A Tool for Studying the Mechanical Behavior of the Bone–Endoprosthesis System Based on Multi-scale Simulation

Alexey Yu. Smolin, Galina M. Eremina, and Evgeny V. Shilko

Abstract The chapter presents recent advances in developing numerical models for multiscale simulation of the femur–endoprosthesis system for the case of hip resurfacing arthroplasty. The models are based on the movable cellular automaton method, which is a representative of the discrete element approach in solid mechanics and allows correctly simulating mechanical behavior of a variety of elastoplastic materials including fracture and mass mixing. At the lowest scale, the model describes sliding friction between two rough surfaces of TiN coatings, which correspond to different parts of the friction pair of hip resurfacing endoprosthesis. At this scale, such parameters of the contacting surfaces as the thickness, roughness, and mechanical properties are considered explicitly. The next scale of the model corresponds to a resurfacing cap for the femur head rotating in the artificial acetabulum insert. Here, sliding friction is explicitly computed based on the effective coefficient of friction obtained at the previous scale. At the macroscale, the proximal part of the femur with a resurfacing cap is simulated at different loads. The bone is considered as a composite consisting of outer cortical and inner cancellous tissues, which are simulated within two approaches: the first implies their linear elastic behavior, the second considers these tissues as Boit’s poroelastic bodies. The later allows revealing the role of the interstitial biological fluid in the mechanical behavior of the bone. Based on the analysis of the obtained results, the plan for future works is proposed.

Keywords Bone · Endoprosthesis · Mechanical behavior · Friction · Computer simulations · Particle-based method

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1 Introduction

Endoprosthetics is an effective way to treat such common degenerative diseases of large human joints as osteoporosis and arthritis. Wear in a pair of friction of the constituent elements of the joint endoprosthesis design has a significant impact on its operational resource. Primarily, this refers to the prostheses of the hip and knee joints. The key role in the wear process belongs to the structure of the surface layers of the contacting elements. To improve the tribological characteristics of metal endoprostheses, which are currently the most widely used, reinforcing coatings are used. In practice, titanium is usually used as a metal and titanium nitride (TiN) as a coating.

Since endoprostheses are intended for a long stay in the human body, they should not lead to any discomfort. Therefore, an important stage in the development of endoprostheses is their testing. Endoprosthesis tests are divided into several stages; these are preclinical and clinical trials. Clinical trials are conducted through the installation of an endoprosthesis in a living human body. Using this test, the final result is determined. However, when conducting clinical trials, there is a danger that a poorly or improperly selected endoprosthesis may adversely affect the patient's health. Therefore, much more attention is paid to preclinical trials when developing endoprostheses. Talking about the mechanical behavior of the endoprosthesis, its preclinical studies can be divided into experimental and theoretical. Experimental studies are tests using special equipment that simulates real dynamic loading experienced by an endoprosthesis in the body. In particular, standard methods, such as instrumented indentation, scratching, and three-point bending, are used to determine the tribological properties of the surface layers of materials. It is worth noting that conventional experimental studies are carried out under standard atmospheric conditions and their results can differ greatly from the behavior of materials in real conditions inside a living body. Therefore, part of the experimental studies is carried out in a medium simulating a living body (*in vitro*), or on test samples placed into the animal (*in vivo*). However, for obvious reasons, the number and possibilities of such studies are very limited.

Theoretical studies of the mechanical behavior of the endoprosthesis are most often carried out using computer simulation. It should be noted that modern numerical methods of solid mechanics allow a detailed study of the mechanical behavior of endoprostheses, which takes into account the influence of a variety of factors. However, to fully utilize all the features of this approach, it is necessary to use special software.

In the last decade, the development of computer-aided tools for studying the mechanical behavior of endoprostheses has been the subject of extensive work by leading world scientific groups in such well-known centers as McGill University (Canada), Liverpool John Moores University (Great Britain), Iowa State University (USA) and many others. The high relevance of this problem is also confirmed by numerous publications on this topic in leading scientific journals.

However, tools taking into account the influence of structural features of surface layers on the wear of contacting surfaces, as well as the effect of wear on the mechanical behavior of the endoprosthesis as a whole, have not yet been developed. The second important factor that has to be considered in modeling the mechanical behavior of living bone is the presence of interstitial fluid in it. The availability of such tools would be very relevant in the study of the durability of a new class of endoprostheses made from new composite materials, including titanium alloys with a nanostructured TiN coating.

2 State-of-the-Art

There are two methods of hip arthroplasty: total hip replacement and hip resurfacing. Total hip replacement suggests cutting the femur head and inserting a prosthetic implant into the bone. In the case of hip resurfacing only a very thin layer of the femur head is replaced by a metal cap, which is hollow and shaped like a mushroom. Despite the more complicated procedure of the operation, the latter method is preferable for young people who lead an active life. Previously, only metals were used for the friction pair of the resurfacing endoprosthesis, in particular, the CoCrN alloy. This led to the fact that during life after the surgical operation, severe wear was observed in the friction pair with a large release of metal particles, which led to necrosis of cells and small phagocytes, and severe allergic vasculitis was also observed [1]. Therefore, in recent years there has been active scientific research on the use of titanium alloys with superthin ceramic coatings in resurfacing endoprosthetics. Moreover, titanium is usually used as a metal and titanium nitride (TiN) as a coating [2, 3]. The structure of the surface layer of the coating plays a key role in the wear process and is determined by the methods and regimes of its application. There are several ways to apply this coating: vacuum spraying (PVD), chemical vapor deposition (CVD), powder nitriding (PIRAC-powder immersion reaction assisted coating nitriding). The coatings obtained by PVD and CVD have insufficient adhesion to the substrate and are prone to delaminating under dynamic loads, while the adhesion of the coating obtained by the PIRAC method is significantly higher. Therefore, the use of metal implants with a PIRAC coating is very promising. Compounds of carbides, borides, nitrides are used as coating materials applied by the PIRAC method [4, 5].

Computer simulation allows one to study the mechanical behavior of endoprostheses, taking into account the influence of a variety of factors on it. Therefore, in preclinical studies, computer simulation is widely used to predict the mechanical behavior of prostheses. For example, modeling based on numerical methods of continuum mechanics allows a detailed study of the behavior of the coating and surface layer under contact loading. Thus, the influence of coating thickness on the load–displacement curve of instrumented indentation of ceramic coatings on a metal substrate was studied in [6–8]. The role of the surface roughness of the ceramic coating in the features of the mechanical behavior of the coating-substrate system during instrumented indentation was numerically studied in [9–12]. The authors of

[13–17] simulated the mechanical behavior of the coating–substrate system in instrumented indentation and scratching and analyzed stress fields in contact areas, as well as features of the load–displacement curves.

