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Mathematical Modeling of Stress in Plasma Coatings Used in Medicine

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To improve the biological compatibility of implants, it is suggested to modify their surface using plasma-spray technology for application of porous scaffold-coating that can serve as a reservoir for active substances. During use, such coatings are often subjected to stress, which, being added to the residual stress, significantly reduces the strength of the coatings. It is virtually impossible to measure the stress values experimentally, so in this work we solve the problem of mathematical modeling of the stress arising in porous coatings in the process of their formation, as well as in the course of their use.

According to the literature, scaffolds based on biological or synthetic materials provide the most effective biological compatibility. Such scaffolds can be filled with stem cells, growth factors, blood plasma proteins, and other active substances including drugs [1-5]. In spite of adequate biological compatibility, such implants cannot be used in organs and tissues subjected to serious stress during functioning (e.g. teeth and joints). This problem can be solved using application of porous scaffold-coatings to metal implants. These scaffold-coatings are based on hydroxyapatite, tricalcium phosphate, and other biologically compatible materials.

Porous coating structure provides for the accumulation of various substances. The coating should include macropores and capillary pores (nanopores) (Fig. 1). A coating modified with pores serves as a container for long-term storage of liquids, whereas capillary pores provide transport of the liquids.

The liquid can contain drugs or other active substances migrating to the pathological focus. Therefore, coating of implants with layers of the required structure is an important problem. However, increase in coating porosity reduces its strength. The technology of implant coating should provide the necessary balance between coating porosity and coating strength.

Plasma coating of powdered materials is a promising approach to coating with porous layers [6]. Control of coating strength is an important component of the coating technology. The coating strength should not exceed a limiting threshold:

$$\sigma_c < [\sigma_c], \qquad (1)$$

where σ_c is the coating material strength; $[\sigma_c]$ is the coating limiting strength.

Methods of adhesion and destruction, as well as the pin method, are conventional methods for monitoring plasma coating strength [7]. These methods do not take into account the coating porosity. However, medical-purpose coatings are characterized by the strength associated with particle-to-particle bonds and particle-to-substrate bonds.

The plasma coating is applied at high temperature with application of particles onto the substrate. The interaction of particles with substrate generates contact strength and so-called residual strength [6]. In addition, the implants are subjected to functional stress (e.g. during

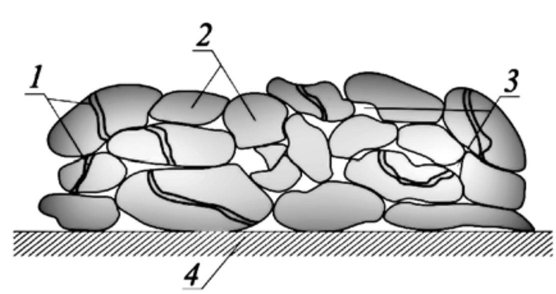

Fig. 1. Scheme of porous plasma coating: 1) nanopores; 2) coated particles; 3) macropores; 4) substrate.

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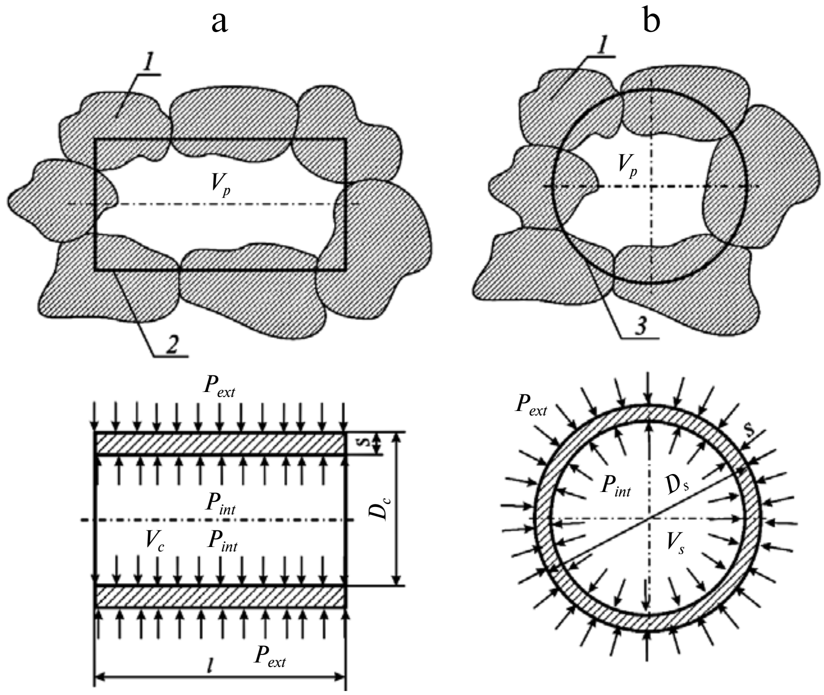

