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FEM APPROACH TO ESTIMATE THE BEHAVIOUR OF BIOCOMPOSITE METAL-SURFACE COATING SYSTEMS

ABSTRACT

A three dimensional (3D) model of biocomposite metal-surface coating system, which is influenced by known external forces, is proposed. This model consists of the metallic substrate (Ti6Al4V) and the hydroxyapatite (HA) coating. Using FEM (finite element method), strain-stress maps of model were generated for investigating relations between the extreme stress of HA coating and the magnitude of external force and the thickness of the coating. The analysis of numerical simulations results confirms that the system with the greatest coating thickness (i.e. 10^{-3} m) has the least extreme stress in this surface coating.

Key words: *biocomposite, FEM analysis, simulation, hydroxyapatite*

INTRODUCTION

Biomechanics and biomaterials must be considered together for elaboration an implant which would be able to transfer physiological loading, ensure stability of fixation and enable long durability and reliability. From the point of view of biomechanics the titanium and its alloys are preferred materials for hard tissue replacements because of their excellent mechanical properties, corrosion resistance and biocompatibility [1]. However titanium and its alloys used in the human body cannot meet all the requirements [2]. In order to improve the biocompatibility of implant its surface is modified by using different types of treatments and coatings [3].

One widely accepted approach to evaluate biocompatibility is the formation of hydroxyapatite (HA) coatings on titanium implants [1,4,5]. Due to the close similarity of chemical composition and high biocompatibility with natural bone tissue HA coating enhances the osseointegration on the metal implant in the early stage of bone healing and provides strong bone-bonding capability [6]. These coatings combine mechanical advantages of metal alloy with the excellent biocompatibility and bioactivity of HA. Despite the strong bonding between HA coating and bone structure, it has been recognized that the mechanical stability of the interface between ceramic coating and the metallic substrate still remains a problem [7,8]. For the purpose of the considered problem it has to be established: 1) the effect of coating thickness on mechanical behaviour of titanium (titanium alloy) - HA coating system; 2) its ability to sustain external loading (forces and moment of forces).

The goal of this work is: 1) to present the three-dimensional (3D) model of biocomposite metal-surface coating system influenced by known external forces; 2) to define the relation between the extreme stress of HA coating and the magnitude of external force and the thickness of its coating. The examined biocomposite metal-surface coating system consisted of metallic substrate (Ti6Al4V) and ceramic surface coating (HA).

NUMERICAL MODEL

A finite element method (FEM) is a numerical tool enabling to achieve solutions of engineering problem which is formulated as a mathematical model. This problem reflects the behaviour of the investigated area under explicitly defined forces. Each investigated area is the continuum medium (i.e. it is a system with infinite number of degrees of freedom) and its behaviour can only be described by a system of complicated differential equations. In many cases solutions of this system cannot be obtained in the form of concrete results. That is why the investigated area has been discretized and its simplified mathematical model (which describes a system with finite number of degrees of freedom) is used in calculations. It has to be bear in mind that using FEM method, only an approximate solution can be obtained, because it needs to use numerical methods for solving the system of differential equations.

The biocomposite system metal-surface coating has been modelled by three numerical models, where the coating *b* adheres to substrate *a* (Fig.1). Each model corresponds to different cases of surface layer placement on the substrate. The substrate *a* has been modelled as a rectangular prism: 150 mm (length) × 20 mm (width) × 20 mm (height). Characteristic dimensions of length and width of surface layer *b* have been assumed to be the same as of metal substrate.

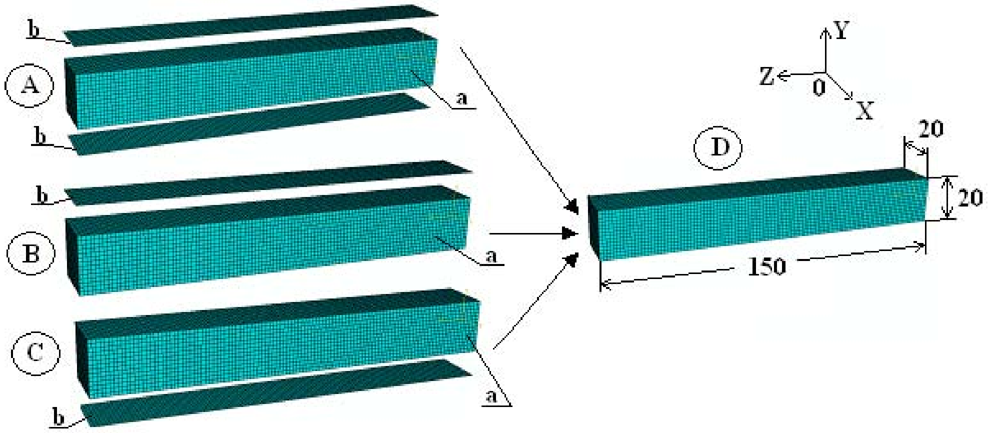


Fig. 1. Three types of numerical models for a substrate with: A) upper and bottom surface coating, B) upper surface coating, C) bottom surface coating, D) dimensions of substrate

