NUMERICAL MODEL OF THE MECHANICAL BEHAVIOR OF COATED MATERIALS IN THE PAIR FRICTION «HEAD - ACETABULUM CUP» OF HIP JOINT

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Abstract

Wear in a friction pair of components of the endoprosthesis has a significant impact on its operational life. The structure of the surface layers of the contacting elements plays a key role in the wear process. To improve the tribological characteristics of metal endoprostheses, hardening nanostructured coatings are used. In this case, titanium is usually used as a metal, and titanium nitride (TiN) is used as a coating. In this paper, an approach is proposed for multiscale modeling of the friction pair of the endoprosthesis "head-acetabulum cup" based on the method of movable cellular automata. The models of materials involved in the friction pair were verified by simulating the nanoindentation process. At the micro level, the process of friction of two rough surfaces is modeled. The results of modeling at the micro level were used in the macromodel of the friction unit as the tribological characteristics of the material surface of contacting pairs after one loading cycle. To test the performance of the micro and macro models, test calculations were performed with a single cycle loading.

Keywords: Nanostructured coatings, indentation, pair friction, simulation, movable cellular automata method

1. INTRODUCTION

For the treatment of pathologies of the hip joint in the modern world, endprosthetics are widely used. Wear in a friction pair of components of the endoprosthesis has a significant impact on its operational life. The structure of the surface layers of the contacting elements plays a key role in the wear process. To improve the tribological characteristics of metal endoprosthesis (EP), hardening nanostructured coatings are used. In this case, titanium is usually used as a metal, and titanium nitride (TiN) is used as a coating. The structure of the coating is determined by the modes of its application. Promising is the coating by powder immersion reaction assisted coating nitriding (PIRAC). Testing of EP has several stages - these are preclinical and clinical trials. Clinical trials are carried out through the installation of an EP in a living human body. Preclinical studies of the mechanical behavior of the EP can be divided into experimental and theoretical. Experimental studies are tests using a technological unit that simulates the dynamic loading experienced by EP. Theoretical studies of the mechanical behavior of the EP using computer simulation make it possible to study the mechanical behavior of EP taking into account the influence of various factors on it. Therefore, in preclinical studies, computer modeling is used to predict the mechanical behavior of endoprostheses. In the numerical study of wear in a friction pair by the finite element method, modeling is used without explicit account of wear particles, first of all this is attributed to high computational costs and the complexity of explicit modeling of material failure. Most modern papers [1-2] concerning the theoretical study of wear in the friction pair of the endoprosthesis are based on the method for calculating the wear proposed in [3]. The surface roughness is taken into account implicitly [4]. In the case of a numerical study of hip joint endoprostheses with modified surface layers or coatings [5], structural features in multilevel modeling are taken into account using the homogenization method (asymptotic averaging), i.e. features of the structure are taken into account implicitly, and are reflected in the integral characteristics of materials [6-7]. However, this approach may give an incomplete pattern of the EP failure, including the improper distribution of stress-strain state in the bone - endoprosthesis system. Therefore, it is promising to develop numerical models of the mechanical behavior of the friction of the endoprosthesis with an explicit account for wear.

The purpose of this work is to develop a multi-level numerical model of the mechanical behavior of the node of EP “head-acetabulum cup”, taking into account such geometric parameters of the TiN coating (PIRAC) as the coating thickness, its roughness and its mechanical characteristics. To achieve the goal, three tasks were set. The first task was to verify the models of materials of the friction unit; for this, a numerical model of the nanoindentation process of the coating - substrate system was built, then numerical calculations were performed, the processing results of which were compared with the data of experiments. It is known that during friction a large contribution to wear is made by the surface roughness. To reduce the computational costs, it was proposed to take into account the tribological characteristics and surface wear, in the macro model, through the coefficient of friction obtained by friction of the contacting surfaces at the micro level. Therefore, the second task was to create a numerical model of friction of materials of the contacting pair at the micro level and to conduct test calculations at the micro level. Wear in the coating was clearly taken into account through the value of the thickness of the layer in which the material was mixed during friction at the micro level. The third task was to create a numerical model of the friction node “head-acetabulum cup” at the macro level using data on the tribological characteristics of materials in the contacting elements obtained from the micromodel and carrying out numerical calculations.

2. METHOD OF MOVABLE CELLULAR AUTOMATA

The method of movable cellular automata [9] is a new efficient numerical method in particle mechanics that is different from methods in the traditional continuum mechanics. Namely, to construct a many-particle interaction model, the expression for the force acting on a discrete element *i* from the surrounding N_i particles should be written in the form (1):

$$\vec{F}_i = \sum_{j=1}^{N_i} \vec{F}_{ij}^{pair} + \vec{F}_i^{\Omega} \tag{1}$$

This force is represented as a superposition of the pair components $\vec{F}_{ij}^{pair}$ dependent on the spatial position or displacement of the automaton *i* relative to the neighbor *j* and the volume-dependent component $\vec{F}_i^{\Omega}$ related to collective effects of the surroundings.