There is practically no theoretical work on the study of wear in a friction pair of a resurfacing endoprosthesis of a hip joint. Most of the work have been devoted to wearing in a friction pair of endoprostheses for total hip replacement. In theoretical studies of the wear process in a friction pair of an endoprosthesis, two approaches are used: with explicit consideration of wear debris and its implicit consideration. In the numerical study of wear in a friction pair by the finite element method, an implicit consideration of wear particles is used. First of all, this circumstance is associated with large computational costs and the complexity of explicit modeling of material failure. Most of the research [18, 19] on the theoretical study of wear in the friction pair of the endoprosthesis are based on the technique proposed in [20], where the ratio of Archard/Lancaster is used to describe the wear via calculating the wear coefficient for adhesive or abrasive wearing. This ratio defines linear wear as a function of contact pressure, loading rate, and wear coefficient, which in turn depends on the tribological characteristics of two contacting surfaces, such as roughness and various physical and mechanical characteristics of the materials of the contacting pair. The surface roughness is taken into account implicitly [21–23].

Most of the works on numerical modeling of the mechanical behavior of the bone–endoprosthesis system is performed using the methods of continuum mechanics. Thus, research of Kuhl and Balle [24], the influence of the type of prosthetics on the stress state in the system was investigated; establishing that the stress field of the system during resurfacing endoprosthetics is close to the stresses in a healthy joint. The results of a numerical study of the mechanical behavior of the bone–endoprosthesis system depending on the geometric characteristics of the implant and its design features are presented in [25], and on the implant material in [26].

Work on studying the mechanical behavior of bone tissue with biological fluid started long ago [27]. At the same time, the Biot model of poroelasticity was most widely used to describe the mechanical behavior of bone tissues. In papers [28–30] the Biot model of the isotropic poroelastic medium was used to describe bone tissues in the framework of continuum mechanics methods.

Taken together, this analysis of the literature shows that for the correct prediction of the mechanical behavior of the bone–endoprosthesis system, the development of numerical models that can describe the bone within the framework of a poroelastic body taking into account possible fracture of bone tissues, as well as wear in the friction pair of the endoprosthesis, is in demand.

3 The Problem Statement

The aim of this chapter is to present recent advances in development of numerical models for multi-scale simulation of the femur–endoprosthesis system for the hip resurfacing arthroplasty. The models are based on the movable cellular

automaton method, which is a representative of the discrete element approach in solid mechanics. According to the chosen multi-scale approach, the model of the lowest scale (mesoscale) describes sliding friction between two rough surfaces of TiN coatings, which correspond to different parts of the friction pair of hip resurfacing endoprosthesis. At this scale, we consider explicitly such parameters of the endoprosthesis friction pair as the thickness, roughness, and mechanical properties of the corresponding TiN coatings. The next scale of the model is a resurfacing cap rotating in the artificial acetabulum insert with an explicit account of sliding friction based on the effective coefficient of friction obtained at the previous scale. At the macroscale, we consider compression of the proximal part of the femur with a resurfacing cap. This macro-model considers the bone as a composite consisting of outer cortical and inner cancellous tissues. Here we use two approaches: the first implies simple linear elastic behavior of both tissues, the second considers these tissues as Boit's poroelastic bodies with accounting for the role of the interstitial biological fluid in the mechanical behavior of the bone. For comparison, we also consider the macroscopic model for healthy bone in compression.

4 Description of the Modeling Method

For simulating the mechanical behavior of the materials for the bone and prosthesis, we use the particle-based method of movable cellular automata (MCA), which was proposed by professors Sergey Psakhie and Yasuyuki Horie in 1994 and firstly published in 1995 [31]. Since that time, the method has been being actively developed in Prof. Psakhie's lab and its latest description can be found, for example, elsewhere in papers [32, 33] as well as in book chapters [34, 35].

MCA is a representative of so-called discrete element methods (DEM). The main principles of the method are as follows. A simulated body is represented by an ensemble of bonded equiaxial discrete elements of the same size (called movable cellular automata), which spatial position and orientation, as well as state, can change due to local interaction with nearest neighbors. Automata interact with each other through their contacts. The initial value of the contact area, as well as the automaton volume, is determined by the size of automata and their packing. The main advantage of the MCA-method in comparison with DEM is the generalized many-body formulas for central interaction forces acting between the pair of elements, similar to the embedded atom force field used in molecular dynamics. It is based on computing components of the average stress and strain tensors in the bulk of automaton according to the homogenization procedure described in [32]. Use of many-body interaction forces allows correct simulation within discrete element approach of such important features of the mechanical behavior of solids like Poisson effect and plastic flow.

When describing the kinematics and dynamics of an automaton motion, its shape is approximated by an equivalent sphere. This approximation is the most widely used in the discrete element method and allows one to consider the forces of central and tangential interaction of automata as formally independent. This makes also possible

to use the simplified Newton–Euler equations of motion to govern translational motion and rotation of the movable automata.

$$\begin{cases} m_i \frac{d^2 \mathbf{R}_i}{dt^2} = \sum_{j=1}^{N_i} \mathbf{F}_{ij}^{\text{pair}} + \mathbf{F}_i^{\Omega}, \\ \hat{J}_i \frac{d\boldsymbol{\omega}_i}{dt^2} = \sum_{j=1}^{N_i} \mathbf{M}_{ij} \end{cases}, \quad (1)$$

where $\mathbf{R}_i$, $\boldsymbol{\omega}_i$, m_i and $\hat{J}_i$ are the location vector, rotation velocity vector, mass and moment of inertia of i th automaton respectively, $\mathbf{F}_{ij}^{\text{pair}}$ is the interaction force of the pair of i th and j th automata, $\mathbf{F}_i^{\Omega}$ is the volume-dependent force acting on i th automaton and depending on the interaction of its neighbors with the remaining automata. In the latter equation, $\mathbf{M}_{ij} = q_{ij}(\mathbf{n}_{ij} \times \mathbf{F}_{ij}^{\text{pair}}) + \mathbf{K}_{ij}$, here q_{ij} is the distance from the center of i th automaton to the point of its interaction (contact) with j th automaton, $\mathbf{n}_{ij} = (\mathbf{R}_j - \mathbf{R}_i)/r_{ij}$ is the unit vector directed from the center of i th automaton to the j th one and r_{ij} is the distance between automata centers, $\mathbf{K}_{ij}$ is the torque caused by relative rotation of automata in the pair.

Movable automata are treated as deformable. Strains and stresses are assumed to be uniformly distributed in the volume of each automaton. Within the framework of this approximation, the values of averaged stresses in the automaton volume may be calculated as the superposition of forces applied to different parts of the automaton surface. In other words, averaged stress tensor components are expressed in terms of the interaction forces with neighbors [32]:

$$\bar{\sigma}_{\alpha\beta}^i = \frac{R_i S_{ij}^0}{\Omega_i^0} \sum_{j=1}^{N_i} \left[f_{ij} (\vec{n}_{ij})_{\alpha} + \tau_{ij} (\vec{t}_{ij})_{\beta} \right] \quad (2)$$

where i is the automaton number, $\bar{\sigma}_{\alpha\beta}^i$ is the component $\alpha\beta$ of the averaged stress tensor, $\alpha, \beta = x, y, z$ (XYZ is the global coordinate system), Ω_i^0 is the initial volume of the automaton i , S_{ij}^0 is the initial value of the contact area between the automata i and j , R_i is the radius of the equivalent sphere (semi-size of automaton i), f_{ij} and τ_{ij} are specific values of central and tangential forces of interaction between the automata i and j , $(\vec{n}_{ij})_{\alpha}$ and $(\vec{t}_{ij})_{\alpha}$ are the projections of the unit normal and unit tangent vectors onto the α -axis, N_i is the number of interacting neighbors of automaton i .