The finite elements meshes for a metal substrate and surface coating FEM models were generated in graphical processor of *Abaqus/CAE 6.6* programming. The substrate was described by 28088 spatial cubic finite elements (C3D8R type) (Fig.2A), thus the coating – 1792 shell finite elements (type S4R) (Fig.2B). Each spatial element had eight nodes and each shell element had five integration points on surface coating width. Moreover, each finite element had three translation degrees of freedom. Using a linear function of shape, displacements inside finite elements and on its nods were matched. Also, it was assumed that the nodes of surface layer *b* and substrate *a* were rigidly jointed (Fig.1D).

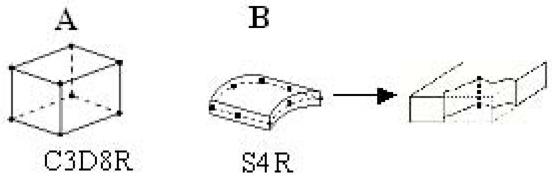


Fig. 2. Finite elements: A) finite element C4D8R type,
B) shell element S4R type with five integration points on surface coating width

The substrate and the surface coating were described as isotropic linear elastic materials by using following material parameters: the Young's modulus of substrate E_{subs} = 115GPa and Poisson's ratio of substrate ν_{subs} = 0,369; the Young's modulus of surface coating E_{shell} = 80 GPa and Poisson's ratio of surface coating ν_{shell} = 0,25. Uniform distributed loading with constant density of 50 kN/m was perpendicularly applied to one surface of numerical model of biocomposite substrate-surface coating system (Fig. 3). The loading was applied to system's nodes placed on the line of symmetry of the whole system that was parallel to the *X* axis. The following boundary conditions were assumed: the left edge of the model was treated as a rigid constraint, and the right edge as sliding constraint.

