of nanocoating are determined in experimental nanotests and using imaging techniques of nanostructures. However, these tests give average values of properties and this information is not sufficient for advanced design of ventricular assist devices. To eliminate this constraint, the multiscale modelling is applied. Developed solution, which is based on application and combination of methods such as finite element method, multiscale approach and inverse analysis, is presented in the paper. These methods are helpful in prediction the location of failure zones in the material of the ventricular assist device and then to analyze the local behaviour of nanocoating. Furthermore, it is possible to identify the parameters of the rheological model of nanocoating and introduce the residual stresses into models.

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

1. INTRODUCTION

Ventricular assist device (VAD) is an artificial organ produced by using the latest achievements in nanomaterials science and nanotechnology in the field of production technology, as well as by applying other fields of technology (control, power supply) and medicine (evaluation of biocompatibility of the surface). However, the application of the VAD is very demanding and leads to increasing commitment to the research.

The first step in Polish mechanical circulatory support made Professor Religa in 1993 who implanted POLVAD. In the "Polish Artificial Heart Programme 2007 - 2011" (Sarna et al., 2010; Milenin & Kopernik, 2010) efforts are made towards the development of such a pump of Polish ventricular assist device (POLVAD) that is low energy consuming and does not cause red blood cell trauma, as well as such a construction of POLVAD that is durable, biocompatible and allows monitoring. The second version of POLVAD was developed in the Programme – POLVAD_EXT (Gawlikowski et al., 2006). The walls of the proposed design of POLVAD_EXT made of polymer are supposed to be covered with a titanium nitride (TiN) nanocoating to improve the biocompatibility (Ebner et al., 2006) and the surface properties of the medical device. The POLVADs are used to keep patients alive with a good quality of life while they wait for a heart

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transplantation which is known as a "bridge to transplantation". However, they are sometimes used as destination therapy and sometimes as a bridge to recovery.

The implantation of blood chamber of POLVAD is needed and considering the current state of knowledge is not necessary to convince anyone. Using biocompatible TiN nanocoating (Ebner et al., 2006) on surface of POLVAD (Sarna et al., 2010) is quite a controversial subject, mainly due to the possibility of loss of cohesion for connection TiN nanocoating/polymer and other negative phenomena that can occur (thrombus formation). These phenomena have very negative consequences for the patient, especially in the cyclic working conditions of blood chamber of VAD.

Thus, the VAD's design used by the Authors of present paper is unique, because of deposited TiN nanocoating by using PLD (pulsed laser deposition) method, what is not realized by other researchers. The multiscale model for analysis the strain and stress states of multilayer wall of blood chambers of POLVADs was developed and tested in previous works (Milenin & Kopernik, 2009; Milenin & Kopernik, 2011). The micromodel was applied in the macromodel of POLVADs where the maximum values of strain and stress were observed – between two connectors (the most probable failure–source regions). This approach allows multiscale analysis of stress and strain states for different versions of POLVADs and investigation of parameters for their constructions.

2. VENTRICULAR ASSIST DEVICE

2.1. Application

Although heart transplantation is the standard for patients who remain in advanced heart failure despite optimal medical therapy, limited donor supplies allow for just more than 2000 transplant each year in the United States (Gray & Selzman, 2006). Recent enthusiasm has developed for the role of mechanical circulatory support for this ever-growing population of sick patients. Although much attention has been directed toward ventricular assist devices, less information is available regarding the role of the total artificial heart. Indeed, efforts in this latter technology have allowed the relatively recent deployment of a variety of complete circulatory assist devices.

The term artificial heart (Korakiantis & Grandia, 2003) is often inaccurately used to describe ventricular assist devices, which are pumps that assist the heart but do not replace it. Total artificial heart (TAH) is another type of mechanical blood pump that replaces the native heart and provides all of the blood pumping action in the body. While considered a success, the use of artificial hearts is limited to patients awaiting transplants whose death is imminent. The devices are unable to reliably sustain life beyond about 18 months. An artificial heart is also distinct from a cardiopulmonary bypass machine (CPB), which is an external device used to provide the functions of both the heart and lungs.

A ventricular assist device, or VAD, is a mechanical circulatory device that is used to partially or completely replace the function of a failing heart. Some VADs are intended for short term use, typically for patients recovering from heart attacks or heart surgery, while others are intended for long term use (months to years and in some cases for life), typically for patients suffering from congestive heart failure (Osaki et al., 2008). VADs (Korakiantis & Grandia, 2003) are designed to completely take over cardiac function and generally require the removal of the patient's heart. They are used to assist either the right (RVAD) or left (LVAD) ventricle, or both at once (BiVAD). Which of these types is applied depends primarily on the underlying heart disease and the pulmonary arterial resistance that determines the load on the right ventricle. LVADs are most commonly used, but when pulmonary arterial resistance is high, right ventricular assistance becomes necessary. Long term VADs are normally used to keep patients alive with a good quality of life while they wait for a heart transplantation which is known as a "bridge to transplantation". However, LVADs are sometimes used as destination therapy and sometimes as a bridge to recovery. In the last few years, VADs have improved significantly in terms of providing survival and quality of life among recipients (Osaki et al., 2008). The pumps used in VADs can be divided into two main categories:

– pulsate pumps, that mimic the natural pulsing action of the heart, and
– continuous flow pumps.

2.2. Polish milestones in cardiosurgery and related biotechnology

The first step in the field of mechanical circulatory support made the U.S. surgeon J.H. Gibbon in 1953 (Nawrat, 2007), who carried out a successful operation, closure of atrial septal defect using cardiopulmonary bypass. The first milestone in Polish cardiosurgery was made by Professor Z. Religa in 1986 (Nawrat, 2007), who together with Vascu team from Brno implanted BRNO LVAD. The most important step in Polish mechanical circulatory support was also made by Proffesor Z. Religa in 1993 (Nawrat, 2007), who implanted Polish POLVAD, which is shown in figure 1 (Nawrat, 2007).

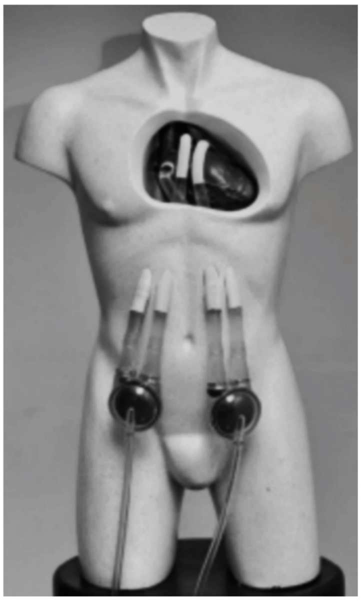


Fig. 1. Biventricular heart supporting by extracorporeal pneumatic VAD (Nawrat, 2007).

The further Polish progress in biomedical technology dedicated to cardiosurgery was led mainly by Professor Religa (Religa & Kustosz, 2002), who said: „Because of the lifestyle, diet, and the complications of influenza each of us can have irreversible cardiac failure. Then the only cure is transplantation. Unfortunately, only every tenth patient has a chance at it (lack of donors). The other must die. The only solution is to implement in clinical practice the total artificial heart."

The consequence of Professor Religa and his team efforts is "Polish Artificial Heart Programme 2007-2011", which is dedicated to the development of the family of heart prostheses that will allow the use of mechanical circulatory support in agreement with the needs of the different treatment of heart disease and levels of failure in both adults and children. The expected result of this research is a group of prostheses, including:

– extracorporal pulsatile ventricular assist device,
– partly implantable pulsatile ventricular assist device,
– totally implantable pulsatile ventricular assist device,
– partly implantable long term impeller pump,
– extracorporal pulsatile, pediatric ventricular assist device.

2.3. Modelled Polish ventricular assist device

The authors of the present paper participate in the "Polish Artificial Heart Programme" and realize the task: „Numerical model of totally implantable pulsate ventricular assist device". The goal of the task is development of numerical model of pulsate ventricular assist device and computer program with the option of a local multiscale modelling, which allows the analysis of the problems posed by the application in terms of blood flow through prosthesis (see Section 4.4). The defined problems include:

– prototype design focused on optimization of selected geometrical and material parameters, as well as its impact on flow and behaviour of the blood,
– development of robust blood rheology model,
– modelling problems concerning the interaction of biological and artificial materials,
– creation of mathematical models of the experimental nanotests for nanocoatings which build wall of the VAD and the identification of mechanical properties for nanomaterials.