Invariants of the averaged stress tensor $\bar{\sigma}_{\alpha\beta}^i$ are used to calculate the central interaction forces (f_{ij} , τ_{ij}) and the criterion of an inter-element bond breaking (local fracture). The components of the averaged strain tensor $\bar{\varepsilon}_{\alpha\beta}^i$ are calculated in increments using the specified constitutive equation of the simulated material and the calculated increments of mean stress.

In [32] it is shown that the relation for the force of central interaction of automata can be formulated based on the constitutive equation of the material for the diagonal components of the stress tensor, while the force of tangential interaction can be formulated on the basis of similar equations for non-diagonal stress components. When implementing the linear elastic model, the expressions for specific values of the central and tangential forces of the mechanical response of the automaton i to mechanical action from the neighboring automaton j are written as follows:

$$\begin{cases} \Delta f_{ij} = 2G_i \Delta \varepsilon_{ij} + D_i \Delta \sigma_i^{\text{mean}} \\ \Delta \tau_{ij} = 2G_i \Delta \gamma_{ij} \end{cases}, \quad (3)$$

where the symbol Δ means increment of the corresponding variable during time step Δt of the numerical scheme of integration of the motion equations, $\Delta \varepsilon_{ij}$ and $\Delta \gamma_{ij}$ are the increments of normal and shear strains of the automaton i in pair $i - j$, G_i is the shear modulus of the material of the automaton i , K_i is the bulk modulus, $D_i = 1 - 2G_i / K_i$.

Due to the necessity of the third Newton's law ($\sigma_{ij} = \sigma_{ji}$ and $\tau_{ij} = \tau_{ji}$), the increments of the reaction forces of the automata i and j are calculated based on the solution of the following system of equations.

$$\begin{cases} \Delta f_{ij} = \Delta f_{ji} \\ R_i \Delta \varepsilon_{ij} + R_j \Delta \varepsilon_{ji} = \Delta r_{ij} \\ \Delta \tau_{ij} = \Delta \tau_{ji} \\ R_i \Delta \gamma_{ij} + R_j \Delta \gamma_{ji} = \Delta l_{ij}^{\text{sh}} \end{cases}, \quad (4)$$

where Δr_{ij} is the change in the distance between the centers of the automata for a time step Δt , $\Delta l_{ij}^{\text{sh}}$ is the value of the relative shear displacement of the interacting automata i and j . The system of equations (4) is solved for finding the increments of strains. This allows calculation of the increments of the specific interaction forces. When solving the system (4), the increments of mean stress and the values of specific forces in the right-hand sides of relations (3) are taken from the previous time step or are evaluated and further refined within the predictor–corrector scheme.

A pair of automata can be in one of two states: bound and unbound. Thus, in MCA fracture and coupling of fragments (crack healing, microwelding etc.) is simulated by the corresponding switching of the pair state. Switching criteria depend on physical mechanisms of material behavior [32, 33]. Note, that knowing stress and strain tensor in the bulk of an automaton, makes possible direct application of conventional fracture criteria written in the tensor form, herein we used von Mises criterion based on a threshold value of the equivalent stress.

5 Results and Discussion

5.1 Modeling Friction Pair of the Hip Resurfacing

We start with the simulation of the friction pair of the hip resurfacing endoprosthesis, which consists of two contacting bodies made of titanium alloy with TiN coating. First, we choose the materials parameters and validate the materials models to compare the simulation results for instrumented indentation with available experimental data. After that, we can simulate friction of the contacting bodies at the mesoscale to get an estimation of the coefficients of friction, which was used in the macroscopic model for rotation a resurfacing cap in the artificial acetabulum insert.

5.1.1 Materials Characterization

The values for the main physico-mechanical properties of the titanium alloy Ti6Al4V that we chose from the literature [36] are shown in Table 1 (corresponding Young's modulus $E = 110$ GPa). Geometric features of the TiN coating and its physico-mechanical properties are determined by the deposition modes at PIRAC forming [37]. So, at a deposition temperature of 700 °C and a treatment time of 48 h, the coating on the titanium substrate has a thickness of 1.3 μm with an average roughness height of 0.15 μm (mode 1) and elastic modulus, depending on the deposition regime, was equal to $E_1 = 258$ GPa; at a deposition temperature of 800 °C and a treatment time of 4 h the coating on the titanium substrate has a thickness of 1.4 μm with an average roughness height of 0.132 μm (mode 2) and an elastic modulus of $E_2 = 258$ GPa; at a deposition temperature of 900 °C and a treatment time of 2 h the coating on the titanium substrate has a thickness of 1.5 μm with an average roughness height of 0.265 μm (mode 3) and an elastic modulus of $E_3 = 321$ GPa. According to this information, we chose the values for the material properties of the TiN coating that are presented in Table 1. Data for yield stress σ_y and ultimate strength σ_b and strain ε_b were obtained using reverse analysis of the load–displacement curve for instrumented indentation [38].

Table 1 Properties of the model materials for the friction pair

Material	Bulk modulus, K , GPa	Shear modulus, G , GPa	Density, ρ , kg/m ³	Yield stress, σ_y , GPa	Ultimate strength, σ_b , GPa	Ultimate strain, ε_b
Ti6Al4V	92	41	4420	0.99	1.07	0.100
TiN mode 1	173	104	5220	4.50	5.50	0.075
TiN mode 2	173	104	5220	4.50	5.50	0.075
TiN mode 3	205	129	5220	4.50	5.50	0.075

5.1.2 Validation of the Models for Materials

The first numerical test, which we performed for validation of the models used for further simulations, was instrumented indentation [39]. General view of the model geometry for this test is shown in Fig. 1a. The model specimen was a parallelepiped consisting of titanium substrate, interface and TiN coating. The loading was simulated by moving all the automata of the Berkovich indenter with constant velocity $V_z = -1$ m/s until the required penetration depth is reached, then we apply them the velocity $V_z = -1$ m/s for unloading (Fig. 1b).

Using the procedure proposed by Oliver and Pharr [40] applied to processing the simulation results we plot the dependence of the material hardness on the penetration depth (Fig. 2) for three kinds of coatings obtained in different regimes. It can be seen from Fig. 2 that the hardest is the coating obtained by mode 3. All the curves correspond to experimental data from [37]. This allows us to conclude that the models of the materials behavior are validated for the normal contact loading conditions and can be used in further steps of our work.

The model specimen for scratch testing was also a parallelepiped consisting of titanium substrate, interface and TiN coating but elongated along the axis Y (Fig. 3). To simulate the force acting on the indenter along axis Z in the experiment, in our calculations we set the velocity of indenter automata to $V_z = -0.5$ m/s (Fig. 3b) until the indenter was immersed into a predetermined penetration depth and after that the vertical velocity was set to zero. Here we considered penetration of the indenter only up to the interface layer; the possibility of the coating to detach from the substrate was not allowed. To move the indenter along the sample surface, a constant velocity of the indenter automata along the axis Y was set to $V_Y = 1$ m/s.