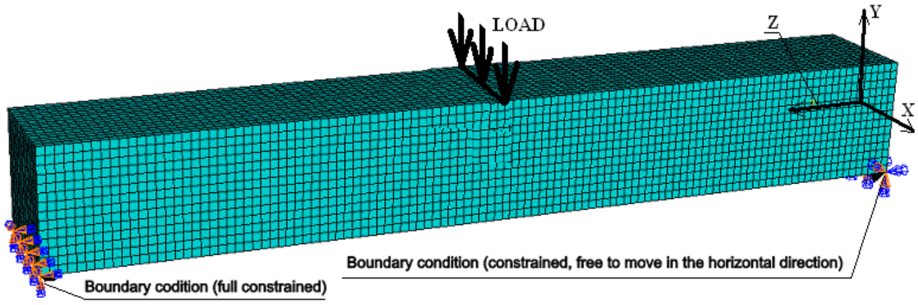


Fig.3. Loading and anchoring method for substrate-surface coating system

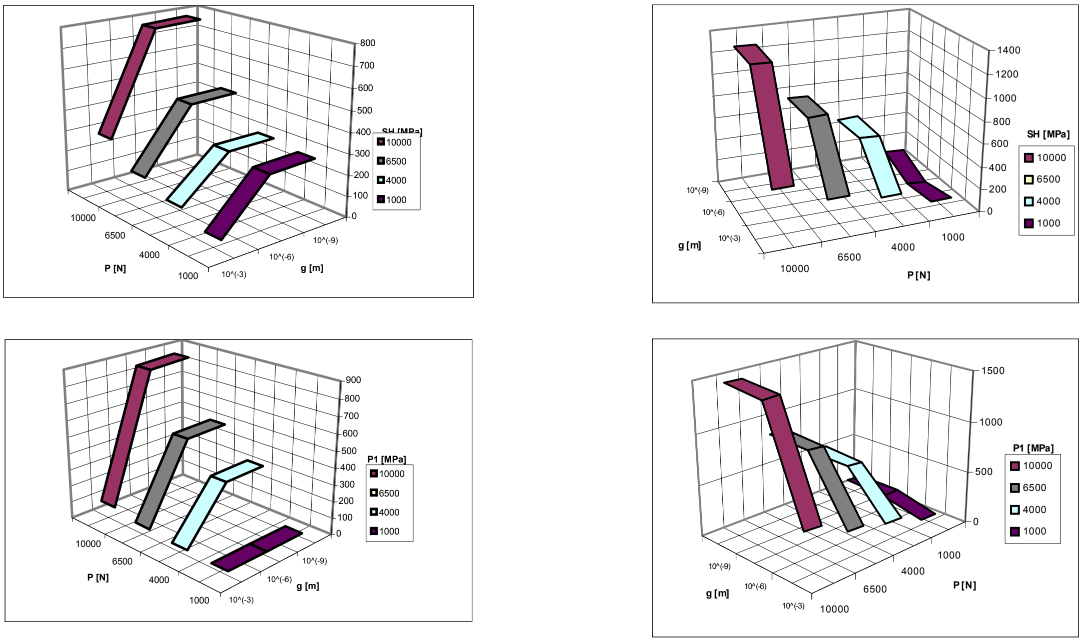
SIMULATION RESULTS

For five values of surface coating thickness (10^{-9} m, 10^{-6} m, 10^{-5} m, 10^{-4} m, and 10^{-3} m) and four magnitudes of external force (10kN, 6,5 kN, 4kN, and 1kN) numerical simulations of each model of biocomposite system metal-surface coating (Fig.1) were conducted. As a result, stress distribution maps were obtained separately for the substrate and the coating. For the substrate there were: 1) maps of reduced stresses calculated by using the Huber-Mises-Hencky criterion (*SH*); 2) maps of three principle stresses; 3) maps of three tangential stresses in planes *XY*, *XZ*, *YZ*. On the other hand, for the surface coating there were: 1) a map of reduced stresses calculated by using the Huber-Mises-Hencky criterion (*SH*); 2) maps of two principle stresses (P_1, P_2); 3) a map of tangential stress in the plane *XZ*.

It is worth noticing that each stress map was generated after previously calculated strain inside every finite element by using node values and shape element functions received as a result of simulation.

The analysis of simulation results based on using strength materials criteria. The accomplishment of described approach is the comparison of extreme value of substrate/coating stress map (estimated as the absolute maximum value between the greatest positive and the biggest negative stress value) with acceptable stresses limits: 1) the yield strength for the substrate R_e (R_e = 1030 MPa [2]); 2) the bending strength for the coating R_g (R_g = 200 MPa [2]). If the extreme value of stress does not exceed the given stress limit, then it concluded that the parameters' set (the extreme stress of HA coating, the magnitude of external force and the thickness of its coating) is describing the acceptable state of the model.

The numerical solutions for coating are presented as diagrams with three related parameters: maximum stresses in the coating, thickness of this coating and the external loading force *P* (Fig.4 and Fig.5). On the basis of received simulation results it can be claimed that acceptable states for each of the three models (the model with upper surface coating, the model with bottom surface coating and the model with upper and bottom surface coating) are assured only when the coating thickness is the greatest (10^{-3} m) and the system substrate – coating surface is loaded with the smallest force (i.e. 1kN). The conclusion formulated on the basis of simulation results is consistent with results given by Lynn and DuQuesnay [9].



A)

B)

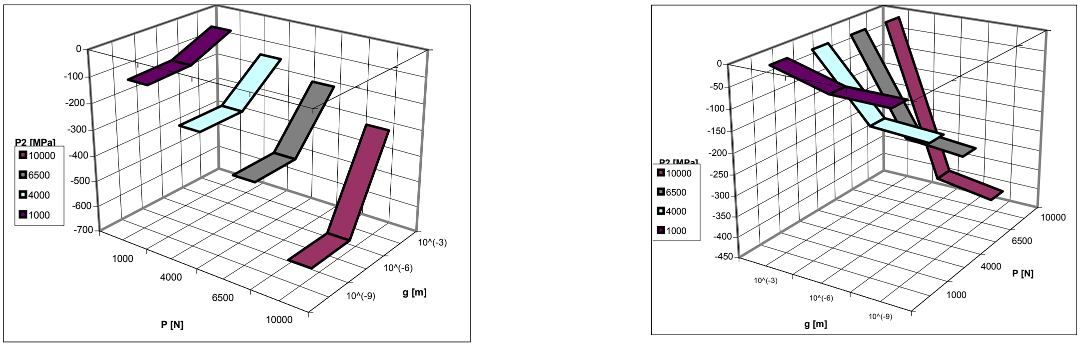


Fig. 4. Relation between the extreme stress in the coating (*SH* – reduced stress calculated from Huber-Mises-Hencky criterion; P_1 – first principal stress; P_2 – second principal stress), the external loading force *P,* and the coating's thickness *g* in the case when: A) the coating is on the tope side of the substrate; B) the coating is on the bottom side of the substrate

