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Effect of Permittivity on the Ionic Boundary Layer upon Protonation of Lithium Niobate

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Abstract. The paper presents the results of a numerical study of the behavior of proton exchange reaction products after they enter benzoic acid, which interacts with a lithium niobate crystal. The theoretical model based on the continuous media approximation considers the convective transfer and diffusion of positively charged lithium ions and negatively charged benzoate ions. Additionally, the possibility of their recombination with the subsequent formation of lithium benzoate molecules is taken into account. The results obtained correspond to stationary, uniform along the interface, profiles of the ion concentration and electric potential. In the process of establishment, benzoate ions form an ionic boundary layer. An analysis is made of the influence of the dielectric constant of the carrier liquid on its characteristics.

Keywords: proton exchange, boundary layer, permittivity, numerical simulation.

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Introduction

Technologies for production planar or channel waveguides [1] are associated with the implementation of the process of replacing positively charged lithium ions belonging to the lithium niobate crystal lattice with hydrogen ions. In many cases, the latter are formed as a result of thermal dissociation of benzoic acid molecules, which are brought into the contact with crystal at characteristic temperatures of ~ 500 K [2, 3]. Other acids, such as palmitic [4], pyrophosphoric [5, 6], etc., can also be a source of protons. The duration of proton exchange can reach several hours. During this time, a near-surface region with an increased hydrogen concentration forms inside the substrate. The value of the refractive index in this region differs markedly from

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that which takes place in the bulk of the crystal. The thickness of the protonation region is $\sim 10^{-6}$ m [7].

Despite the fact that this technology has been known for several decades, during which a large number of both experimental [1] and theoretical [8,9] works have been accumulated, there are still many questions related to the physical and chemical nature of the processes taking place during the mentioned reaction of substitution. So, at the moment, not all regularities of the formation of many crystalline phases in the protonated region of lithium niobate have been studied. It is known that the phase diagram is affected by both the addition of lithium benzoate to benzoic acid [10], and the temperature at which proton exchange occurs, as well as its duration [11]. In addition, the subject of research at the moment is the preliminary plasma treatment of the crystal surface and its effect on the final characteristics of the waveguide [12].

From a fundamental point of view, it seems important to study not only the processes that take place inside the crystal, but also those that occur in the acid. According to the results obtained during the experiments, the properties of the acid and its impurities have a very strong influence on the final result. For example, dilution of benzoic acid with lithium benzoate reduces the intensity of proton exchange. Already at 5% impurity concentration, the substitution reaction does not occur [10]. The addition of water to benzoic acid, which intensifies the exchange process, has a strong effect on the final waveguide [13].

In [14] a mathematical model that allows one to describe the behavior of ions, which are the products of the proton exchange reaction, in benzoic acid is presented. It was shown that despite the smallness of the region in which the reaction under consideration takes place, the processes occurring in it can be described using the equations of continuum mechanics. This model included the diffusion mechanism of impurity propagation and the recombination mechanism of ion interaction. In the course of solving the problem formulated in [14], the possibility of the existence of stationary ion concentration profiles was discovered. It should be noted that benzoate ions, which have a much lower diffusion coefficient than lithium ions, form the boundary layer. The disadvantages of this work may be that it did not consider the dynamics of the formation of concentration profiles, and also used the model value of the permittivity of the carrier liquid. In [14] it was equal to unit, which, obviously, does not correspond to the realistic value of the permittivity of benzoic acid, which is known to be a polar dielectric. This makes it necessary to refine the previous calculations in terms of quantitative determination of the parameters of the boundary layer.

1. Formulation of the problem

Let us consider a homogeneous surface of a lithium niobate crystal, on which a photolithographic mask is partially deposited (Fig. 1). This configuration is used to create channel waveguides. The resulting cavity, shown in Fig. 1, has dimensions $h = 10^{-6}$ m, $l = 5h$ [15] and is filled with benzoic acid heated to a temperature of $T = 500$ K. This temperature favors the conditions for thermal dissociation of molecules acids into benzoate ions $C_7H_5O_2^-$ and hydrogen ions H^+ . The latter tend to penetrate deep into the crystal with further replacement of lithium ions Li^+ . Thus, from the side of the interface there is a flow of positively charged lithium ions into the acid. After some time, they should meet with benzoate ions and form a lithium benzoate $C_7H_5O_2Li$ molecule.