Within the frame of MCA, it is assumed that any material is composed by a certain amount of elementary objects of finite size (automata) which interact among each other and can move from one location to another, thereby simulating a real deformation process. The automaton motion is governed by the Newton-Euler equations (2):

$$\begin{cases} m_i \dfrac{d^2\vec{R}_i}{dt^2} = \sum\limits_{j=1}^{N_i} \vec{F}_{ij}^{pair} + \vec{F}_i^{\Omega}, \\ \hat{J}_i \dfrac{d\vec{\omega}_i}{dt} = \sum\limits_{j=1}^{N_i} \vec{M}_{ij}, \end{cases} \tag{2}$$

where $\vec{R}_i$, $\vec{\omega}_i$, m_i and $\hat{J}_i$ are the location vector, rotation vector, mass and moment of inertia of *i*th automaton respectively, $\vec{M}_{ij} = q_{ij}(\vec{n}_{ij} \times \vec{F}_{ij}^{pair}) + \vec{K}_{ij}$, here q_{ij} is the distance from the center of *i*th automaton to the point of its interaction ("contact") with *j*th automaton, $\vec{n}_{ij} = (\vec{R}_j - \vec{R}_i)/r_{ij}$ 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, $\vec{K}_{ij}$ is the torque caused by relative rotation of automata in the pair.

The total force acting on automaton *i* can be represented as a sum of explicitly defined normal $\vec{F}_{ij}^{n}$ and tangential (shear) $\vec{F}_{ij}^{\tau}$ components (3):

$$\vec{F}_i = \sum_{j=1}^{N_i}\left(\vec{F}_{ij}^{pair} - AP_i S_{ij}\vec{n}_{ij}\right) = \sum_{j=1}^{N_i}\left[\left(F_{ij}^{pair,n}\left(h_{ij}\right) - AP_j S_{ij}\right)\vec{n}_{ij} + F_{ij}^{pair,\tau}\left(\vec{l}_{ij}^{shear}\right)\vec{t}_{ij}\right] = \sum_{j=1}^{N_i}\left(\vec{F}_{ij}^{n} + \vec{F}_{ij}^{\tau}\right) \tag{3}$$

where $F_{ij}^{pair,n}$ and $F_{ij}^{pair,\tau}$ are the normal and tangential pair interaction forces depending respectively on the automata overlap hij and their relative tangential displacement $\vec{l}_{ij}^{shear}$ calculated with taking into account rotation of the both automata. Note, that although the last expression of equation (3) formally corresponds to the form of element interaction in conventional discrete element models, it differs fundamentally from them in many-particle central interaction of the automata.

Using homogenization procedure for stress tensor in a particle described in [10], the expression for components of the average stress tensor in automaton i takes the form (4):

$$\bar{\sigma}_{\alpha\beta}^{i} = \frac{1}{V_i}\sum_{j=1}^{N_i} q_{ij} n_{ij,\alpha} F_{ij,\beta} \, , \tag{4}$$

where α and β denote the axes *X, Y, Z* of the laboratory coordinate system, V_i is the current volume of automaton *i*, $n_{ij,\alpha}$ is the α-component of unit vector $\vec{n}_{ij}$ and $F_{ij,\beta}$ is β-component of the total force acting at the point of "contact" between automata *i* and *j*.

The equations of motion (2) for the system of movable cellular automata are numerically integrated with the use of velocity Verlet algorithm modified by introducing a predictor for estimation of $\bar{\sigma}_{\alpha\beta}^{i}$ at the current time step.

3. CALCULATIONS

For verification of materials models, a nanoindentation model was built (**Figure 1, a**) of the "coating-substrate" system. The indenter was defined as a rigid non-deformable diamond. The movement of the indenter was set through the velocity in the vertical direction. Next, a micromodel of the friction process was created for the contacting surfaces of the EP taking into account the average height of the surface layer roughness, depending on the mode of coating on the substrate. Since the knowledge of the tribological characteristics of the coating surface after loading cycles necessary for use in the macromodel, the substrate and the transition layer were not taken into account in the micromodels, the contacting blocks with roughness were located on bases that were a fixed base and a piston (**Figure 1, b**), for visibility contacting blocks are shown in different colors. The piston movement was set through the velocities. At the first stage, the velocity was applied in the vertical direction to contact the friction surfaces, then the speed was set in the horizontal direction to simulate friction. The macromodel consisted of acetabulum cup with an outer diameter of 52 mm and an EP head with a diameter of 28 mm (**Figure 1, c**). At the first stage, the head of the EP moved in the direction of the acetabulum cup and the contact of the surfaces, then one cycle of rotational movement along one direction was set using speed.