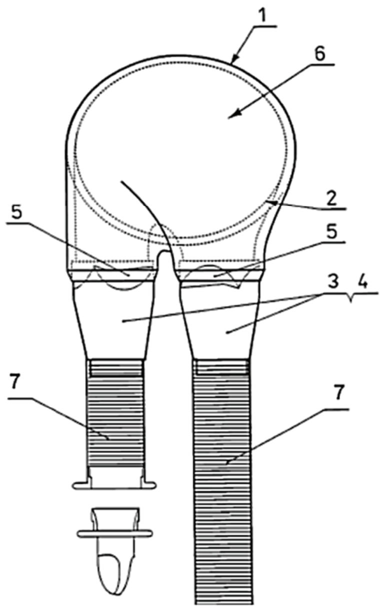


Fig. 2. Pneumatic ventricular assist device (Ebner et al., 2007) (1): (2) – chamber, (3) and (4) – connectors, (5) – valves, (6) – membrane, (7) – cannulae.

The modelled ventricular assist device is presented in figure 2 (Ebner et al., 2007). Pneumatic ventricular assist device has a blood chamber equipped with two connectors, in which valves regulating blood flow are placed (see Section 4.4). Additionally, a flexible membrane dividing the chamber in bloody and air parts, is mounted.

3. CONSTRUCTION NANOMATERIALS OF VENTRICULAR ASSIST DEVICE

3.1. Biocompatible nanocoatings

In the present section of paper the biocompatible properties of nanocoatings applied in VADs are described. All numerical models developed by the Authors are dedicated to investigation of the mechanical properties of nanocoatings. The selected mechanical properties are also considered as the biocompatible properties. The mechanical properties of the coatings are discussed in further sections of the paper.

The early genesis of the concept of nanomedicine sprang from the visionary idea that tiny nanorobots and related machines could be designed, manufactured, and introduced into the human body to perform cellular repairs at the molecular level was introduced by R.P. Feynman in 1959 (Freitas, 2005). Without losing sight of Feynman's original long-term vision of medical nanorobotics, nanomedicine today has branched out in hundreds of different directions, each of them embodying the key insight that the ability to structure materials and devices at the molecular scale can bring enormous immediate benefits in the research and practice of medicine. According to the partial nanomedicine technologies taxonomy proposed by (Freitas, 2005) the biocompatible surfaces and thin-film coatings are categorized as control surfaces, which are applied in the next category of nanomedicine technologies – biotechnology, especially in nanomedicine subcategory artificial organs.

Titanium coating, which is called the buffer layer, has been deposited by laser ablation on the whole outer surface of the VAD's blood chamber (Ebner et al., 2007) made of polyurethane (PU). It is caused by the fact, that the polymer exhibits the change in stiffness in the long term clinical application thus the need of the surface modification. Then, also by using the PLD (Pulsed Laser Deposition) method the titanium nitride and/or titanium carbo-nitride coating is deposited. The whole thickness of outer layers covering the PU elements is from 5 nm to 500 nm, profitably from 20 nm to 100 nm and the most profitably 50 nm. The buffer titanium layer is equal from 1 to 50% thickness of whole outer covering layers.

Biomaterials such as titanium Ti and stoichiometric titanium nitride TiN, as well as titanium carbo-nitride Ti(C,N), seem to be good candidates for future blood-contact applications such as VADs (Sarna et al., 2010).

The single most important factor that distinguishes a biomaterial from any other material is its ability to exist in contact with tissues of the human body without causing an unacceptable degree of harm to that body. There are very many different ways in which materials and tissues can interact such that this co-existence may be compromised, and the search for biomaterials that are able to provide for the best performance in devices has been based upon the acquisition of knowledge and understanding about these interactions. These are usually discussed in the broad context of the subject of biocompatibility. There are many definitions of biocompatibility, but the best known and accepted are these which were formulated by David F. Williams. The following definition of biocompatibility is proposed by Williams (Williams, 2008): „The biocompatibility of a long term implantable medical device refers to the ability of the device to perform its intended function, with the desired degree of incorporation in the host, without eliciting any undesirable local or systemic effects in that host."

The major material characteristics that may conceivably influence the host response are listed in (Williams, 2008), as well as the major characteristics of the generic host response to biomaterials. The main biocompatibility determinants of titanium, stoichiometric titanium nitride and titanium carbonitride deposited by PLD method applied in VADs were tested by (Ebner et al., 2006; Sarna et al., 2010). According to classification of biocompatible properties introduced by Williams (2008) the following conclusions can be formulated on the basis of (Ebner et al., 2006; Sarna et al., 2010) results:

1) material variables that could influence the host response:
   - The high quality of microstructure, lack of cracks and elastic properties,
   - Nanocrystalline structure,
   - The uniform distribution of element content in the layer,
   - High hydrophobic properties,
   - The thinner coating, the greater the residual stress. The thickness of coating equal 50 nm gives the full range of deformability.

2) characteristics of the generic host response to biomaterials:
   - Titanium nitride exhibits low cell-material interaction in dynamic cell detachment test which increased with the carbon introduction into the Ti(C,N) phase, what can be crucial in platelet adhesion.
   - Cell-material interaction in static conditions revealed stoichiometric titanium nitride as biocompatible material and this behaviour was damaged by non-stoichiometry.
   - Chemical composition (stoichiometry) and crystallographic orientation has influence on cell adhesion, because of diversification of atomic density on crystallographic planes.
   - The bigger the smoothness of surface is, the greater is stress between cell and materials surface.

Additionally, recent studies extended the view on promising biocompatible parameters of TiN and TiCN coatings deposited by other beyond PLD recommended physical deposition methods. Many works dedicated to biocompatibility research of these coatings confirm the results obtained by (Ebner et al., 2006; Sarna et al., 2010), but also more biocompatible parameters were measured and according to Williams's classification they are as follows:

1) material variables that could influence the host response:
   - All of the coatings exhibited increased contact angles compared with the substrate (Ti). The TiN showed the lowest contact angle (wettability) of the examined coating layers (Jones et al., 2000; Serro et al., 2009). It is also shown that TiN is slightly more hydrophilic.
   - The corrosion property of TiN layers is expected to be very good (Park et al., 2003).
   - The TiN coating resulted in values of roughness higher than the substrate Ti on which it was grown (Jones et al., 2000). There was no observable correlation between the surface roughness of the structures and the change in measured contact angle.
2) characteristics of the generic host response to biomaterials:
   - No significant differences in the cytotoxicity were observed in (Chien et al., 2008) and therefore, all coatings are not cytotoxic (Park et al., 2003) and may be used as biomaterials (Serro et al., 2009).
   - The cell viability, adherence and proliferation increase significantly (Chien et al., 2008; Serro et al., 2009).
   - The titanium substrate and deposited coatings (Jones et al., 2000) produced variable results in terms of hemocompatibility. All of these surfaces caused some degree of platelet activation. Thrombus formation was also seen on all of these surfaces. The greater spreading of platelets on these surfaces is thought to occur as a result of a lower ratio of adsorbed albumin-to-fibrinogen proteins. Although many of the reports in the literature of TiN coatings in biomedical applications are favourable, there must remain doubts as to its suitability in blood interfacing applications.

3.2. Deposition process

The thickness of biomaterial coatings could be changed from submicron to several hundred micrometers depending on the usage, and therefore, an appropriate coating process should be chosen (see, figure 3) due to lower process temperature and stronger adherence (Goto, 2005).

The deposition techniques fall into categories:

- Chemical – a fluid precursor undergoes a chemical change at a solid surface, leaving a solid layer. Chemical deposition is categorized by the phase of the precursor: plating, chemical solution and chemical vapour deposition.
- Physical - uses mechanical or thermodynamic means to produce a thin film of solid. Examples of physical deposition include: thermal evaporation, sputtering, pulsed laser and cathodic arc deposition.
- Mixture of chemical and physical – examples: reactive sputtering, molecular beam epitaxy and topotaxy.