Fig. 2. Diagram of particle configuration transformation into abstract geometrical figure: a) hollow cylinder; b) hollow sphere; l – cylinder length; V_p – pore volume; V_c – hollow cylinder volume; V_s – hollow sphere volume; D_c – cylinder diameter; D_s – sphere diameter; 1 – coated particles; 2 – abstract cylinder; 3 – abstract sphere.

chewing or walking). Therefore, the coating strength is a sum of plasma coating strength and functional coating strength:

$$\sigma_c = \sigma_r + \sigma_f, \tag{2}$$

where σ_r is residual coating strength; σ_f is functional coating strength.

The value of the strength in the contact area is an important parameter of implant quality. However, direct measurement of this strength is virtually impossible. To solve this problem, a method for measuring strength based on statistical simulation in the contact area is suggested in this work. According to this method, several coated particles are isolated in the porous segment. An abstract porous structure in the shape of a hollow cylinder or hollow sphere is formed on the basis of the porous segment (Fig. 2).

The parameters of the geometric structure are set based on averaged pore configuration:

$$V_p \sim V_c \sim V_s. \tag{3}$$

The abstract structures were regarded as models of cylindrical or spherical envelopes with contacting edges [8].

External forces induce normal stress U (meridional) and T (circular), transverse stress Q, as well as bending moments M_m (meridional) and M_t (circular) (Fig. 3).

External force p, thrust load Q, and edge loads Q_0 and M_0 are applied to the envelope (Fig. 4).

External and internal envelope stresses are calculated from [9]:

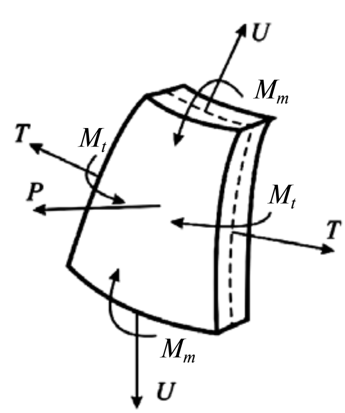

Fig. 3. Diagram of external forces applied to envelope element.

$$\begin{cases} \sigma_{m_0} = \sigma_{m_0}^{p} + \sigma_{m_0}^{(Q_0-Q)} + \sigma_{m_0}^{M_0}; \\ \sigma_{t_0} = \sigma_{t_0}^{p} + \sigma_{t_0}^{(Q_0-Q)} + \sigma_{t_0}^{M_0}; \\ \sigma_{\max} = \max\left\{\sigma_{m_0}; \sigma_{t_0}\right\}, \end{cases} \quad (4)$$

where σ_{m_0} is meridional stress; σ_{t_0} is tangential (circular) stress; $\sigma_{m_0}^{p}$, $\sigma_{m_0}^{(Q-Q_0)}$, $\sigma_{m_0}^{M_0}$ are meridional stresses caused by p, $(Q - Q_0)$, M_0; $\sigma_{t_0}^{p}$, $\sigma_{t_0}^{(Q-Q_0)}$, $\sigma_{t_0}^{M_0}$ are tangential stresses caused by p, $(Q - Q_0)$, M_0.

It was reported in [9] that Q_0 and M_0 were calculated from:

$$\begin{cases} \Delta_p^c - \Delta_{Q_0}^c + \Delta_{M_0}^c = \Delta_p^s + \Delta_{(Q_0-Q)}^s + \Delta_{M_0}^s; \\ \Theta_p^c - \Theta_{Q_0}^c + \Theta_{M_0}^c = -\Theta_p^s - \Theta_{(Q_0-Q)}^s - \Theta_{M_0}^s, \end{cases} \quad (5)$$

where Δ_p^c, $\Delta_{Q_0}^c$, $\Delta_{M_0}^c$ are, respectively, p, Q_0, and M_0 load-induced radial and angular deformations of cylindrical envelope; Δ_p^s, $\Delta_{(Q_0-Q)}^s$, $\Delta_{M_0}^s$; Θ_p^s, $\Theta_{(Q_0-Q)}^s$, $\Theta_{M_0}^s$ are p, Q_0, and M_0 load-induced radial and angular deformations of spherical envelope.