The estimations in [14] make it possible to say that the equations of concentration convection written in the electroconvective approximation allow to describe the process of ion transport and

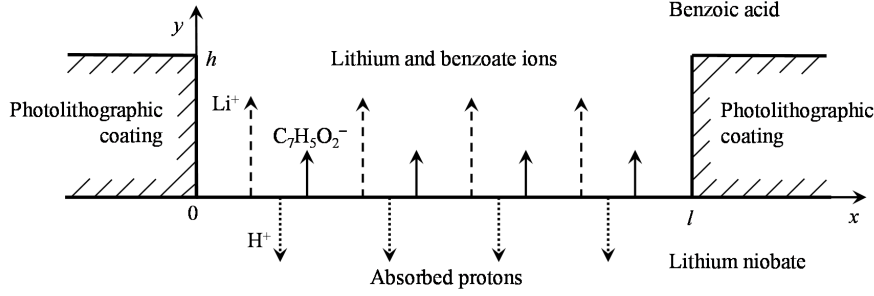


Fig. 1. Statement of the problem. System of coordinate

their further recombination using the following system of equations [16, 17]:

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \nabla) \mathbf{v} \right) = -\nabla p + \eta \Delta \mathbf{v} + e(n_+ - n_-) \mathbf{E}, \quad (1)$$

$$\operatorname{div} \mathbf{v} = 0, \quad \operatorname{div}(\varepsilon_0 \varepsilon \mathbf{E}) = e(n_+ - n_-), \quad \mathbf{E} = -\nabla \varphi, \quad (2)$$

$$\frac{\partial n_{\pm}}{\partial t} + (\mathbf{v} \nabla) n_{\pm} = D_{\pm} \Delta n_{\pm} \mp \nabla(k_{\pm} n_{\pm} \mathbf{E}) - k_R n_+ n_-, \quad (3)$$

where \mathbf{v} , \mathbf{E} , φ , p , n_{\pm} are the fields of velocity, electric field strength and electric potential, pressure, concentration of positively and negatively charged ions. Parameters η , e , ε , ε_0 are the dynamic viscosity of benzoic acid, electron charge, electrical constant and permittivity. In turn, D_{\pm} , k_{\pm} , and k_R set the diffusion coefficients of lithium and benzoate ions, their mobility and the recombination coefficient, the value of which was estimated according to [17]:

$$k_R = \frac{e(k_+ + k_-)}{\varepsilon_0 \varepsilon}. \quad (4)$$

The concentration fluctuations that may occur in such hydrodynamic system are not able to cause gravitational convection [18], therefore, there is no corresponding term in equation (1). However, unlike the statement presented in [14], the system of equations (1)–(3) will be solved without neglecting the convective terms, as well as the time derivative, which will allow us to study the dynamics of the formation of concentration and electric field profiles.

The walls of the photolithographic mask and the crystal surface were considered to be solid; therefore, the no-slip condition was imposed on them. A constant mass flow of ions of both signs $J = 10^{18} \text{ m}^{-2} \text{ s}^{-1}$ [14] was maintained at the lower boundary. The remaining boundaries for ions were impenetrable. The electric potential was measured relative to the lower limit.

$$x = 0, l: \quad \mathbf{v} = 0, \quad \frac{\partial n_{\pm}}{\partial x} = 0, \quad \frac{\partial \varphi}{\partial x} = 0. \quad (5)$$

$$y = 0: \quad \mathbf{v} = 0, \quad \frac{\partial n_{\pm}}{\partial y} = -\frac{J}{D_{\pm}}, \quad \varphi = 0. \quad (6)$$

The upper bound of the region in question was free, so

$$y = h: \quad \frac{\partial v_x}{\partial y} = 0, \quad v_y = 0, \quad \frac{\partial n_{\pm}}{\partial y} = 0, \quad \frac{\partial \varphi}{\partial y} = 0. \quad (7)$$