Irrespective of thin film preparation methods such as PVD and CVD, the thin film process is comprised of three elementary stages including decomposition, transport and nucleation, and growth mechanisms (Taga, 2001). Figure 4 shows the flow charts of the thin film process, where starting materials are successively modified to the resulting films.

Using temperature-sensitive materials like polymers, especially substrates in VADs, requires low-temperature coating techniques to deposit biocompatible coatings Ti, TiN and TiCN (Lackner, 2005), but there is a lack of industrially scaled vacuum coating techniques at temperatures below 50°C. An alternative for overcoming this problem is the PLD technique (Lackner, 2005) shown in an advanced version as HybridPLD system in figure 5.

atomic clusters is then deposited on the substrate. The outstanding advantage of this technique is the possibility to deposit coatings of very high chemical

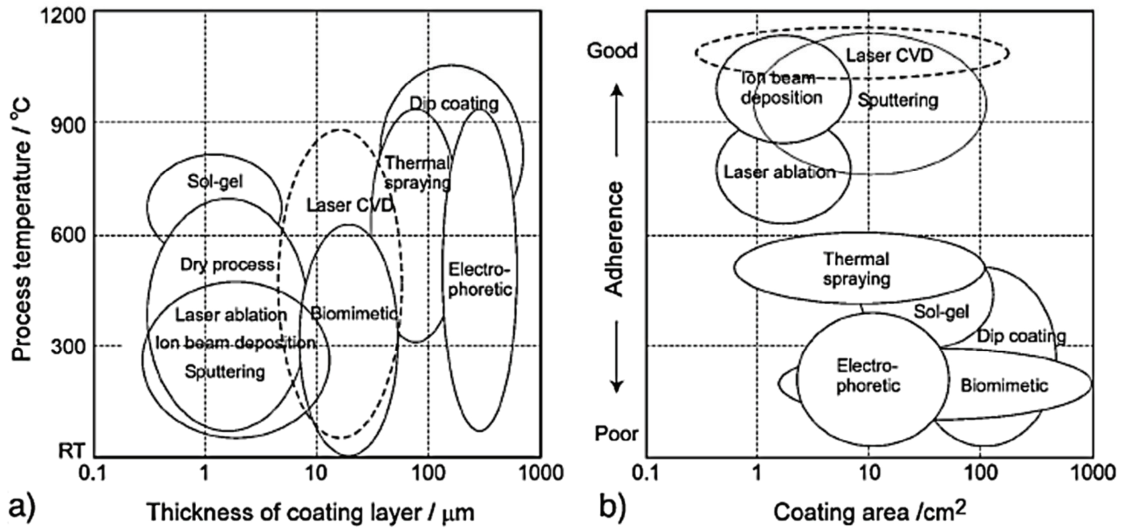


Fig. 3. Schematic diagram of coating processes for biomaterials (Goto, 2005): a) process temperature versus thickness of coating layer, b) adherence versus coating area.

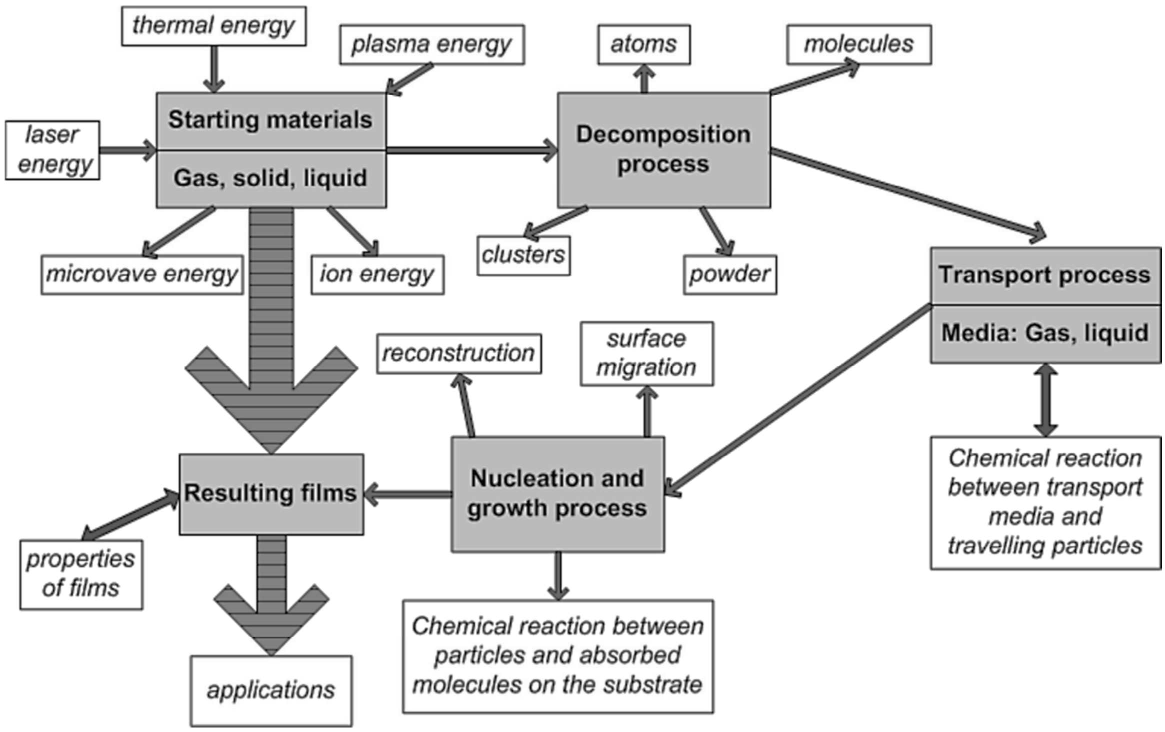


Fig. 4. Flow chart of thin film process (Taga, 2001).

In the PLD technique (Lackner, 2005) a Nd:YAG laser operating at the fundamental harmonics is used to deposit the coatings on PU substrates in VADs by ablation of high purity titanium nitride target. In the PLD technique a pulsed laser beam is focused on a target in order to evaporate its surface layers under vacuum or low pressure process gas conditions. The vaporized material consisting of atoms, ions and

purity and adhesion to various substrate materials at room temperature. The application of reactive process gases leads to the opportunity of varying the film stoichiometry in a wide range.

In VADs the multilayer or graded coatings are also expected, therefore, the hybrid coating technologies are involved, because they allow the modification and deposition of complex coatings structures in one deposition plant. Since the process of material ejection at the target surface using PLD is not that sensitive to the background gas or other system parameters, it is relatively easy to incorporate simultaneous or successive applications of different processing techniques in PLD systems. Based on the principle of multi-beam evaporation from a static target position onto moved substrates an industrially-scaled PLD coating facility was built at Laser Center Leoben (Lackner, 2005).

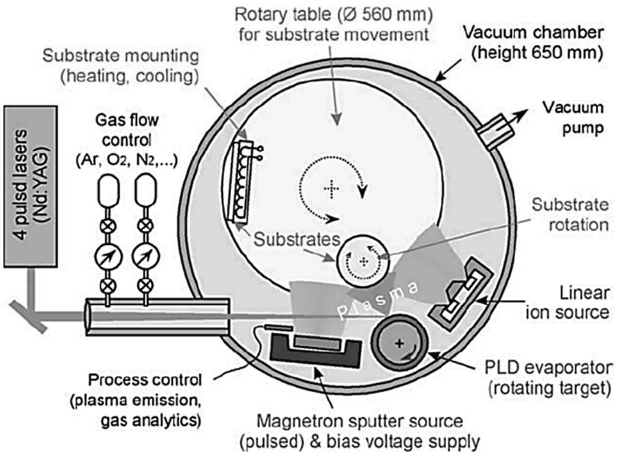


Fig. 5. *Example for a versatile industrially-scaled hybrid PLD coater including an ion source, pulsed DC magnetron sputtering, substrate biasing, plasma diagnostics, substrate heating and substrate rotation/manipulation (HybridPLD coater, Joanneum Research Forschungsgesellschaft mbH, Laser Center Leoben) (Lackner, 2005).*

The system, shown schematically in figure 5, comprises the hybrid coating approach (thus, HybridPLD), allowing simultaneous deposition from several coating sources:

- PLD coating is performed from rotating (metal) targets using a pulsed Nd:YAG laser system of four laser beams of 1064 nm wavelength, operating at a repetition rate of 50 Hz and providing 10 ns pulses of 600 mJ pulse energy.
- Additionally, magnetron sputtering (bias-supported) from a 40 cm high rectangular sputter target provides a second high-rate coating technique in the HybridPLD equipment. By using pulsed DC (diode) sputtering the reactive deposition of a wide range of metals is possible.
- A linear ion source completes the available coating techniques, allowing substrate cleaning and activation as well as plasma-assisted chemical vapour deposition (PACVD) at low substrate temperatures.