The radial and angular deformations are calculated from [9]:

$$\begin{cases} \Delta_p^c = \dfrac{(2-\mu)R^2}{2Es}p; \ \Delta_p^s = \dfrac{pa^2}{2Es}\left(2 - \mu - \dfrac{a^2}{b^2}\right); \\ \Delta_{Q_0}^c = \dfrac{2\beta R^2}{sE}Q_0; \ \Delta_{Q_0}^s = \dfrac{2\beta a^2}{sE}Q_0; \\ \Delta_{M_0}^c = \dfrac{2\beta^2 R^2}{sE}M_0; \ \Delta_{M_0}^s = \dfrac{2\beta^2 a^2}{sE}M_0; \\ \Theta_{Q_0}^c = \dfrac{2\beta^2 R^2}{sE}Q_0; \ \Theta_{Q_0}^s = \dfrac{2\beta_e^2 R^2}{s_e E}Q_0; \\ \Theta_{M_0}^c = \dfrac{4\beta^3 R^2}{sE}M_0; \ \Theta_{M_0}^s = \dfrac{4\beta_e^3 R^2}{s_e E}M_0; \\ \beta = \sqrt[4]{3(1-\mu^2)}\sqrt{Rs}; \ \beta_e = \sqrt[4]{3(1-\mu^2)}\sqrt{as_e}; \\ R = \dfrac{D_c}{2}; \ a = \dfrac{D_s}{2}; \ b = \dfrac{D_s}{4}, \end{cases} \quad (6)$$

where μ is Poisson coefficient; D_c is cylinder diameter; D_s is spherical envelope diameter; s_e, b, a are thickness, width, and radius of spherical envelope, respectively.

Edge stress is calculated from [9]:

$$\begin{cases} \sigma_{m_0}^{p} = \dfrac{pR}{2s}; \ \sigma_{t_0}^{p} = \dfrac{pR}{s}; \\ \sigma_{m_0}^{M_0} = \dfrac{6M_0}{s^2}; \ \sigma_{t_0}^{M_0} = \dfrac{2M_0\beta^2 R}{s}; \\ \sigma_{m_0}^{Q_0} = 0; \ \sigma_{t_0}^{Q_0} = \dfrac{2Q_0\beta R}{s}. \end{cases} \quad (7)$$

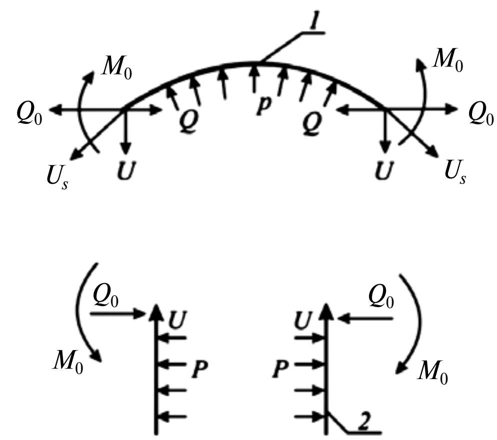

Fig. 4. Diagram of edge load: 1 – spherical envelope; 2 – cylindrical envelope.

Let the vital activity of the human body be the source of liquid motion in pores. This causes excessive pressure calculated from [10]:

$$P = \rho C_p v = \rho C_p \frac{1}{t}, \quad (8)$$

where ρ is liquid density; C_p is liquid wave propagation rate; v is liquid flow velocity; l is liquid length; t is pulsation wave time. The P value calculated from Eq. (8) is accepted as the value of the external stress.

The residual stress is calculated from the Hertz equation [11]:

$$\sigma = 0.418\sqrt{q\frac{E}{\rho}}, \quad (9)$$

where q is normal load in contact area; E is the elasticity modulus of coated particles; ρ is curvature radius of particles ($\rho = R_1R_2/(R_1 - R_2)$); R_1 and R_2 are radii of interaction of particles.

The stress of porous coatings is calculated using the following algorithm.

1. Coating strength is specified as scale of physical values.

2. The Monte-Carlo model gives numerical values of model parameters.

3. The stress values in pores are calculated from Eqs. (1)-(8).

4. Multiple statistical calculations give average values of coating strength.

5. The results of statistical tests are compared with experimental data.

6. In case of the difference between the results, the coating procedure is corrected.

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