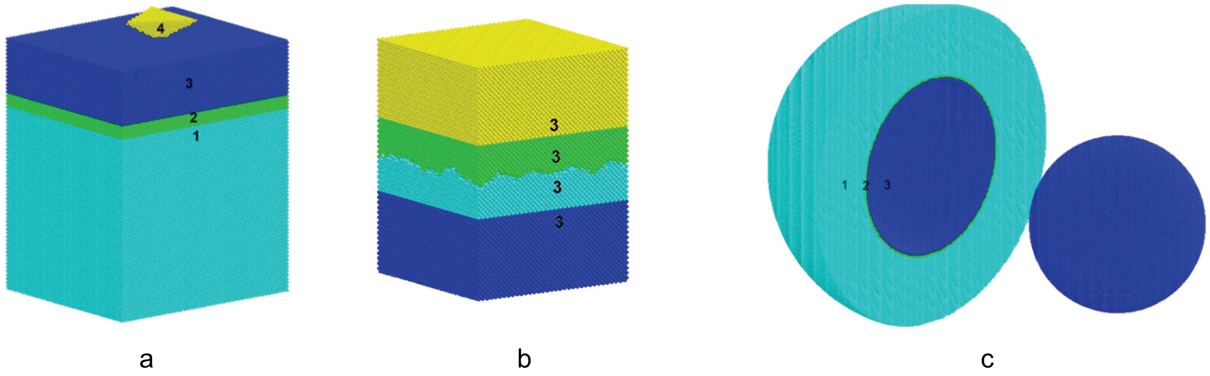

Figure 1 The numerical models, presented in the form of a package of automaton a-nanoindentation, b-friction, c-friction unit "head-acetabulum cup" of hip joint implant (numbers indicate the model materials: 1-titanium, 2-interface, 3-coating, 4- diamond)

According to literature data [11], the following parameter values were chosen for calculating Ti6Al4V samples: ρ = 4420 kg / m^3, G = 41 GPa, K = 92 GPa, E = 107, $\sigma_{y0.02}$ = 0.99 GPa, σ_y = 1.07 GPa and ε_b = 0.10. The geometrical features of the TiN coating and its mechanical properties are determined by the deposition regimes during PIRAC [8] formation. So, at a deposition temperature of 700 ºC and a processing time of 48 hours of coating on a titanium substrate, it has a thickness of 1.3 μm with an average roughness height of 0.15 μm (1 mode) and an elastic modulus, and the elastic modulus values were E_1 = 258 GPa; at a deposition temperature of 800 ºC and a processing time of 4 hours of coating on a titanium substrate, it 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 ºC and a processing time of 2 hours of coating on a titanium substrate, it has a thickness of 1.5 μm with an average roughness height of 0.265 μm (3 mode) and an elastic modulus of E_3 = 321 GPa. In accordance with this, the following values of the coating parameters were set: ρ = 5220 kg / m^3, G1 = 104 GPa, G_2 = 104 GPa, G_3 = 129, K_1 = 173Gpa, K_2 = 173GPa, K_3 = 205 GPa. The data on the yield stress σ_y = 7.5 GPa, σ_b = 8.5 GPa, ε_b = 0.075 were obtained using the inverse analysis of the indentation curve [12].

4. RESULTS AND DISCUSSION

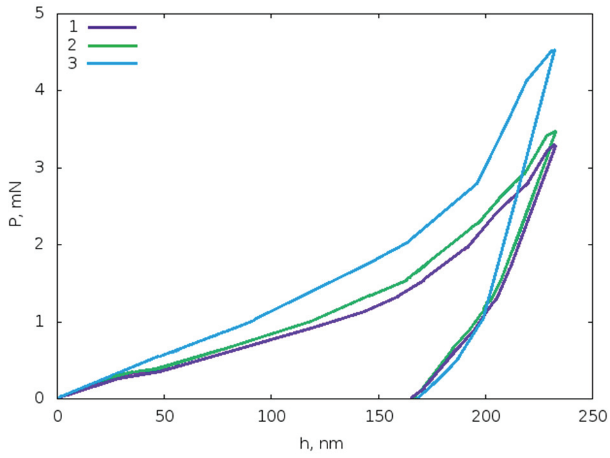

Figure 2 Load-displacement curve P(h) for different application modes (numbers indicate the coating application modes)

