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NUMERICAL MODEL OF THE MECHANICAL BEHAVIOR OF COATED MATERIALS IN THE FRICTION PAIR OF HIP RESURFACING ENDOPROSTHESIS

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Abstract. The paper is devoted to the theoretical study of the mechanical behavior of materials in the friction pair of hip resurfacing endoprosthesis. The investigation was based on three-dimensional computer simulation by the movable cellular automaton (MCA) method, which is a representative of the methods of particles in the mechanics of materials. The results indicate the promising use of metallic alloys with biocompatible ceramic coatings in friction pairs to increase the service life of hip resurfacing.

1 INTRODUCTION

For the treatment of pathologies of the hip joint in the modern world, endoprosthesis (EP) are widely used. Two types of endoprosthesis are used for hip: total hip replacement and hip resurfacing arthroplasty. For the treatment of osteoporosis and other diseases of the hip joint, a hip resurfacing arthroplasty is preferable. The advantage of using hip resurfacing is the possibility of maintaining healthy bone and the possibility of revision operations [1].

An important factor affecting the durability of the hip joint endoprosthesis is wear in pair of friction “acetabular cup-femur head”. In the case of resurfacing, just the surface of the femur head is replaced by the cap, which is specially shaped like a mushroom [2-3]. The difference in the diameters of the hip resurfacing cup and the acetabular cup averages about 2 mm [4]. Polyethylene-metal friction pairs were the first generation of a pair of materials used in a friction pair of hip resurfacing endoprosthesis, however, a large degree of wear led to look for other materials suitable for use in the friction pair [5]. Metal friction pairs based on cobalt-chromium alloys are suitable for the manufacture of endoprosthesis even for young physically active people, since due to their mechanical behavior they are able to withstand high dynamic loads. However, during wear, metal endoprosthesis excrete particles that induce inflammatory processes in the surrounding tissues [6–7]. The use of titanium alloys is a good alternative to the use of cobalt-chromium alloys due to its biocompatible properties, however, these alloys are prone to increased wear. Another group of materials with good biocompatibility are ceramic products, however, this type of prosthesis is applicable mainly to people with low and medium physical activity due to their tendency to brittle failure under high dynamic loads. Therefore, at present, the directions of hip resurfacing endoprosthesis based on metallic titanium alloys with ceramic coatings [8], which combine good biocompatibility and wear resistance, are being actively developed.

Endoprosthesis testing of has two main stages: preclinical and clinical trials. Clinical trials are carried out by installing the endoprosthesis in a living human body. However, when conducting clinical trials there is a danger that poor-quality or incorrectly chosen endoprosthesis may adversely affect the patient's health, therefore, great attention is paid to preclinical trials in the development of endoprosthesis. Preclinical studies of the mechanical behavior of the endoprosthesis can be divided into experimental and theoretical. Experimental studies are tests using a technological installation that simulates the dynamic loading experienced by the endoprosthesis. Theoretical studies of the mechanical behavior of the endoprosthesis using computer simulation make it possible to investigate the mechanical behavior of endoprosthesis taking into account the influence of various factors.

Most of the work on modeling the mechanical behavior of materials in friction pairs is devoted to total hip replacement. Works on modeling hip resurfacing are mainly devoted to studying the mechanical behavior of a single-component endoprosthesis and the system “bone-endoprosthesis” under dynamic loads without rotation in a friction pair [9-11]. In [12], a force action scheme with rotation of the head in the acetabular cup with and without friction is presented. However, there is no work to simulate the rotational motion of the resurfacing cap in the acetabulum; therefore, it is important to build a numerical model for the rotation of the resurfacing cap in the acetabulum consisting of one-component and two-component materials.

This paper proposes a numerical study of the mechanical behavior of contacting elements of a friction pair consisting of a homogeneous material and a material with a coating during rotational motion using the method of movable cellular automata.