Based on the results of our simulations, images of the deformed sample were created, and the values of the critical force characteristics at certain stages of fracture were obtained. It was found that the value of the critical force for the onset of fracture

Fig. 1 The model specimen for indentation (a) and its cross-section with loading parameters (b) represented by automata packing (the numbers indicate the model materials: 1—titanium, 2—interface, 3—coating, 4—diamond)

Fig. 2 Dependence of the hardness on the depth of penetration (the numbers indicate the modes of coating deposition)

Fig. 3 The model specimen for scratch testing (a) and its cross-section with the loading parameters (b) represented by automata packing (the numbers indicate the model materials: 1—titanium, 2—interface, 3—coating, 4—diamond)

and cracking is largest for the coating thickness of $1.4 \mu\text{m}$ and roughness of $0.132 \mu\text{m}$, and smallest for the thickness of $1.5 \mu\text{m}$ and roughness of $0.265 \mu\text{m}$. At delamination of the coating, the maximum of critical force is typical for the specimen with a coating thickness of $1.5 \mu\text{m}$ and roughness of $0.265 \mu\text{m}$, and the minimum for the specimen with a coating thickness of $1.3 \mu\text{m}$ and roughness of $0.15 \mu\text{m}$ (Fig. 4).

Critical loads obtained by modeling scratch testing are in very good agreement with the experimental data [41].

5.1.3 Modeling of Sliding Friction at the Meso-scale

At the next step, we developed a meso-model of sliding friction of the contacting surfaces of the endoprosthesis that explicitly accounts for the surface roughness, mean height of which is determined by the regime of the coating deposition [42].

Fig. 4 The force acting on the indenter from the coating P versus the scratching path l of the indenter (the numbers indicate the modes of coating deposition)

Because at the macroscale we need just effective value of the friction coefficient, whereas the substrate and interface were not considered in this model.

Geometrically, the model for studying friction consists of two bodies in the form of parallelepipeds (Fig. 5). Each parallelepiped is usually divided into two parts: one is the contact surface, and the other is its base. The different roughness relief of the two contacting surfaces was set in the preprocessor of the MCA_3D software package. To simulate the environment of the developed meso-scale simulation box during sliding friction, periodicity conditions along the X and Y axes were set on its side faces.

In the initial state, the interacted bodies are separated in spaced so that the asperities of the rough surfaces do not touch each other. For their approaching and the beginning of contact interaction, the velocity V_z along the Z -axis was applied to the automata of the top and bottom layers of the sample. After touching the upper and lower parts of the sample, traction forces (pressure $P = 0.75\sigma_y$) directed along the Z -axis, as well as horizontal velocity $V_y = 1$ m/s along the Y -axis, were applied to the automata of the top and bottom layers of the sample (Fig. 5b). The specified loading conditions at the top and bottom of the model had symmetrical character and the same magnitude, but the directions of the action were opposite. To avoid too hard loading in the friction zone, a gradual increase in the applied loads was implemented. To imitate the length of the real bodies along the vertical direction, it is necessary to damp the elastic waves arising in the friction zone and propagating along this direction. To this end, a special viscous damping force along the Z -axis was introduced for the automata of both loading regions.

According to the simulation results obtained, the dependence of the friction coefficient on the calculation time was plotted for different combinations of the roughnesses and reliefs (Fig. 6). Figure 6a shows that at the moment of contact of two

Fig. 5 The model sample for sliding friction at mesoscale (a) and its cross-section with loading parameters (b), the colors indicate different geometry blocks of the model

Fig. 6 Plots of the friction coefficient in the model at meso-scale versus the calculation time with the same (a) and different (b) modes of coating deposition (the numbers indicate these modes)

rough surfaces of different relief, but of the same roughness, the peak of the friction coefficient occurs, then the process goes to the stationary mode and the friction coefficient becomes almost constant. The plot shows that the greatest coefficient of friction $\mu_3 = 0.3$ is observed on the surfaces of the TiN coating in the first and third deposition modes, which corresponds to the experimental data [43], and the minimal $\mu_2 = 0.25$ in the second deposition mode. The thickness of the quasi-liquid mixing layer for the first and second regime is $0.08 \mu\text{m}$, for the third regime— $0.12 \mu\text{m}$.

It is known that an increase in the hardness of materials in contact with friction leads to a decrease in the friction coefficient, and an increase in the surface roughness leads to an increase in the friction coefficient [44, 45]. However, the materials used for the manufacture of endoprostheses should have increased hardness. Therefore, we have aimed to identify the most effective materials used in a friction pair. For this purpose, the calculations were carried out for the samples with different roughness and mechanical characteristics. According to the results of these numerical calculations, it was found that in the friction pair of the second and third modes $\mu_{2-3} = 0.27$; for the first and third modes $\mu_{1-3} = 0.28$ (Fig. 6b). The results indicate the promising use of materials obtained under different application conditions for different parts of the friction pair. At the modes 1–3 and 2–3, the thickness of the mixing layer is $0.1 \mu\text{m}$, and for the pair of the modes 1–2— $0.8 \mu\text{m}$.

5.1.4 Modeling Friction in the Rotating Friction Pair

The next step in the numerical study of the friction in the hip joint with resurfacing endoprosthesis was the development of the macro-model of friction between the endoprosthesis casing cap rotating in the artificial insert of acetabular cup [46].

In the case of a one-component material, the geometric model consisted of a hemisphere simulating a casing cap for the femur head with an external diameter $D_{\text{ext_cap}} = 36 \text{ mm}$ and an interior diameter $D_{\text{int_cap}} = 33 \text{ mm}$; a hemisphere simulating an acetabular cup of the hip prosthesis with an outer diameter of $D_{\text{ext_insert}} = 41 \text{ mm}$ and an interior diameter of $D_{\text{int_insert}} = 38 \text{ mm}$; and also a conical “shell” for the cup imitating the surrounding bone tissue (Fig. 7b). In the case of a two-component (coated) material, the hollow hemispheres were additionally specified for a casing cap with an outer diameter of 35.9 mm and an inner diameter of 33.1 mm (Fig. 7a).

The load was applied by specifying the translational and rotational velocities for the automata of the resurfacing cap. These velocities corresponded to rotation of the cap as perfectly rigid body around the axis of symmetry of the corresponding sphere, which in our case was parallel to the axis OX . The value of the corresponding rotational velocity gradually increases from 0 to 10 s^{-1} . The bottom layer of the automata of the conical shell of the bone tissue was rigidly fixed (Fig. 7b).

When simulating a single rotational cycle, the maximum reaction force was not greater than 3 kN , which corresponds to the load of a walking man, and the angle of rotation of the resurfacing cap was 120° , which is typical for standard daily physical activities for a healthy person.