3.3. Mechanical properties of nanocoatings

Knowledge about the mechanical properties of nanomaterials, which are used in the VADs, is crucial for the accuracy of numerical simulations. Mechanical properties (hardness, stiffness, fracture resistance, toughness, load support) and tribological properties (friction coefficient, adhesion, resistance to: abrasive wear, sliding wear, brittle fracture, fatigue wear, dynamic loading and corrosion of coating/coating systems) of coatings are obtained in the following experimental nanotests (Fischer-Cripps, 2002):

- nanoindentation,
- nano-scratch,
- nano-impact,
- high temperature testing.

The technical reasons for applying nanoindentation instead of tensile test for coatings are briefly justified below. Tensile tests, before necking begins, have the advantage of uniform stress and strain fields, which is why they are the most common way to determine mechanical properties at larger scales. They provide stress-strain curve and thus one can measure the mechanical properties easily and reliably. However, they have disadvantages at smaller scales. Since, larger forces are required, a specimen gripping may be difficult. Also specimen preparation can be expensive and time-consuming. Gripping and alignment are fraught with potential errors. Strain measurement requires unique approaches. The second known method, which is the nanoindentation test, is easy to use and requires little specimen preparation. The principal goal of this testing is to extract elastic modulus and hardness of the specimen material from experimental readings of indenter load and depth of penetration. For these reasons, this method is widely used in testing especially of thin films up to nanometer scale thickness. On the other hand, there are many factors to consider for extracting quantitatively reliable mechanical properties from a nanoindentation test. Thus, there has been considerable interest in the last two decades in the mechanical characterization of coatings using nanoindentation test (Fischer-Cripps, 2002), because standard experimental methods performed in macro scale are not highly recommended by specialists and test gives the information about key mechanical parameters:

- mechanical properties (hardness, elastic modulus),
- creep resistance,

– temperature-dependent properties.

No other known nanotechnique provides information about both the elastic and plastic properties of coatings. The example of results obtained in nanoindentation test as force-displacement data measured for TiN nanocoating deposited by PLD method on ferritic steel are presented in figure 6 (Kopernik et al., 2011). Using these raw data the calculated Martness hardness is 6.04 GPa and reduced Young modulus is 155 GPa for TiN.

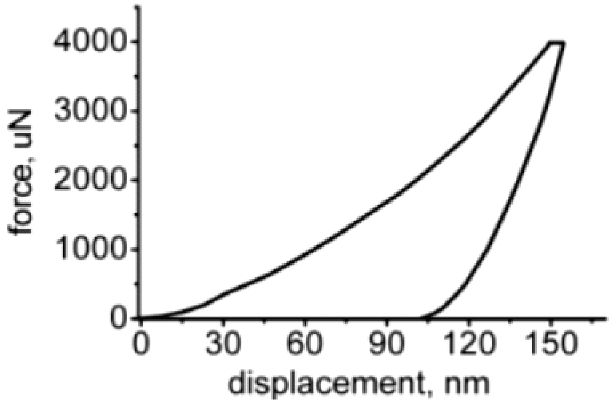


Fig. 6. *Example of force-displacement curve measured for TiN (Kopernik et al., 2011).*

The analysis of nanoindentation test raw data gives the elastic-plastic properties of TiN coating and, therefore, confirm purposefulness of identification the parameters in material models of coatings by numerical procedures (see section 4.3.3).

The four most commonly used pyramidal indenter geometries are:
– Vickers,
– Berkovich,
– modified Berkovich,
– cube corner.

The Martens hardness is defined for Vickers and Berkovich indenter geometries, but not for spherical or Knoop indenters. Nanoindentation testing is performed in load-controlled mode using appropriate experimental system (Fischer-Cripps, 2002). The indentation test can be controlled either in force or in depth. Indentations are cycle load-controlled load-partial unload experiments from 1 mN to 20 mN maximum load. An uncoated substrate wafer is tested for comparison.

The validity of the results for hardness and modulus depends largely upon the analysis procedure used to process the raw data. The two most commonly used methods are:
– Oliver and Pharr (Oliver & Pharr, 1992; Kopernik et al., 2008; Kopernik et al., 2011),
– Field and Swain (Field & Swain, 1993).

The main difference between the two mentioned methods is that the Field and Swain method fits a single pair of data points (maximum load and some percentage unload) to the Hertz equation (Fischer-Cripps, 2000), where the Oliver and Pharr method uses a series of data points and fits the slope of the initial unloading to the derivative of the Hertz equation. The Oliver and Pharr method is more time-consuming, since a number of unload points must be measured, but less susceptible to errors in the data. The choice of method depends upon the circumstances of the test. For example, where the test is being performed in an environment where there are undesirable mechanical or thermal influences, the Field and Swain method may be more appropriate. These two procedures are concerned not only with the extraction of modulus and hardness, but also correcting the raw data for various systematic errors that have been identified for this type of testing. However, methods to estimate mechanical properties are limited to the hardness and Young modulus. These properties do not describe the complete material models of coatings. Due to strong inhomogeneities of the tests, extracting these additional model parameters from the tests is difficult. Therefore, additional attempts towards the development of the numerical model of nanoindentation test are still undertaken.

The recently examined problems of nanoindentation measurements by applying modelling, scaling and dimensional analysis provide better understanding of fundamental questions specified by (Cheng & Cheng, 2004), including (see, figure 7):
– What information is contained in the indentation load-displacement curves?
– How does hardness depend on the mechanical properties and indenter geometry?
– What are the factors determining piling-up and sinking-in of surface profiles around indents?
– Can stress-strain relationships be obtained from indentation load-displacement curves?
– How to measure time dependent mechanical properties from indentation?
– How to detect or confirm indentation size effects?

According to Pauleau (2001) residual stresses in coatings produced by physical vapour deposition (PVD) techniques result from the contribution of thermal, intrinsic and extrinsic stresses. Tensile intrinsic stresses are usually observed in not fully dense films deposited by thermal evaporation from non-energetic particles. Compressive intrinsic stresses develop in relatively dense films deposited at low temperatures under energetic particle bombardment.

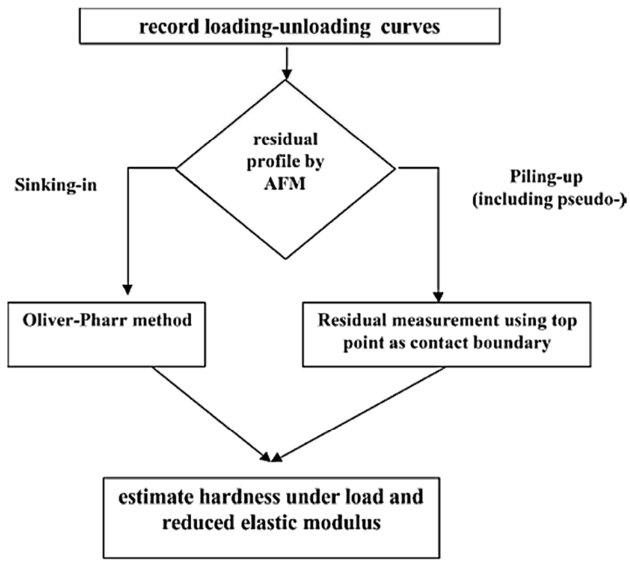


Fig. 7. *Flow chart describing a methodology for obtaining hardness and elastic modulus by instrumented indentation and surface profile measurements by using AFM (Atomic Force Microscopy) (Cheng & Cheng, 2004).*

The comparison between literature studies and results obtained for biocompatible TiN nanocoating deposited on PU by using PLD method shown in (Kopernik et al., 2011) leads to conclusion that compressive residual stresses are bigger, when TiN nanocoating is deposited by PLD method. The residual stress for different thickness of TiN nanocoatings is from 1.5 GPa to 2.4 GPa. 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 layer formation. Therefore, the compressive residual stress distribution obtained in (Kopernik et al., 2011) is further introduced as the initial stress in the numerical model of nanoindentation test (see Section 4.4).