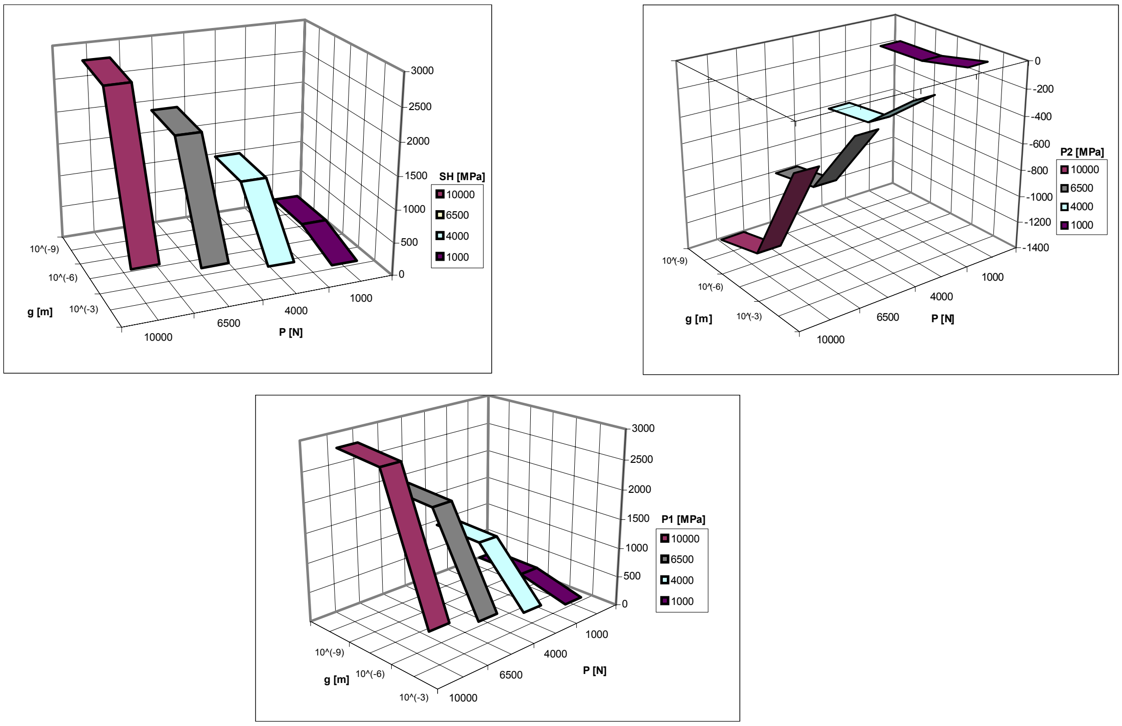


Fig. 5. Relation between the extreme stress in the coating (*SH* – reduced stress calculated from Huber-Mises-Hencky criterion; P_1 – first principal stress; P_2 – second principal stress), the external loading force *P,* and the coating's thickness *g* in the case when the coating is on the top and the bottom side of the substrate

CONCLUSIONS

The proposed FEM models are very useful to estimate the behaviour of biocomposite metal-surface coating systems influenced by external loading. Especially, proposed models are useful to establish relations between surface coating thickness, magnitudes of external loading and extreme stresses of coating/substrate. On the basis of received simulation results of FEM model it is possible to established acceptable states for each of the different cases of the metal-surface coating system, namely: the model with upper surface coating, the model with bottom surface coating and the model with upper and bottom surface coating.

The proposed model of biocomposite metal-surface coating systems is going to be improved by considering an additional number of factors that can decide about endurance characteristics of the whole system, namely: 1) surface flaws [10]; 2) micropores [10] and mikrocracks [11]; 3) inclusions [10]; 4) the degree of porosity [12] and the deleterious influence of porosity [11]; 5) the degree of crystallization [12]; 6) the degree of amorphous and crystalline phase [11] (because amorphous HA rapidly dissolves in the physiological fluids environment, changing the properties of coating, which become weak and can also promote inflammatory responses [13]); 7) residual stresses in coating, which play an important role in the adhesion, fatigue and stress corrosion behavior [12] (residual stress is mainly caused by the mismatch in thermal properties between the coating and the substrate material in conjunction with complicated solidification for ceramic coating [13]).

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