2 METHOD OF MOVABLE CELLULAR AUTOMATA

MCA is a new efficient numerical method in particle mechanics that is different from methods in the traditional continuum mechanics [13,14]. Within the frame of MCA, it is assumed that any material is composed of a certain amount of elementary objects (automata) which interact among each other and can move from one place to another and rotate, thereby simulating a real deformation process. The automaton motion is governed by the Newton-Euler equations:

$$
\begin{gathered}
\text{¿}\\
m_i \frac{d^2 R_i}{\mathrm{dt}^2} = \sum_{\mathrm{j}=1}^{N_i} F_{\mathrm{ij}}^{\mathrm{pair}} + F_i^{\Omega},\\
\text{¿} \qquad \hat{J}_i \frac{d\omega_i}{\mathrm{dt}^2} = \sum_{\mathrm{j}=1}^{N_i} M_{\mathrm{ij}} \qquad\qquad (1)\\
\text{¿}\{\\
\text{¿}
\end{gathered}
$$

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, F_{ij}^{pair} is the interaction force of the pair of *i*th and *j*th automata, F_i^{Ω} 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, $M_{ij}=q_{ij}\left(n_{ij}\times F_{ij}^{pair}\right)+K_{ij}$, here q_{ij} is the distance from the center of *i*th automaton to the point of its interaction ("contact") with *j*th automaton, $n_{ij}=\left(R_j-R_i\right)/r_{ij}$ 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, K_{ij} is the torque caused by relative rotation of automata in the pair.

The forces acting on automata are calculated using deformation parameters, i.e. relative overlap, tangential displacement and rotation, and conventional elastic constants, i.e. shear and bulk moduli. A distinguishing feature of the MCA method is calculating of forces acting on the automata within the framework of multi-particle interaction [15,16], which provides for an isotropic behavior of the simulated medium regarded as a consolidated body rather than a granular medium. Moreover, stress tensor components can be calculated for the automaton taking into account all the forces acting on the automaton [15-17], which enables the realization of various models of the plastic behavior of materials developed in the frame of continuum mechanics.

A pair of elements might be considered as a virtual bistable cellular automaton, which permits simulation of fracture and cracks healing and micro welding by the MCA. In this work, a fracture criterion based on the threshold value of von Mises stress was used [15,16]. A criterion based on the threshold value of plastic work was used for making a new bond between contacting automata [16]. Switching of a pair of automata from bonded to non-bonded state and vice versa would result in a changeover in the forces acting on the elements; in particular, non-bonded automata would not resist moving away from one another.

3 DESCRIPTION OF THE MODEL

3.1 Material characterization

From the literature [18] we chose the following values for the material properties of the titanium alloy Ti6Al4V: density ρ = 4420 kg/m^3, shear modulus G = 41 GPa, bulk modulus K = 92 GPa, Young's modulus E = 110 GPa, yield stress σ_y = 0.99 GPa, ultimate strength σ_b = 1.07 GPa and ultimate strain ε_b = 0.10. The mechanical properties of the TiN coating [19]: density ρ = 5220 kg/m^3, shear modulus G = 104 GPa, bulk modulus K = 129 GPa, Young's modulus E = 258 GPa, yield stress σ_y = 3.00 GPa, ultimate strength σ_b = 3.5 GPa and ultimate strain ε_b = 0.075.

3.2 Geometry of the model and scheme of loading

In the case of a one-component material, the geometric model consists of a hemisphere simulating the resurfacing cap for femur head, with an external diameter D_ext_cap=36 mm and an interior diameter D_int_cap=33 mm, a hemisphere simulating the acetabulum cup insert, with an outer diameter of D_ext_insert=41 mm and an iterior diameter of D_int_insert=38 mm, and also a prismatic shell for the insert imitating the surrounding bone tissue (fig. 1). In the case of a two-component coated material, hollow hemispheres are additionally specified for the resurfacing cap with an outer diameter of 35.9 mm and an inner diameter of 33.1 mm (fig.2, a).