The review of major models proposed in the literature to explain the origin of residual stresses in PVD films was prepared by (Pauleau, 2001). The method selected in (Kopernik et al., 2011) to calculate the residual stress in biocomaptible TiN nanocoating deposited in VADs is presented in (Pauleau, 2006) and it finally leads to substituting the Stoney's equation on the basis of observations of TEM (Transmission Electron Microscopy) images.

4. MULTISCALE MODELLING

4.1. Motivation

The development of reliable material models for simulations of loading of nanocoatings has been of interest to scientists for several years. The main objective is to realistically describe the phenomena occurring in materials at lower length scales under the complex conditions of deformation and to incorporate this into the continuum based approaches. Several of these phenomena are stochastic in nature and their realistic description by deterministic models is limited. Thus, the search for models that account more accurately for microscale and even nanoscale phenomena is the objective of research. The improvements in experimental techniques are major factors stimulating this research. New experimental techniques make it possible to visualize physical processes and to measure relevant parameters at fine scales. Examples connected with new experimental equipment allowing research on mechanics of deformation are atomic force microscopy (AFM), nanoindentation tests, computer tomography, etc. These techniques are supported by the established approaches such as scanning and transmission electron microscopy. The knowledge about mechanisms of phenomena obtained from these experiments is combined with the idea of multiscale modelling of materials to develop models with new predictive capabilities.

4.2. Classification of multiscale modelling methods

The multiscale methods are classified into two groups: upscaling methods and concurrent multiscale computing (De Borst, 2008). In the upscaling class of methods, constitutive model at higher scale is constructed from observations and models at lower, more elementary scales. The idea of the representative volume element (RVE) is employed. By an interaction between experimental observations at different scales and numerical solutions of constitutive models at larger scale, physically based models and their parameters are derived at the macroscale. The computational homogenisation is considered to belong to this group of methods.

In concurrent multiscale computing the problem is solved simultaneously at several scales by an *a priori* decomposition of the domain. The two-scale methods, whereby the decomposition is made into coarse scale and fine scale, have been considered so far.

Various discrete methods are applied to describe material behaviour at micro- and/or nanoscales, eg. cellular automata (CA), molecular dynamics (MD), Monte Carlo (MC) methods. In the concurrent multiscale computing the method used to describe the fine scale is applied to a part of the whole domain. It can be either the same method, which is used in the coarse scale, (eg. the FE method), or it can be one of the earlier mentioned discrete methods (CA, MC).

4.2.1. Multiscale models

The extended finite element (XFE) and the multiscale extended finite element (MS-XFE) methods are examples of the concurrent multiscale models. In the XFE solution special elements capable to accommodate a discontinuity are introduced. In the MS-XFE method a very fine mesh is generated in the area of particular interest that is selected before simulation. The example is the area around the front of crack propagation in a simulation of fracture, as shown in (Allix, 2006). An example of the upscaling approach based only on the FE method is presented in (Milenin & Muskalski, 2007). The two-scale model based on the FE method combined with the representative volume element approach is proposed to simulate the influence of colony composed of ferrite and cementite on the macroscopic behaviour during wire drawing. The macroscale model uses a FE solution that provides the boundary conditions for the microscale model. This work, which is classified as upscaling method based on the FE solutions in the two different scales, is applied in the present work for analysis of phenomena occurring in the nanocoatings due to loading of the ventricular assist device in the macroscale.

4.3. Modelling methods selected for VAD's multiscale model

4.3.1. FEM

The first work, which introduced a main conception of finite element method, was that of R. Courant in 1943. Finite element method (FEM) is now a basic tool for numerical modelling of mechanical processes, such as deformation of VAD. Base conception of FEM for elastic and elastic-plastic problems is widely described, for example, in (Zienkiewicz & Taylor, 2000). The implementation of FEM is applied in many works dedicated to modelling of the following processes observed in VADs:

- Blood flow in different phases of artificial VAD working (Moosavi et al., 2009);
- Modelling of human heart valve function (Sacks et al., 2009);
- Multiscale modelling of fibre structure of human heart (Sacks et al., 2009).

Basing on literature, the example of result obtained for pneumatic VAD's numerical simulation in macroscale in 2D is presented in (Moosavi et al., 2009). The velocity vectors of blood and driving fluid during the systole phase are shown in figure 8.

The following conclusions are formulated basing on (Moosavi et al., 2009):

- The results show how the membrane in blood chamber moves downward and upward to generate the velocity field.
- Wakes occur in the blood chamber, what prevents the blood from being coagulated. The review of the blood flow domain at different time steps shows that the wakes are periodically generated during the diastolic phase and continuously move from the inlet to the outlet during the systolic phase. Therefore, in the analysed type of VAD with membrane, blood is washed out properly and there is no zone in which the blood is coagulated due to remaining in the chamber.

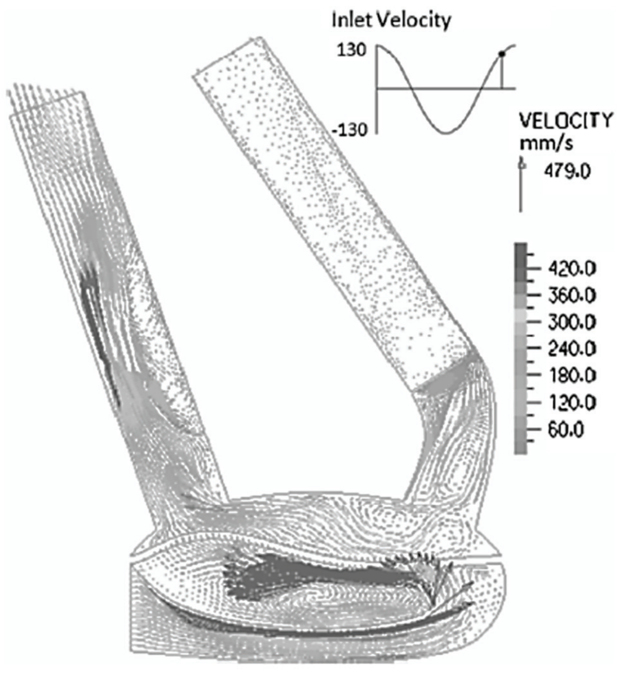


***Fig. 8.** Velocity vectors of blood and driving fluid during the systole phase (Moosavi et al., 2009).*

- The opening and closing of the inlet and outlet valves can be clearly distinguished in the investigated model of VAD. In this model, the valves leaflets were also considered and their effect to flow pattern were analysed. The configuration of generated wakes near the valves indicates that the type of the valve plays an essential role in the wakes' generation. The type of the valve used in this simulation provides the proper conditions for the generation of blood wakes and prevents the appearance of the stagnation regions.
- Additionally, the results show that the magnitude of the maximum shear stress at each time step occurred at the end of the leaflet. The model of the leaflets does not perform a critical shear stress on the red blood cells.
- Summarizing, the numerical FEM simulation in macroscale shows the performance of the VAD with membrane and valves for satisfying the standard design consideration of the blood flow device.