The fact that the same flux density J is used in boundary conditions (6) for both negatively charged and positively charged ions is due to the overall electroneutrality of the system, since

one hydrogen ion replaces one lithium ion. In other words, the fulfillment of condition (6) is associated with the equality

$$\int_0^l \int_0^h n_+ dx dy = \int_0^l \int_0^h n_- dx dy. \quad (8)$$

The boundary value problem, which includes the system of equations (1)–(3) in combination with boundary conditions (5)–(7), was solved in dimensionless variables. $h, \nu/h, h^2/\nu, Jh/D_+, eJh^3/\varepsilon_0\varepsilon D_+, \rho\nu^2/h^2$, respectively. In these units, $\nu = \eta/\rho$ is the coefficient of kinematic viscosity.

After the exclusion of the electric field strength and procedure of adimensionalization, the equations and boundary conditions have the form:

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\nabla)\mathbf{v} = -\nabla p + \Delta \mathbf{v} + A(n_+ - n_-)\nabla\varphi, \quad (9)$$

$$\operatorname{div} \mathbf{v} = 0, \quad \Delta\varphi = (n_+ - n_-), \quad (10)$$

$$\frac{\partial n_{\pm}}{\partial t} + (\mathbf{v}\nabla)n_{\pm} = \frac{1}{\operatorname{Sc}_{\pm}}\Delta n_{\pm} \mp B_{\pm}\nabla(n_{\pm}\nabla\varphi) - Cn_+n_-, \quad (11)$$

$$x = 0, l: \quad \mathbf{v} = 0, \quad \frac{\partial n_{\pm}}{\partial x} = 0, \quad \frac{\partial\varphi}{\partial x} = 0, \quad (12)$$

$$y = 0: \quad \mathbf{v} = 0, \quad \frac{\partial n_+}{\partial y} = -1, \quad \frac{\partial n_-}{\partial y} = -\frac{D_+}{D_-}, \quad \varphi = 0, \quad (13)$$

$$y = h: \quad \frac{\partial v_x}{\partial y} = 0, \quad v_y = 0, \quad \frac{\partial n_{\pm}}{\partial y} = 0, \quad \frac{\partial\varphi}{\partial y} = 0. \quad (14)$$

The dimensionless control parameters are defined as follows:

$$A = \frac{e^2 h^6 J^2}{\varepsilon_0 \varepsilon \rho \nu^2 D_+^2}, \quad B_{\pm} = \frac{k_{\pm} e J h^3}{\varepsilon_0 \varepsilon \nu D_+}, \quad C = \frac{k_R J h^3}{\nu D_+}, \quad \operatorname{Sc}_{\pm} = \frac{\nu}{D_{\pm}}. \quad (15)$$

The formulated problem admits a two-dimensional solution in terms of the stream function ψ and the vorticity ϕ :

$$v_x = \frac{\partial\psi}{\partial y}, \quad v_y = -\frac{\partial\psi}{\partial x}, \quad \phi = \frac{\partial v_x}{\partial y} - \frac{\partial v_y}{\partial x}. \quad (16)$$

After eliminating velocity and pressure using (16), equations (10)–(13) take the final form:

$$\frac{\partial\phi}{\partial t} + \frac{\partial\psi}{\partial y}\frac{\partial\phi}{\partial x} - \frac{\partial\psi}{\partial x}\frac{\partial\phi}{\partial y} = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + A\left(\frac{\partial\Delta}{\partial y}\frac{\partial\varphi}{\partial x} - \frac{\partial\Delta}{\partial x}\frac{\partial\varphi}{\partial y}\right), \quad (17)$$

$$\frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} = n_- - n_+ = \Delta, \quad \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = \phi, \quad (18)$$

$$\begin{aligned} \frac{\partial n_{\pm}}{\partial t} + \frac{\partial\psi}{\partial y}\frac{\partial n_{\pm}}{\partial x} - \frac{\partial\psi}{\partial x}\frac{\partial n_{\pm}}{\partial y} &= \frac{1}{\operatorname{Sc}_{\pm}}\left(\frac{\partial^2 n_{\pm}}{\partial x^2} + \frac{\partial^2 n_{\pm}}{\partial y^2}\right) + \\ + B_{\pm}\left(\frac{\partial n_{\pm}}{\partial x}\frac{\partial\varphi}{\partial x} + \frac{\partial n_{\pm}}{\partial y}\frac{\partial\varphi}{\partial y} + n_{\pm}\left(\frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2}\right)\right) &- Cn_+n_-, \end{aligned} \quad (19)$$