Fig. 7 General view of the model for friction pair of hip resurfacing endoprosthesis (a) and its cross section with loading parameters (b), represented by automata packing

Table 2 Properties of the model cortical bone

Material	Bulk modulus, K , GPa	Shear modulus, G , GPa	Density, ρ , kg/m ³	Ultimate strength, σ_b , GPa
Cortical bone	14	3.3	1850	0.12

Friction of Bone-Bone Pair

For comparison, based on the developed model we also studied friction between two cortical bone hemispheres (assuming them as a healthy joint) [47]. Cortical bone was considered as a linear elastic brittle material with the properties taken from [48] and shown in Table 2.

The simulation results for healthy friction pair of bone tissues showed that in the contact interaction zone of the acetabulum and femur head and behind this zone at extreme positions (the edge of the acetabulum), large compressive stresses aroused in the head and in the acetabulum with a maximum value not reaching 10 MPa. Such a load does not exceed the strength and, therefore, reduces the likelihood of premature wear of the femoral joint (Fig. 8).

Friction of Ti–Ti Pair

Then we considered stress fields in the simulated specimens for the titanium endoprosthesis joints without any coating, which are depicted in Figs. 9 and 10. The simulation results showed that in the case of a friction pair of a homogeneous metal material a large tensile stress with a maximum value not reaching 990 MPa appeared in the cap. Namely, it was observed at extreme positions in the zone of contact interaction of the acetabulum insert and resurfacing cap and behind it (edge of the

Fig. 8 Field of mean stress in the friction pair of the healthy hip joint (bone)

Fig. 9 Field of mean stress in the friction pair of the hip resurfacing endoprosthesis made of titanium alloy

Fig. 10 Field of mean stress in the friction pair of the hip resurfacing endoprosthesis made of titanium alloy with TiN coating

acetabulum). Such a load exceeds the yield strength and, therefore, can lead to rapid wear of the surface of the resurfacing cap of the femur head of the joint (Fig. 9). These results are consistent with the data on the stress distribution in the metal head obtained in [49]. At the same time, the stress in the acetabulum insert did not exceed 100 MPa.

Friction of Ti–NiTi Pair

In the case of a coated endoprosthesis, a zone of tensile stresses with a maximum value of 1.1 GPa was observed in the contact zone, but this area was significantly smaller and concentrated mainly in the coating (Fig. 10). In addition, when using two-component materials in the friction pair, there was no noticeable increase in stress values in the cap when it was in the extreme positions. Consequently, the use of titanium alloys with a ceramic coating allows avoiding premature wear at the extreme positions of the femur head in the acetabulum. In the insert consisting of titanium alloy and coating, the value of compressive stresses reached 300 MPa. It should be noted that the magnitude of such stresses is not critical for the coating.

Thus, the presented results of the numerical simulations and their analysis suggest that the use of titanium alloy coated by TiN in the friction pair of hip resurfacing endoprosthesis can help avoiding premature wear of the endoprosthesis.

5.2 Modeling Bone–Endoprosthesis System

Finally, we developed a macromodel of hip resurfacing endoprosthesis with proximal part of the femur bone shown in Fig. 11. The geometry of the model was based on the so-called 3rd generation composite femur [50], which provides geometries of the cortical and cancellous bones as different solid bodies. A numerical model of the bone-endoprosthesis system was constructed for the resurfacing endoprosthesis with real geometric parameters. A CAD model from [50] was taken as a tubular femur, according to the parameters of which a personalized solid model for the endoprosthesis was created using FreeCAD software. For our purpose, we cut the top part of the bone geometry, added the resurfacing endoprosthesis (colored in cyan, and its coating colored in blue) and special loading part (colored in red) (Fig. 11b). Based on these solid models of the femur and endoprosthesis, mesh models were constructed in STL format, which then were imported into the MCA preprocessor as it shown [39].

Based on the developed model we simulated compression of the proximal part of the femur with resurfacing endoprosthesis, which can have a hardening coating or have not. The loading was applied by setting constant velocity in both horizontal and vertical directions as shown in Fig. 11b up to reaching the critical values of the resisting force of 3 and 10 kN [51]. The simulation results are presented in Fig. 12 as fields of mean stress.

It is reported in [52] that strength limit for the cancellous bone of healthy people reaches about 10 MPa in compression and 5 MPa in tension; and may be lower than 5 MPa and even 3 MPa for some diseases, respectively. Analysis of the stress field in the model system showed that maximum tensile stress was observed near the endoprosthesis, and did not reach critical values. Therefore, herein we tried to analyze the compression stress in the scale up to 5 MPa. From Fig. 12 one can see

Fig. 11 The model of hip resurfacing endoprosthesis (a) and its cross-section with the scheme of loading (b)

Fig. 12 Fields of mean stress in the cross-section of the system “bone-endoprosthesis” loaded by the force of 3 kN (a, c) and 10 kN (b, c) for titanium endoprosthesis (a, b) and titanium with TiN coating (c, d)

that maximum compression stress, which that can lead to fracture, is observed in the femoral neck.

5.3 Modeling of Biomaterials Based on Poroelastic Approach

It is well known, that the main difference of the living bone from one stored for a long time after removal from the body is the presence of the biological fluid. This is one of the reasons for the difference in the mechanical properties of living and “dead” bones. Moreover, this biological fluid may transfer across the whole bone and dramatically change its mechanical behavior under dynamic loading. That is why the next step in the further development of the numerical model described above is taking into account the biological fluid and its influence on the mechanical response of the femur.

5.3.1 Modification of the MCA Method to Enable Simulating Fluid-Saturated Materials

Automata that model fluid-saturated material are considered as porous and permeable. Pore space of such an automaton can be saturated with liquid. The characteristics of the pore space are taken into account implicitly through the specified integral parameters, namely, porosity ϕ , permeability k , and the ratio $a = 1 - K/K_S$ of the macroscopic value of bulk modulus K to the bulk modulus of the solid skeleton K_S . The mechanical influence of the pore fluid on the stresses and strains in the solid skeleton of an automaton is taken into account on the basis of the linear Biot's model of poroelasticity [53, 54]. Within this model, the mechanical response of a "dry" automaton is assumed linearly elastic and is described based on the above-shown relations. The mechanical effect of the pore fluid on the automaton behavior is described in terms of the local pore pressure P^{pore} (fluid pore pressure in the volume of the automaton). In the Biot model, the pore pressure affects only the diagonal components of the stress tensor. Therefore, it is necessary to modify only the relations for the central interaction forces in Eq. (3):

$$\Delta f_{ij} = 2G_i \left(\Delta \varepsilon_{ij} - \frac{a_i \Delta P_i^{\text{pore}}}{K_i} \right) + D_i \Delta \sigma_i^{\text{mean}} \quad (5)$$

Interstitial fluid is assumed to be linearly compressible. The value of fluid pore pressure in the volume of an automaton is calculated based on the relationships of Biot's poroelasticity model with the use of the current value of the pore volume. The pore space of the automata is assumed to be interconnected and provides the possibility of redistribution (filtration) of the interstitial fluid between the interacting elements. A pore pressure gradient is considered as the "driving force" of filtration. The fluid redistribution between automata is carried out by numerical solution of the classical equation of the fluid density transfer [55]. This equation is numerically solved using the finite volume method adopted for the ensemble of automata.