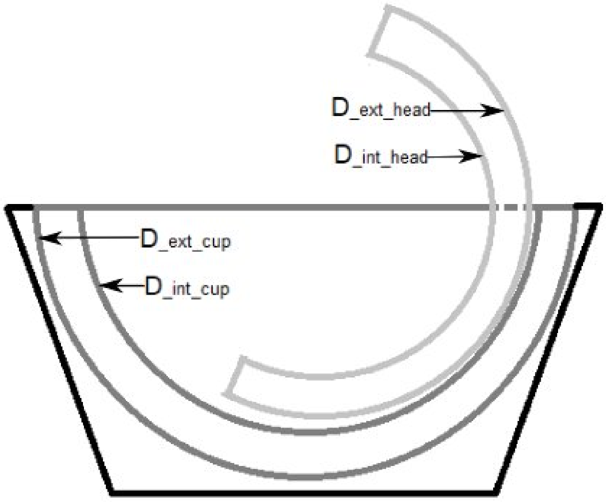
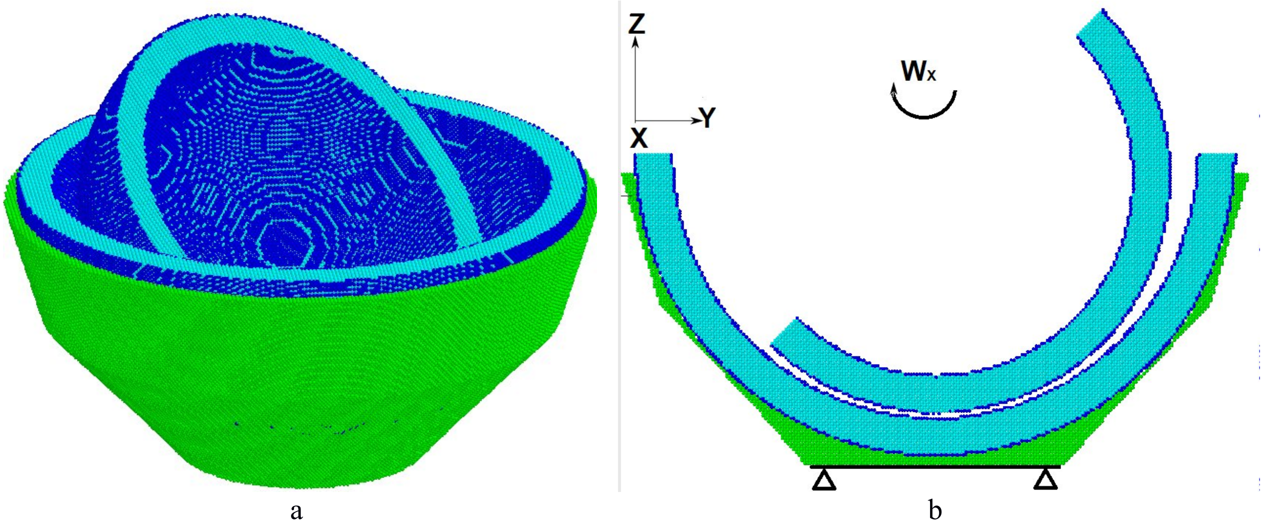


Figure 1. Schematic representation of the model of friction pair of the resurfacing endoprosthesis in cross-section

The load is applied by specifying the translational and rotational velocity of the resurfacing cap automata, corresponding to its rotation as an absolutely rigid body around the axis of symmetry of the corresponding sphere and parallel to the axis *X*.