2. Solution technique

The boundary value problem (17)–(19), (12)–(14) was solved numerically by the two-field [19] method implemented using an explicit scheme in the Fortran programming language. One-sided differences were used in the approximation of derivatives with respect to coordinates at the boundaries and derivatives with respect to time. Spatial derivatives in the internal nodes of the computational domain were approximated by central differences. To solve the Poisson equations (18), the method of successive upper relaxation was used. The method of establishment was used in the calculations. The time step was chosen from considerations of the stability of the numerical procedure. The stream function at all boundaries was equal to zero. The vorticity value at the upper boundary was also equal to zero. The vorticity at solid boundaries was determined using the Thom condition. To resolve the boundary layer, the computational domain was discretized using a uniform grid consisting of 40 nodes along the x axis and 100 nodes along the y axis.

The choice of control parameter values was made in accordance with [14]: $h = 2 \cdot 10^{-6}$ m, $k_+ = 1.5 \cdot 10^{-7}$ m²/s·V, $k_- = 2 \cdot 10^{-8}$ m²/s·V, $D_+ = 10^{-8}$ m²/s, $D_- = 10^{-9}$ m²/s, $\nu = 5 \cdot 10^{-7}$ m²/s, $\rho = 10^3$ kg/m³, $J = 10^{18}$ s⁻¹m⁻².

Separately, it is necessary to comment on the choice of values of the permittivity. At the moment, there are no data in the literature on direct measurements of this value for pure benzoic acid, even under normal conditions, when it is in the solid state. Moreover, according to the available data, the permittivity of benzoic acid varies greatly when impurities are added to the acid [20], which only complicates the search for specific values, given the wide variety of ways to create waveguides [1]. To estimate ε , it only remains to find an analogue of a substance whose molecules are identical in their properties to those of benzoic acid and whose permittivity would be measured at the required temperatures corresponding to the proton exchange regimes. Thus, considering the values of dipole moments d of molecules, one can compare benzoic acid ($d = 1.78$ D [21]) with methanol ($d = 1.70$ D [22]). The permittivity of the latter was measured over a very wide range of temperatures and pressures in [23]. According to these results, ε at temperatures ~ 500 K can be taken equal to 10. It should be noted that this value was obtained at a pressure ~ 200 atm, which is very different from the proton exchange conditions. However, according to [23], the dielectric constant of methanol does not strongly depend on pressure, so we can stop at this estimation. When solving the problem, several values of the permittivity were used to potentially consider different ways of protonation. Based on these values, the recombination coefficient k_R was also recalculated.

3. Results of numerical simulation

The performed calculations demonstrate a very fast damping of all hydrodynamic perturbations and reaching a stationary regime, regardless of the value of the permittivity (Fig. 2). In dimensional units, the system needs $\sim 10^{-4}$ s to settle in a stationary state. It should be noted that these results confirm the assumptions made in [14] regarding the absence of convective mass transfer in the stationary case, since all fields after reaching this regime are uniform along the interface. In other words, this problem can be solved with good accuracy in a one-dimensional approximation. In the future, to visualize the results, only profiles along the y axis for the center of the computational domain will be presented.