5.3.2 Choosing Poroelastic Parameters for Bone Tissues

The aim of this section is to choose the correct values of the model for both cortical and cancellous bone tissues. The first who considered bones like poroelastic bodies was Cowin [27]. In paper [56] he with co-authors provided the values of the main parameters of poroelastic body for cortical and cancellous tissues of the human bone. These parameters are as follows: Young's modulus, Poisson's ratio, the permeability, Biot's coefficient (or bulk modulus of the solid phase), the porosity, densities of the solid grain and the fluid. Later, several authors have made experimental and theoretical studies aimed to get the values of poroelastic parameters for some specific bones of humans and animals [48, 57–60]. Based on data published in the literature, one may conclude that there is a large scatter of the main poroelastic properties of the bone tissues. For example, geometric permeability estimates span across several

Table 3 Poroelastic properties of the model bone tissues

Bone tissue	Bulk modulus of the solid phase, K_S , GPa	Bulk modulus of the matrix, K , GPa	Shear modulus of the matrix, G , GPa	Density of the matrix, ρ , kg/m ³	Porosity ϕ	Geometric permeability, k , m ²
Cortical	17.0	14.0	5.55	1850	0.04	1.0×10^{-16}
Cancellous	17.0	3.3	1.32	600	0.80	3.5×10^{-13}

orders of magnitude ($10^{-25} - 10^{-10}$ m²), and values for Young's modulus vary from 1 up to 25 GPa [48]. That is why it is of special interest to study the peculiarities of the mechanical behavior of small model specimens in compression depending on the variation of these properties.

Basic values of the poroelastic properties chosen for our numerical models for both cortical and cancellous bone tissues are shown in Table 3. The fluid in both bone tissues is assumed to be the same and equivalent to salt water, with a bulk modulus $K_f = 2.4$ GPa, and density $\rho_f = 1000$ kg/m³.

The developed model was applied to study the dynamic mechanical behavior of the fluid-saturated porous materials under uniaxial compression at a constant speed. We studied and analysed the dependences of the effective Young's modulus of fluid-saturated materials on the strain rate and the characteristic time of fluid redistribution in the pore space. In our calculations, the material parameters and the strain rate varied within wide limits: the permeability of the material varied within 4 orders of magnitude, the viscosity of the fluid varied within 2 orders of magnitude, the sample size changed within the order of magnitude, and the strain rate varied within 3 orders of magnitude [61].

We simulated uniaxial compression of 3D cubic specimens along the vertical axis (Z). The size of the automata for all models in this study was equal to 2 mm. The base size of the cubic specimens was chosen to be 5 cm. The initial pore pressure of interstitial fluid was assumed to be equal to atmospheric. Fluid could freely flow out from the compressed specimen through the side surface.

Analysis of the simulation results showed that under compression, the values of the mechanical characteristics of the fluid-saturated material are determined by the balance of two competing processes [62, 63]:

- deformation of the solid skeleton, providing compression of the pore space and a corresponding increase in the pore pressure of the interstitial fluid;
- outflow of the interstitial fluid through the side surface, which leads to the inverse effect of lowering pore pressure.

We revealed a key control parameter that determines the specific dynamic value of the mechanical characteristics of fluid-saturated materials, namely the dimensionless Darcy number:

$$D_a = \frac{T_{\text{Darcy}}}{T_{\text{load}}} \sim \frac{\eta_{\text{fl}} L^2}{k \Delta P} \dot{\varepsilon}_{\text{def}}, \quad (6)$$

where T_{Darcy} is the characteristic time of fluid filtration (Darcy time scale), $T_{\text{load}} \sim 1/\dot{\varepsilon}_{\text{def}}$ is the time scale of the specimen deformation, $\dot{\varepsilon}_{\text{def}}$ is the specimen strain rate, η_{fl} is the dynamic viscosity of the pore fluid, L is the characteristic length of the pore pressure difference ΔP (a half of length of the cubic side in the considered case). The parameter D_a characterizes the ratio of the timescales of deformation of the fluid-saturated porous specimen and filtration of the pore fluid.

The simulation results showed that the effective Young's modulus of fluid-saturated bone tissues non-linearly depends on the strain rate $\dot{\varepsilon}_{\text{def}}$, the specimen size L , the dynamic viscosity of pore fluid η_{fl} , and the permeability of solid skeleton k . In particular, Young's modulus of a fluid-saturated sample is minimal (equal to E_{min}) at infinitely small strain rates and tends to the maximum value (Young's modulus of undrained sample E_{max} [54]) at large ones. The key result is the established ability to build single “gauge” dependence applicable to specimens of porous materials of various sizes, characterized by different permeability of solid skeleton, different fluid viscosities, and deformed at different strain rates. An argument of such a “master curve” is the dimensionless Darcy number D_a (Fig. 13):

$$E = E_{\text{max}} + \frac{E_{\text{min}} - E_{\text{max}}}{1 + (D_a/D_{a_0})^p}, \quad (7)$$

where E_{min} corresponds to $D_a \rightarrow 0$ (“dry” specimen), E_{max} corresponds to $D_a \rightarrow \infty$ (undrained specimen), D_{a_0} and p are the fitting constants. This master curve has a logistic (sigmoidal) form but the fitting values of D_{a_0} and p (as well as E_{min} and E_{max}) are different for cortical and cancellous bones.

Based on the presented results we chose the values of the poroelastic parameters for both bone tissues applied to the model proximal femur corresponding to Darcy

Fig. 13 Dependences of the normalized Young's moduli of the modeled specimens of cortical (a) and cancellous (b) bone tissues with different poroelastic properties on the Darcy number. Crosses show numerically obtained values, lines are approximating curves

numbers about 50, i.e. the middle of the plots range shown in Fig. 13. This means that at the loading rate of the model femur the effect of interstitial fluid flow is expected to be well pronounced.

5.3.3 Validation of the Materials Model

During life, the properties of the human bones change considerably; usually they become fragile. In [64], the concept of bone fragility was formulated as follows: bone tissue can adapt its shape and size in response to mechanical stress through a remodeling mechanism, during which the bones are formed or rearranged under the independent action of osteoclasts and osteoblasts. Remodeling is a process that supports the mechanical resistance of the skeleton, allowing you to selectively restore and replace damaged bone tissue. During the period of growth, these processes form a structure capable of adapting to the loads and maintaining strength. With age, the natural remodeling processes slow down under the influence of such factors as decreasing muscle mass and physical activity, malnutrition. Consequently, bone embrittlement occurs. Osteoporosis is a systemic skeletal disease characterized by low bone mass and impaired microarchitecture of bone tissue, which leads to increased bone fragility (reduced bone density) and a tendency to fractures. Researchers and clinicians continue to persist in finding ways to prevent the 8 million osteoporotic fractures occurring annually around the world [65]. An early and accurate assessment of the risk of fracture, with timely initiated treatment—this approach seems to be the most appropriate for reducing this number of fractures and associated personal and social losses.