4.3.2. RVE

Multiscale FEM belongs to the group of homogenization methods so that it is applicable only in the case of statistically uniform materials (Mura, 1993; Nemat-Nasser & Hori, 1993; Torquato, 2002; Willis, 1981; Willis, 1982; Zohdi & Wriggers, 2005). For this kind of materials, it is typical that they possess a representative volume element, whose analysis yields the effective material parameters, but the limiting condition is that the ratio of the characteristic lengths of RVE and the simulated body has to tend to zero. The representative volume element is an intermediate scale between the nano and the macroscopic ones. Inhomogeneities of the nanostructure are supposed to be small compared to the RVE, and the RVE should be small compared to the item, to which belongs this nanostructure. The latter assumption means that the averages of all the gradients vanish in the RVE. The method is based on the principle of volume averaging, leading to the definition of the macro stress tensor in the form:

$$\bar{\sigma} = \frac{1}{V_{RVE}} \int_{V_{RVE}} \sigma dV \quad (1)$$

where: $\bar{\sigma}$ – average stress; the integration is carried out over the RVE with the volume V_{RVE}.

Note, that within the scope of modelling of TiN coating, consideration is given to the theory of small elastic-plastic deformations. The well-posed problem in the nanoscale also requires the equality of macrowork with the average volume of nanowork:

$$\bar{\sigma} \cdot \bar{\varepsilon} = \frac{1}{V_{RVE}} \int_{V_{RVE}} \sigma \varepsilon dV \quad (2)$$

which is known as Hill-Mandel macrohomogeneity condition (Hill, 1963; Hill, 1972) and where: $\bar{\sigma}$ – average stress, $\bar{\varepsilon}$ – average strain, V_{RVE} – volume of RVE.

Equation (1) is satisfied by three types of boundary conditions in the nanolevel: static, kinematic and periodic. In (Thibaux et al., 2000) the effects of different boundary conditions are compared and the minimum number of grains needed to obtain a representative volume element is investigated. It is assumed that volume element is representative if different kinds of boundary conditions lead to the same result in terms of mechanical behaviour. Another way to assess this requirement is checking whether a bigger number of grains inside the RVE would not affect the results for the mechanical behaviour for identical properties. The periodic boundary conditions are the following: velocity component perpendicular to the side of the cube is imposed, but ones parallel to the side are let free. With these boundary conditions, each side of the cube is a symmetry plane (Thibaux et al., 2000). Two ways to compute the average properties are presented: averaging over all integration points, or excluding the points within a minimum distance from the boundary of the representative volume element. Finally, it appears that the best boundary conditions are periodic, using an average computed on the whole mesh.

4.3.3. Inverse analysis

Numerical simulation of any process or phenomenon requires information about material properties and accuracy of simulations depends strongly on the correctness of description of mechanical and/or thermal boundary conditions. In the present work the former problem is directly connected with the evaluation of mechanical and rheological properties of nanocoatings. One of the challenges in simulations of loading of VAD is an evaluation of these parameters in various exploitation conditions by performing nanoindentation tests. Advantages and disadvantages of these tests and difficulties with the interpretation of the results are known (Kopernik & Pietrzyk, 2007). The main disturbances are inhomogeneities of strains, localization of strains and effect of friction. Following this, the goal of many researches is development of the method that eliminates the disturbances occurring in experimental tests and that allows estimation of material parameters independently of these disturbances. The problem of parameters evaluation is defined as an inverse problem. Inverse algorithm can be applied to solve any of thermal, mechanical and boundary problem in material deformation (Malinowski et al., 1994; Boyer & Massoni, 2001; Fourment et al., 1998; Szeliga et al., 2006). Any nanoindentation test is described by the set of equations:

$$\mathbf{d} = F(\mathbf{x},\mathbf{p}), \qquad F: R^k \to R^r \quad (3)$$

where: $\mathbf{d} = \{d_1,..,d_r\}$ – vector of measured output parameters, $\mathbf{x} = \{x_1,..,x_l\}$ – vector of model parameters, $\mathbf{p} = (p_1,..,p_k\}$ – vector of test variables. If vector $\mathbf{x}$ is unknown, the problem (3) is called the inverse problem. The examples of measured output parameters are: loads monitored during the test and shape of the sample after the test. The examples of model parameters are: material mechanical and rheological coefficients. The examples of process variables are: displacement, die velocity, and temperature of sample.

The objective of the inverse analysis is an evaluation of optimum values of vector $\mathbf{x}$ components. It leads to minimization, with respect to the vector $\mathbf{x}$, of the distance between vectors containing calculated and experimental values:

$$\Phi(\mathbf{x}) = \sum_{i=1}^{n} \beta_i [\mathbf{d}_i^c(\mathbf{x},\mathbf{p}_i) - \mathbf{d}_i^m]^2 \qquad (4)$$

where: $\mathbf{d}^m = \{\mathbf{d}_1^m, \mathbf{d}_2^m,.., \mathbf{d}_n^m\}$ – vector of measured data, $\mathbf{d}^c = \{\mathbf{d}_1^c, \mathbf{d}_2^c,.., \mathbf{d}_n^c\}$ – vector of calculated data, β_i – weights (i = 1 .. n), n – number of sampling points. Measured data $\mathbf{d}^m$ is obtained from the test and values $\mathbf{d}^c$ are calculated using direct problem model. The flow chart of the inverse method is shown in figure 9 (Szeliga et al., 2006).

The goal function (4) is usually defined as an average square root error (error in Euclid's norm), but another norms can be used, as well.

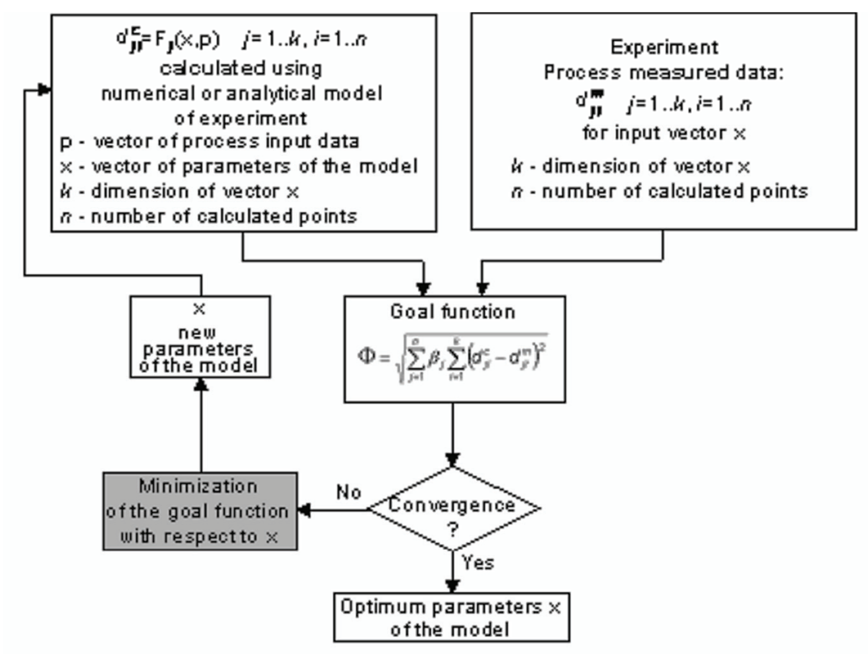


Fig. 9. *Flow chart of the inverse algorithm (Szeliga et al., 2006).*

Regardless of the type of the experiment and independently of the applied method of the solution, the algorithm of the inverse problem consists of three parts:

– Experiment. Measured data from the experiment is input information for the goal function of the inverse algorithm.
– Simulation for direct problem, usually based on finite element method.
– Optimization procedure to minimize the defined goal function. Classical non-gradient and gradient algorithms as well as heuristic methods like evolution algorithms can be applied.

In the present work, the inverse algorithm is used to identification of properties of nanocoatings (parameters in material model and residual stress distribution) on the basis of results of nanoindentation tests, analytical equation, TEM and AFM images. The applied non-gradient simplex Nelder-Mead method was described by the Authors in details in (Kopernik et al., 2008).