An analysis of the concentration profiles shows that negatively charged benzoate ions form a boundary layer, the thickness of which increases with permittivity growth (Fig. 3). This is mainly due to the fact that the recombination coefficient depends on ε . An increase in permeability

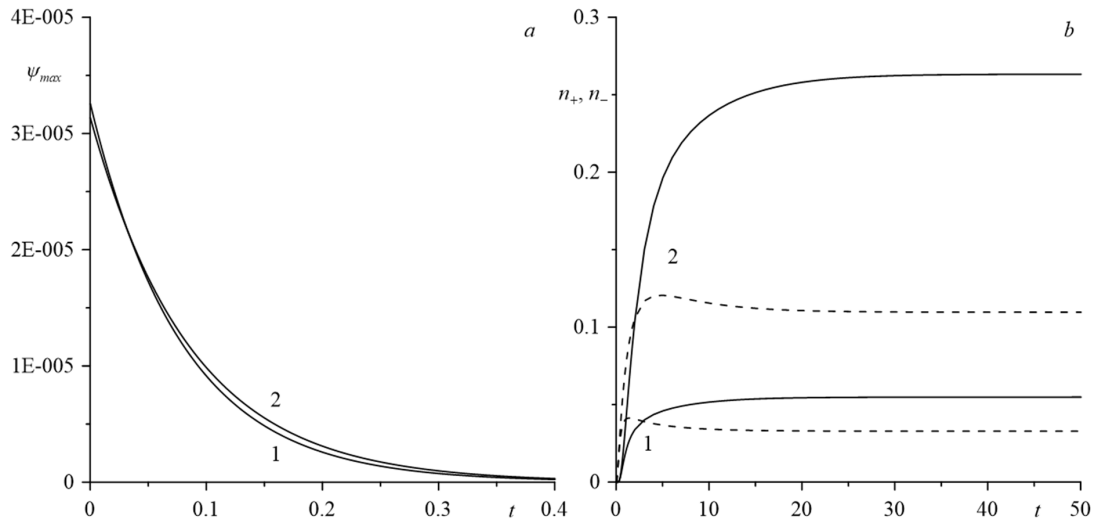


Fig. 2. Dependencies of stream function maximum value (a) and concentration in the point with coordinates $x = 2.5$, $y = 0.2$ (b) on dimensionless time: 1 — $\varepsilon = 1$, 2 — $\varepsilon = 10$. On the figure b solid lines — benzoate ions concentration, dashed lines — lithium ions concentration

reduces k_R , which makes it more likely that benzoate ions are located at large distances from the crystal. As the results show, on average, the thickness of this layer lies in the range from $\sim 10^{-7}$ m to $\sim 10^{-6}$ m. On the other hand, lithium ions, which have higher mobility, have the ability to penetrate deep into benzoic acid at much greater distances. In fact, they occupy the entire computational domain and are held by the electric field that arises according to (11) due to the difference in ion concentrations. The intensity of this field is directed towards the substrate, i.e. the ionic boundary layer is slightly stretched. At the same time, in the concentration profiles of lithium ions, one can notice a bend in the region where benzoate ions are no longer present. This bending is also associated with the action of the electric field, which, on the contrary, tends to "press" the positively charged ions to the substrate.

The electric field also undergoes changes when the permittivity is taken into account (Fig. 4). As can be seen from Fig. 3 an increase in ε leads to an increase in the concentration difference. As a result, the potential difference at realistic permeability values can be increased by an order of magnitude compared to the model value $\varepsilon = 1$: from $\sim 10^{-4}$ V to $\sim 10^{-3}$ V.

Conclusion

The calculation results allow us to state that taking into account realistic values of the permittivity increases the thickness of the ionic boundary layer formed by benzoate ions during proton exchange. If in the model case $\varepsilon = 1$ the layer thickness was $\sim 2 \cdot 10^{-7}$ m, then as the permeability value increases to $\varepsilon = 10$, negatively charged ions can be detected at a distance of $\sim 4 \cdot 10^{-7}$ m from the crystal. Thus, the thickness of the boundary layer becomes comparable with the thickness of the protonated region inside the substrate. In addition, it can be concluded that the use of acids with a high dielectric permittivity makes it possible to influence the "outer" boundary layer to a greater extent during protonation by generating an acid flow along the substrate by swinging the workpiece, which is often used in production.