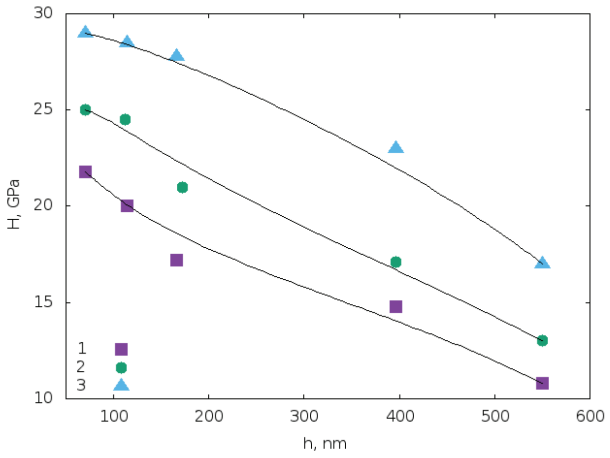

Figure 3 Dependence of the values of hardness on the depth of penetration (numbers indicate the coating application modes)

According to the results of processing the simulation data by the Oliver - Farr method [13], the dependences of the hardness of the systems under consideration on the depth of penetration of the indenter were obtained (**Figure 2**) for three types of coatings obtained with a different method of application.

From the dependence shown in **Figure 3**, it can be seen that the hardest system is the composition of the substrate with the coating applied in the third mode. The results obtained correspond to the data published in [8], which in turn suggests that the material models are developed correctly and can be used to create a multi-level numerical model of the friction node of the “head-acetabulum cup” of EP.

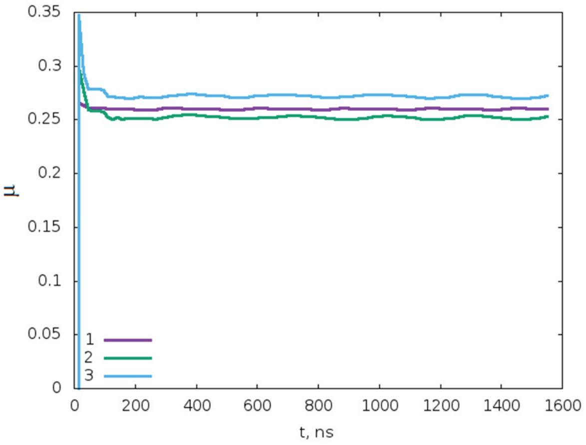

Figure 4 Dependence of friction coefficient on the calculation time when modeling the process of friction at the micro level (numbers indicate the coating application modes)

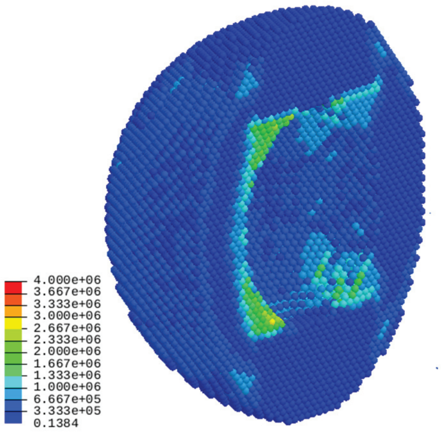

Figure 5 The stress intensity distribution in the friction unit of the EP with a coating obtained by the 3 application mode

According to the results of test calculations the mechanical behavior of two contacting surfaces during friction at the micro level, the values of the friction coefficient and the thickness of the layer in which mixing occurred after one cycle were obtained. Further, obtained values were used in the macromodel of the friction node of the EP to describe the tribological properties of the contacting surfaces after one cycle, thus it was proposed to take into account the wear in the macromodel explicitly. Then, the motion of the EP head in the acetabulum cup was simulated and the stress-strain state of the friction unit was analyzed (**Figure 5**). According to the results of simulation 1 of the friction unit loading cycle, taking into account the data on the tribological state of the surfaces of the contacting elements obtained from the simulation results of the friction at the micro level, it was found that the highest stress value was observed in a friction pair with a coating applied at mode 3, and the minimum value for friction pairs obtained in the second mode of application.

5. CONCLUSION

This article presents a numerical multilevel model of the friction unit of friction of the EP of hip joint. For verification of models of EP materials, numerical nanoindentation experiments were performed. It is shown that the use of friction results for the contacting surfaces of the EP at the micro level in the macromodels of the friction unit hip joint is promising, since it allows one to explicitly take into account the wear in the macromodels through the value of the friction coefficient and the wear of the coating obtained in the micromodels. In the future, it is planned to carry out calculations for the multi-cycle loading of the friction unit of the EP using the proposed multilevel modeling approach.

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