There are many methods for the direct assessment of the structural strength and the material composition of the bone, such as testing of whole bone, bone mass, strength assessment using microindentation [66]. However, all of these methods are used for in vitro or in vivo research and are therefore not suitable for clinical practice. Recently, however, indentation has become positioned as a procedure for clinical use with minimal invasiveness [67]. In the indentation method, the bones are penetrated using an indenter tip with a depth sensor. Among the advantages of this method, there is an ability to measure material properties and microstructural features and identify local changes in bone material caused, for example, by disease or medication [68]. However, the method remains invasive and extremely local, therefore, at present, the development of methods for non-invasive diagnostics of the strength properties of local bone tissue is actively underway.

One of the new directions in this area is the combination of methods for visualizing the structure of bone tissue (CT and MRI) with computer modeling [69]. Therefore, the development of numerical models of the mechanical behavior of bone tissue during micro and macroindentation is relevant.

Here we describe a numerical model of the mechanical behavior of fluid-saturated cancellous tissue during indentation used for validation of the developed model of fluid-saturated bone tissues [70].

Geometrically, the bone tissue indentation model was a parallelepiped with a Berkovich pyramid (Fig. 1). During indentation, the counter-body was set as the rigid non-deformable indenter, which motion was set through the velocity in the vertical direction. This velocity was set to $V_z = -1$ m/s until the indenter was penetrated at a given depth, after which the velocity $V_z = 1$ m/s was set to simulate unloading. The simulation results were processed using the Oliver-Farr method [40].

The mechanical properties for the cancellous bone were chosen from Table 3, and the fluid in bone tissue is assumed to be equivalent to salt water as before.

It is known that bone tissue, when indented, behaves like a soft material, and gives an error in determining the elastic modulus using a standard experimental procedure; thus, indentation with a time delay of indentation depth (holding) looks to be better for this material [71]. Therefore, one of the first experiments to test the developed model was aimed to establish the fact of the influence of holding time on the mechanical properties of bone tissue. Three variants of loading were considered: (1) without holding $t_{\text{hold}} = 0$; (2) holding time corresponded to loading time $t_{\text{hold}} = t_{\text{loading}}$; (3) holding time was two times longer than loading time $t_{\text{hold}} = 2 \cdot t_{\text{loading}}$ (Fig. 14a).

When analyzing the load–displacement curves (Fig. 14b) using the Oliver-Farr method, the following values of recoverable characteristics were obtained: the hardness of 47 MPa for all loading regimes, the elastic modulus 3.7 GPa for no holding, $E = 3.5$ GPa for $t_{\text{hold}} = t_{\text{loading}}$, $E = 3.33$ GPa for $t_{\text{hold}} = 2 \cdot t_{\text{loading}}$. The obtained results showed that the elastic modulus is determined correctly at $t_{\text{hold}} = t_{\text{loading}}$ and corresponds to the specified input value. In addition, these calculations suggest that at constant deformation, stress relaxation occurs, which indicates that the model specimen of cancellous bone tissue possesses viscoelastic properties.

At the next stage, the effect of interstitial fluid flow in the porous skeleton of the material was investigated. According to the simulation results (Fig. 15a), it was established that the hardness of the undrained bone tissue specimen was 55 MPa, while the hardness of the fluid-saturated bone was 47 MPa, and the elastic moduli

Fig. 14 **a** The indenter penetration depth versus time; **b** load–displacement curve for different holding times; numbers indicate loading regimes: (1) $t_{\text{hold}} = 0$, (2) $t_{\text{hold}} = t_{\text{loading}}$, (3) $t_{\text{hold}} = 2 \cdot t_{\text{loading}}$

Fig. 15 Load–displacement curves for undrained (a), numbers indicate loading rates: (1) undrained, (2) fluid-saturated and fluid-saturated model specimens (b), numbers indicate loading rates: (1) $v = 1$ m/s, (2) $v = 5$ m/s, (3) $v = 10$ m/s

were 3.9 and 3.6 GPa, respectively. The results obtained correspond qualitatively to the data on the influence of fluid on the mechanical response of bone tissue by other authors [72–74].

Further calculations were carried out to study the effect of porosity value of the bone tissue and its permeability on the mechanical response of the bone in indentation. However, the results obtained indicate that with the chosen values of porosity (80%), the above factors do not have a significant effect on the mechanical response of the fluid-saturated bone tissue.

The viscoelastic behavior of the bone tissue is also characterized by the dependence of the mechanical characteristics on the loading rate; therefore, at the next stage of testing the numerical model development, experiments were performed on the indentation of a model specimen of cancellous bone tissue with different loading rates. The study of the effect of loading rate on the mechanical response of fluid-saturated bone tissue showed that an increase in loading rate leads to an increase in the values of recoverable characteristics (Fig. 15b), thus at the speed of $V = 1$ m/s we got $H = 47$ MPa, $E = 3.5$ GPa, at the speed of $v = 5$ m/s we got $H = 53$ MPa, $E = 3.7$ GPa, and at the speed of $v = 10$ m/s we got $H = 56$ MPa, $E = 3.95$ GPa. The obtained values, again, corresponds qualitatively to the results of other authors [75–77].

5.3.4 Modeling the Bone Compression

Similar as in the previous section, the geometry of the bone is based on the 3rd generation composite femur [50], which consists of the cortical and cancellous parts as different solid bodies. General view of the model represented as fcc packing of automata and its cross-section are shown in Fig. 16.

Fig. 16 General view of the model for proximal femur (a) and its cross-section (b)

At the bottom of the model, we place a disk with properties of the cortical bone; the automata of this disk are fixed. For compressing the femur, we place a special cylindrical “cap” on the femur head. This “cap” is shown in blue color in Fig. 16. Automata of the “cap” have the properties corresponding to cartilage. Loading is applied by setting the constant velocity $V = 1$ m/s to the automata of the upper face of the “cap”. The velocity vector is directed along the face normal. Note, that this loading results in both compression and small bending of the bone.

To reveal the role of the interstitial fluid flow in the model femur under compression, we studied three different cases. In the first case, all bone tissues contained no fluid, i.e. were “dry” (so-called drained test). In the second case, we used the chosen poroelastic parameters from Table 3. In the third case, all pores containing fluid were assumed to be closed, which means no permeability of the materials (undrained test). Then we analyzed the distributions of mean stress, equivalent stress and pore fluid pressure at the final point at the total strain about 2%.

Fields of mean stress in the cross section of the model femur for all three cases are shown in Fig. 17. One can see that fluid filtration cause the increase in mean stress in the cortical part of the femur head, especially in the area of its contact with the loading “cap”. At the same time, the drained and undrained tests do not differ considerably from each other. However, fields of equivalent stress in the cross section of the model for these cases shown in Fig. 18, clearly demonstrate that shear stress in the same area is much smaller for the undrained test, while for the two other cases are practically the same.