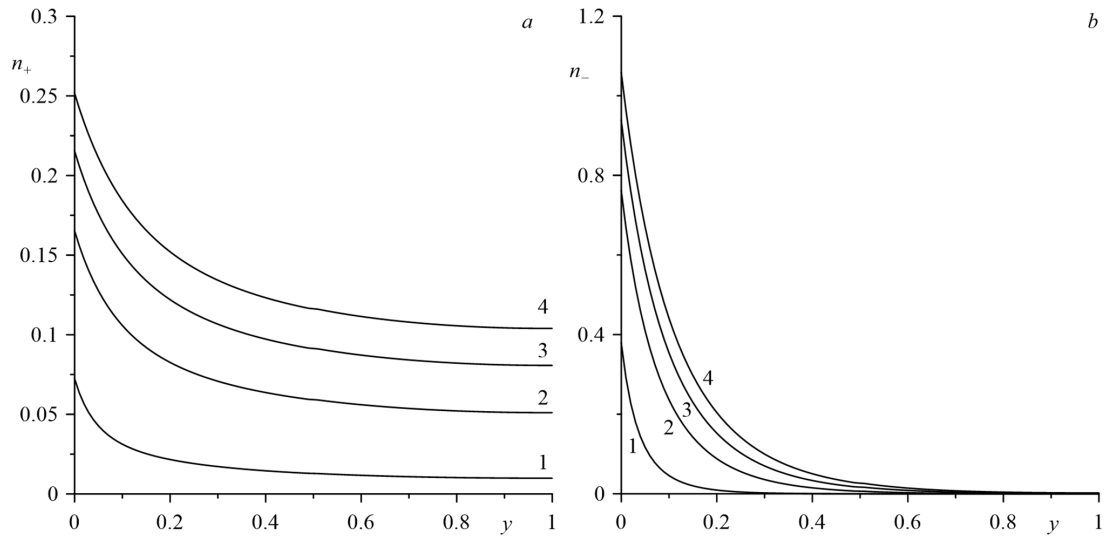


Fig. 3. Concentration profiles of lithium ions (a) and benzoate ions (b) in the point $x = 2.5$ at the time $t = 50$. 1 – $\varepsilon = 1$, 2 – $\varepsilon = 10$, 3 – $\varepsilon = 20$, 4 – $\varepsilon = 30$

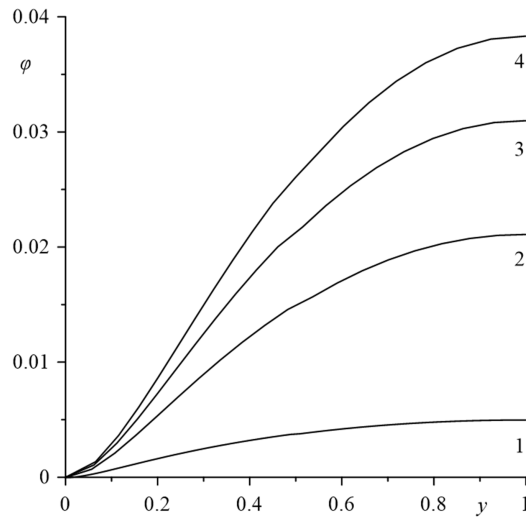


Fig. 4. Electric potential profiles in the point $x = 2.5$ at the time $t = 50$. 1 – $\varepsilon = 1$, 2 – $\varepsilon = 10$, 3 – $\varepsilon = 20$, 4 – $\varepsilon = 30$

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Влияние диэлектрической проницаемости на ионный пограничный слой при протонировании ниобата лития

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Аннотация. В работе представлены результаты численного исследования поведения продуктов реакции, попадающих в бензойную кислоту, которая взаимодействует с кристаллом ниобата лития при протонном обмене. В теоретической модели, построенной в приближении сплошной среды, рассматривается конвективный перенос и диффузия положительно заряженных ионов лития и отрицательно заряженных бензоат-ионов. Дополнительно учитывается возможность их рекомбинации с последующим формированием молекул бензоата лития. В процессе установления бензоат-ионы образуют ионный пограничный слой. В этом пределе полученные результаты отвечают стационарным, однородным вдоль межфазной поверхности профилям концентрации ионов и электрического потенциала.

Ключевые слова: протонный обмен, пограничный слой, диэлектрическая проницаемость, численное моделирование.