4.4. Proposed approach to multiscale model of VAD

TiN is an elastic-plastic coating and is deposited by laser ablation on the whole surface of the modelled VAD's blood chamber made of nonlinear elastic polyurethane (Chronothane 55D; Young's modulus E = 470 MPa and Poisson's ratio ν = 0.4). The FEM solution is focused on strain and stress analysis for macromodel of VAD's blood chamber with option of local strain and stress analysis in nanomodel by applying RVE (compare, Modelling methods selected for VAD multiscale model). The RVE nanomodel also includes residual stress distribution (see, Mechanical properties of nanocoatings) and modelling unloading in nanomodel of wall of VAD's blood chamber. The introduced multiscale model leads to two associated additional problems, which are defined as:

– Automatic fragmentation of FEM mesh generated in any commercial and authors' program in macroscale to set precisely loadings and boundary conditions in any place of macromodel of VAD's blood chamber;
– Identification of parameters in material model of TiN by development nanomodel and program to simulation the nanoindentation test for TiN/PU with the option of inverse analysis and modelling unloading (see, Modelling methods selected for VAD multiscale model) (Kopernik et al., 2011).

The purpose of this approach is 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 multiscale solution is shown in figure 10 and is composed of two stages:

– residual stresses modelling and
– active loadings modelling.

In the first stage (figure10a), the residual stress is reached by applying experimental results and the inverse method (Kopernik et al., 2011) in nanoscale. In the second step (figure 10b), 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, the boundary conditions are moved from solution in nanoscale to macroscale.

The macromodel of VAD's blood chamber is composed of the geometry model, which was created and refined in CAD program. The 3D FEM model of the blood chamber was generated in authors'

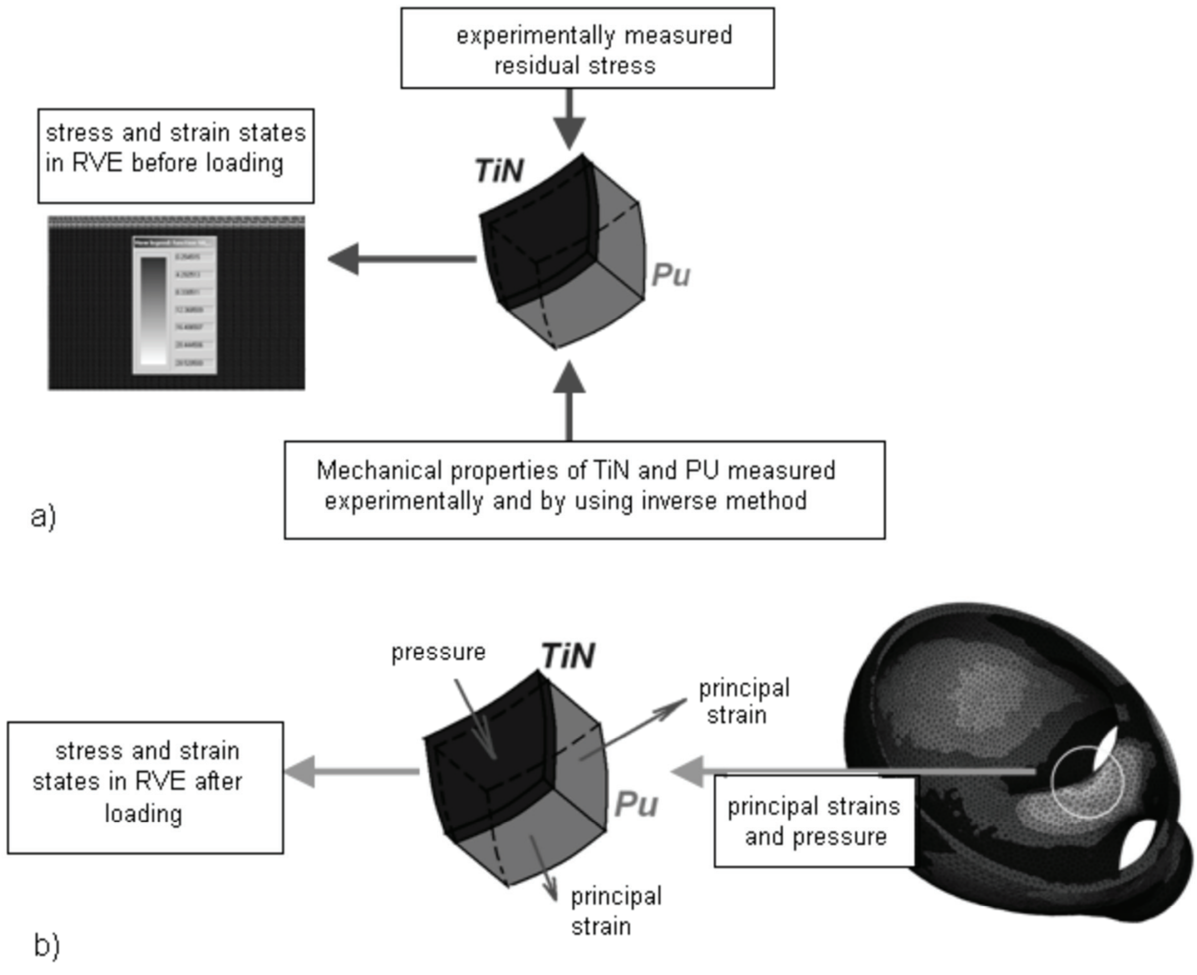


Fig. 10. *General conception of multiscale model of blood chamber: a) residual stress modelling, b) active loading modelling.*

code and is presented in figure11. The 30 000 elements are used to solve the boundary problem for the analysed model. The FEM mesh fragmentation by applying algorithms (Irons, 1975; Milenin, 1998) was performed to set properly boundary conditions (Milenin & Kopernik, 2011) in the model. The static loading equal to 16 kPa (maximum physiological blood pressure in the ventricle) is uniformly distributed on the inner surface of the chamber.

The selected results are shown in figure 12 as distributions of effective strain and effective stress in wall of blood chamber under working loadings, which are observed on the inner surface of bottom part of blood chamber in side view of cross-section between the two connectors. The results of simulations show that values of stress equal tens of kPa on wall of the blood chamber, what in comparison with applied outer working loadings and material properties of chamber can be assumed as correct. Besides, the previous studies based on ABAQUS FEM code (Milenin & Kopernik, 2009) confirmed places of concentration of the maximum values of stress and strain, which are computed in the bottom parts of blood chamber POLVAD between inlets of both connectors.

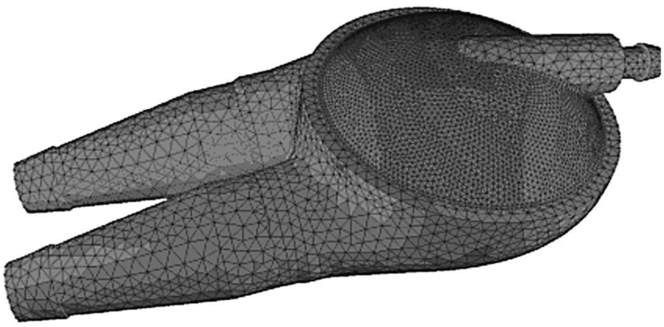


Fig. 11. The 3D FEM model of the blood chamber performed in authors' code.

The 2D nanomodel of TiN/PU specimen prepared in authors' code has 3800 elements. The parameters of bilinear elastic-plastic material model selected for TiN (figure 13) and identified in the inverse analysis by using authors' 2D model of nanoindentation test are as follows (Kopernik et al., 2011): ε_1 = 0.009, σ_1 = 2,614 MPa, ε_2 = 0.166 and σ_2 = 9,107 MPa. According to this solution, the elastic modulus of TiN is equal to 290.4 GPa. The obtained elastic modulus is in the range of values given in literature.