It can be clearly seen from Figs. 16 and 18 that the maximum stresses occur in the cortical part of the femur. Figure 19 shows the 3D view of both equivalent and mean stresses distribution in the model (particularly, the outer part of the cortical bone). It is obvious that the main stresses are localized in the femoral neck. The shear stresses propagate along the loading direction into the main part of the bone up to the

Fig. 17 Distribution of mean stress in cross-section of the model femur at drain test (a), test with chosen poroelastic parameters (b), and undrained test

Fig. 18 Distribution of equivalent stress in cross-section of the model femur at drained test (a), test with chosen poroelastic parameters (b), and undrained test

Fig. 19 Distribution of equivalent stress (a) and mean stress (b) in the model femur with chosen poroelastic parameters

Fig. 20 Distribution of pore pressure in the model for the test with chosen poroelastic parameters (a, c) and undrained test (b, d), c and d are corresponding cross-sections

supporting plate. But the most dangerous seems the tensile mean stress in the upper part of the femoral neck (Fig. 19b).

Figure 20 shows fields of the pore pressure in the cases with interstitial fluid. It can be seen that ability to flow results in filtration of the fluid to the regions of large tensile and shear stresses of the cortical bone, but not the maximum tensile mean stress (upper part of the femoral neck). At the same time, one can see negligible pore pressure in the cancellous bone in the case of fluid filtration (Fig. 20c).

5.3.5 Modeling the Bone-Endoprosthesis System

In the last sub-section, we consider the femur–endoprosthesis system, where the bone is described using poroelastic approach and the implant is made of the TiN-coated

Fig. 21 Model system “bone-endoprosthesis”. **a** 3D view; **b** cross-section view with scheme of loading

titanium alloy Ti6Al4V. The values for the main physico-mechanical properties of the titanium alloy and TiN coating produced by the PIRAC deposition mode 2 are taken from Table 1. The properties for the bone tissues are taken from Table 3. A model of the bone-endoprosthesis system was constructed by analogy with Sect. 5.2 and is shown in Fig. 21a.

The main feature of this section is that here we vary the loading similar to the different types of human activity. Thus, dynamic loading F_{res} , which is equivalent to the physiological one for a person weighing 75 kg, was applied to the upper part of the implant (Fig. 21b). According to [78], this force lies in the medial plane ZX and is inclined under different angles relative to the bone axis Z for different kinds of activity. Standing up load is characterized by the total force of 3.6 kN and applied at the angle of 24° ; sitting down load of 3 kN is applied at the angle of 20° ; a load of walking is 3 kN and applied at the angle of 17° ; jogging is characterized by 4.5 kN and applied under angles of 15° ; stance position is characterized by 3.2 kN and applied under angle of 16° . Here, the loading is simulated through the setting constant velocity to the automata of the external surface of the loading block marked by the blue color in Fig. 21 up to the moment when the required loading value of the resistance force is reached, similarly as it was done in [78, 79]. The value of the loading velocity is 1 m/s for walking, sitting, standing up and position while standing, for jogging the loading velocity is 2 m/s [79].

Typical patterns of the mean stress fields obtained by simulations are shown in Fig. 22. According to the presented results, the highest tensile and compressive stresses are concentrated in the upper and lower parts of the femur neck, respectively.

Analysis of the images also shows that the angle of the load application for the same value of the resulting force significantly affects the distribution of compressive stresses in the proximal femur (Fig. 22a–c). Thus, an increase in the angle of the load application by 4° with a simultaneous increase in the force by 20% leads to an increase

Fig. 22 Fields of mean stress in the system “bone-endoprosthesis” under different physiological loading: **a** standing up, **b** sitting down, **c** walking, **d** jogging and **e** stance position

in the area of compressive stresses by 20% (Fig. 22b, a, respectively). A decrease in the angle of the load application by 3° at the same value of the force (the cases of sitting down and walking) causes an increase in the localization area of maximum compressive stresses by about 15% (Fig. 22b, c, respectively). At the same time, a decrease in the angle of the load application by 2° relative to the nominal direction with an increase in the loading force by 7% (the cases of walking and standing position) leads to a decrease in the localization area of maximum compressive stresses by 5% (Fig. 22c, e, respectively). The highest stress concentration is observed for

Fig. 23 **a** Plots of the loading force versus time for the considered types of physiological loading; **b** fracture pattern of the bone–endoprosthesis system (the lines connect bonded automata, the cracks correspond to the white zigzag “curves” in the network of the bonded automata)

jogging: compressive stresses are observed in the lower part of the neck under the implant pin, as well as in the femoral head area under the casing cap (Fig. 22d).

Analysis of the loading plots shown in Fig. 23a and the corresponding fracture patterns (one example is depicted in Fig. 23b) allows us to conclude that for all types of physiological loads microcracks arise at the loading of 5–6 kN, while formation of a macrocrack is observed at the force above 6 kN. When the force value reaches 14–16 kN the complete failure of the femoral neck takes place; according to [80] the resulted pattern of crack depicted in (Fig. 23b) may be defined as the subcapital fracture. It worth noting that the least probability of fractures occurs at walking, while the greatest when sitting down.

One more interesting peculiarity that can be seen from the loading curves depicted in Fig. 23a, is a lower failure force at jogging (red curve). It can be explained by the minimum angle of the load inclination for this case, which means the maximum arm of the force for breaking the femoral neck. Failure, in this case, occurs earlier because of the higher loading velocity.

Thus, we finally considered the mechanical behavior of the femur bone with hip resurfacing under conditions of real physiological loads. The simulation data obtained, indicate that with a decrease in the angle of the force application relative to the femur axis, an increase in the area of compressive stresses is observed, as well as the appearance of such stresses in the femur head in the region closed to the prosthesis cap. With a further increase in loading force, corresponding to an increase in the body weight or the performance of physical exercises with weighting, a tendency to fracture is observed. Furthermore, the accumulation of micro and macro-cracks in the bone tissue under the loading force values, slightly exceeding the natural physiological levels, can also under certain circumstances lead to failure. A critical physiological load, in which the destruction of bone tissue starts to appear in the case of resurfacing endoprosthesis, corresponds to sitting down in excess weight conditions or using additional weights.

6 Conclusions and Future Work

This chapter presents the multiscale numerical models that can be used as a simulation tool for the virtual analysis of the femur–endoprosthesis system for the case of hip resurfacing arthroplasty. The movable cellular automaton method, which is used for simulation of the mechanical behavior of the materials, allows explicit accounting for contact loading of rough surfaces of the TiN coatings used in the friction pair of the endoprosthesis as well as fracture of the bone tissues at different scales of the model. The implementation of the Boit theory of poroelasticity within the movable cellular automaton method allows revealing the role of the interstitial biological fluid in the mechanical behavior of the bone tissues.

Based on the analysis of the obtained simulation results, the following plan for future works is proposed. First, it is necessary to use real geometry of the bone and endoprosthesis, which are more complicated than was considered here. This means that we need to consider not only the proximal part of the femur, but at least a whole bone, and maybe with the knee joint. Real resurfacing caps have many geometrical features that also have to be included in future models. All these requirements lead to the use of the small size of the automata and hence the huge number of them and large computational costs. Second, the loads have to be also refined in order to be more realistic. The third important problem that has to be considered in the future is the detained description of the interface between an implant and bone, including osseointegration.

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