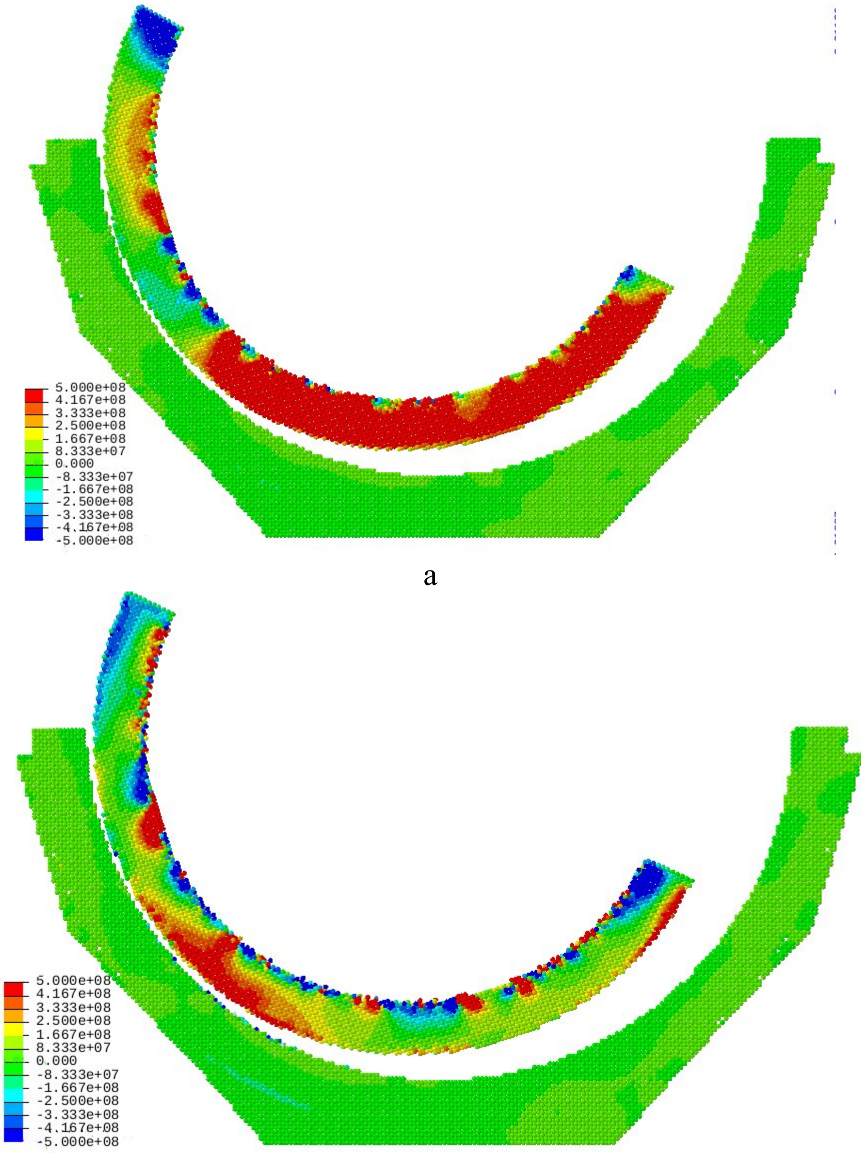
a b

Figure 2. 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

In this case, the value of the corresponding rotational velocity gradually increases from 0 to 10 1/s. The bottom layer of the automata of the cylindrical shell of the bone tissue is rigidly fixed (fig 2, b).

4 SIMULATION RESULTS

When simulating a single rotational cycle, the maximum reaction force was not greater than 3000 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 an ordinary healthy person.



a

b

Figure 3: Distributions of mean stress in the friction pair of the hip resurfacing endoprosthesis of titanium alloy (a) and titanium alloy with TiN coating (b)

The simulation results showed that in the case of a friction pair of a homogeneous material in the zone of contact interaction of the acetabulum insert and resurfacing cap and behind it at extreme positions (edge of the acetabulum) a large are of tensile stress with a maximum value not reaching 990 MPa appeared in the cap. 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.3, a). These results are consistent with the data on the stress distribution in the metal head obtained in [20]. At the same time, the stress in the acetabulum insert did not exceed 100 MPa.

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.3, b). 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.

In general, the results of the numerical simulations suggest that the use of coated materials in the friction pair of hip resurfacing endoprosthesis can help avoiding premature wear of the endoprosthesis.

5 CONCLUSIONS

A three-dimensional model of the mechanical behavior of materials in a friction pair of hip resurfacing endoprosthesis during rotational motion is presented based on the method of movable cellular automata. The obtained simulation results allow us to draw the following conclusions.

The greatest value of tensile stresses in the cap made of titanium alloy during rotation is observed at the extreme positions of the resurfacing cap, in the case of the cap made of TiN coated titanium, this tendency is avoided.

The use of a hardening coating would help to avoid premature wear of the contacting elements of the hip resurfacing endoprosthesis.

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