In simulations performed for nanomodel of TiN/PU specimen, the biggest values of effective strain are located in a very thin zone between two main material layers TiN and PU (figure 14 a). The

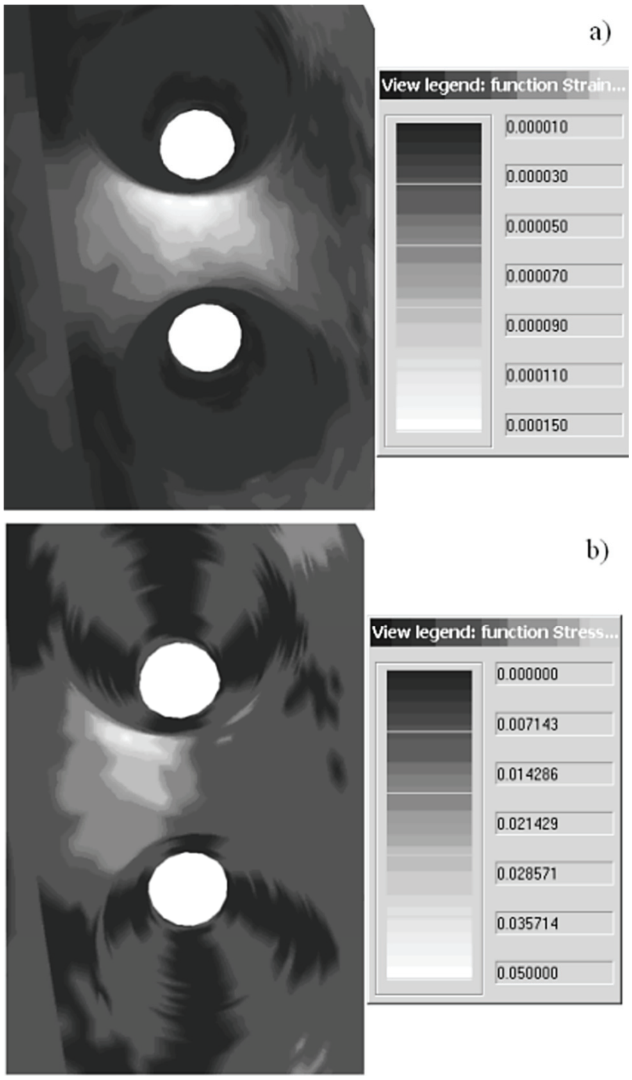


Fig. 12. Tested distribution of a) effective strain and b) effective stress in material of blood chamber POLVAD computed in own code, which are observed on inner surface of bottom part of blood chamber in side view of cross-section between two connectors.

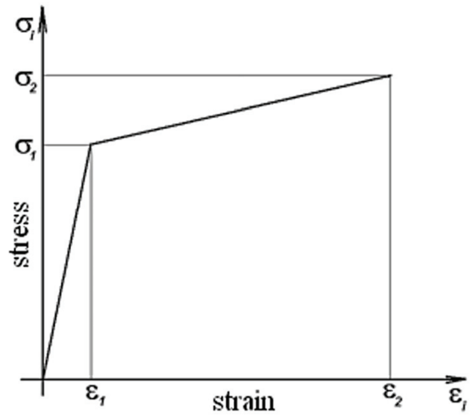
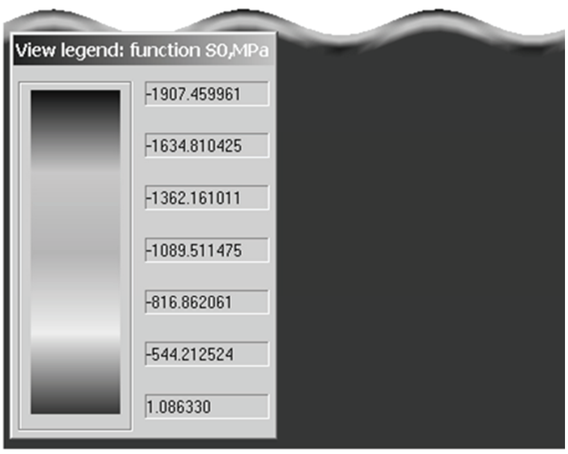


Fig. 13. Bilinear elastic-plastic material model selected for TiN.

average stress in layers TiN (figure 14b) is equal 1.9 GPa (respectively 1 GPa 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.

a)



b)

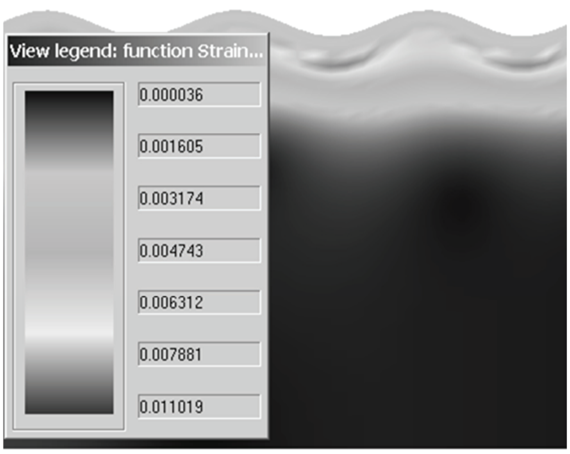


Fig. 14. *Distribution of: a) effective strain and b) average stress in nanomodel of specimen PU/TiN.*

5. CONCLUSIONS

Conclusions based on the multiscale solution dedicated to blood chamber:

- The FEM solutions reached in the commercial code ABAQUS and in Authors' code reproduce the strain and stress states in the blood chamber. Predicted distributions of selected parameters help to define precisely the regions of chamber, which can be defined as the failure-source areas. Thus, the extended multiscale modeling is needed for these areas. Additionally, the calculated values of strain after loading are the input for the nanomodel.
- The nanomodel based on the authors' FEM code is composed of main material layer (PU) and very thin outer coating (TiN). The observed distributions of stress and strain states help to determine precisely the critical values of these parameters, which can be achieved in the investigated materials.
- In macromodel the region with the biggest tendency to fracture is located at the inner surface of the bottom part of the blood chamber between two connectors.
- In the nanomodel the region with the biggest tendency to fracture is identified as a very thin region between two main material layers TiN and PU at inner surface of the bottom part of blood chamber between two connectors.
- The developed FEM computer program allows simulation and optimization for any construction of multilayer blood chamber of ventricular assist device in macro and microscale.

The more advanced solution will be obtained in the future and will be combined with the solution for flow in the blood chamber. This fluid structure interaction should enable an analysis of phenomena occurring in the ventricular assist device and to model exactly these problems that are unattainable to model in commercial software.

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NOWY WIELOSKALOWY MODEL MES WIELOWARSTWOWEJ KOMORY WSPOMAGANIA PRACY SERCA ZBUDOWANEJ Z POLIURETANU I NANOPOWŁOKI TiN OSADZONEJ METODĄ ABLACJI LASEROWEJ

Streszczenie

Komora wspomagania pracy serca jest sztucznym narządem, który jest wykorzystywany do leczenia chorób serca. Na świecie, jak i w Polsce, czynione są wysiłki zmierzające do opracowania takiego urządzenia, które jest biokompatybilne, trwałe, zużywa mało energii, pozwala na monitorowanie i nie wprowadza zamian w morfologii krwi. Niniejszy artykuł omawia rodzaje komór wspomagania pracy serca, łącznie z komorą wspomagania zaproponowaną w Polsce. Szczególnie nacisk jest położony na modelowanie numeryczne i komputerowe wspomaganie projektowania takiego sztucznego narządu. Ściany komory wspomagania pracy serca są pokryte nanopowłoką TiN za pomocą nowoczesnych technik (ablacja laserowa) w celu poprawy biokompatybilności. Nanopowłoka modyfikuje własności powierzchniowe takiego urządzenia. Własności mechaniczne nanopowłoki są określane w doświadczalnych nanotestach i za pomocą technik obrazowania nanostruktur. Jednakże, te testy podają średnie wartości własności i taka informacja nie jest wystarczająca dla zaawansowanego projektowania komory wspomagania pracy serca. Aby wyeliminować to ograniczenie, zastosowano modelowanie wieloskalowe. Opracowane rozwiązanie, które jest oparte na zastosowaniu i kombinacji metod takich jak: metoda elementów skończonych, podejście wieloskalowe i analiza odwrotna, zostało przedstawione w artykule. Te metody są pomocne przy przewidywaniu lokalizacji stref uszkodzenia w materiale komory wspomagania pracy serca i potem, aby analizować lokalne zachowanie nanopowłoki. Ponadto, jest możliwa identyfikacja parametrów modelu reologicznego nanopowłoki i wprowadzenie naprężeń własnych do modeli.

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