UDC 004.772+539.2+537.226

V.A. Kalytka[1], M.V. Korovkin[2], A.I. Aliferov[3], A.V. Bashirov[4], D.R. Talaspekov[1]

[1]Karaganda State Technical University, Kazakhstan;
[2]National Research Tomsk Polytechnic University, Russia;
[3]Novosibirsk State Technical University, Russia;
[4]Karaganda Economic University of Kazpotrebsoyuz, Kazakhstan
(E-mail: kalytka@mail.ru)

The scheme of numerical optimization of the parameters of electrophysical processings in heterogeneuos solid elements

Describing the conceptual basis of universal mathematical model of the nonlinear physical processes in heterogeneous systems (bodies) perturbed by field and temperature influences. Determined the main directions of practical application (in the future) constructed upon based this model method for software and hardware. As an example, describing the algorithm of numerical calculation and optimization of the parameters of the relaxation processes during the polarization in compound dielectric lattice structure (in particular in proton semiconductors and dielectrics (PSCD)) with the help of minimizing comparison function method (MCF) of theoretical and experimental results. The basis of the MCF-method is necessary for the numerical comparison maxima points calculated by the formulas of the existing theory of proton relaxation and measured in the experiment.

Keywords: mathematical model of non-linear processes, elements of technologies schemas, proton semiconductors and dielectrics (PSCD), minimizing comparison function method (MCF- method).

Introduction

In the last decade, intensive development of computing, digital equipment and software and hardware has contributed to a significant improvement in numerical methods for solving equations of mathematical and theoretical physics, methods for statistical processing of laboratory results and experiments, methods for comparative numerical analysis of the degree of accuracy of the theory with respect to experiment and methods of computer prediction results of experiments [1-6].

The method of minimizing the comparison function (MFS method) used in the mathematical modeling of various physical processes that occur in heterogeneous physical systems evolving in time under the influence of various field factors is effective from the point of view of optimizing the computational process, the method of comparing the results of experimental and theoretical studies. MFS – is the method that has become quite widespread in various fields of science and technology. It remains relevant in the numerical optimization of the operation parameters of technological schemes of various information and communication systems and industrial installations confirmed by a number of recent works [1-12].

In [1] the method of minimizing the time of idle of user processes during their migration in «cloud hosting» is considered. Implementation of this method is carried out by: predicting the time of stopping processes; reduce the amount of RAM used during migration [1].

In [2] the question of using the method of modified Lagrangian functions (MPF) for numerical optimization of processes, with allowance for holonomic constraints in mechanical systems, is investigated. The development of methods for accounting for additional geometric and kinematic relationships makes it possi-

ble to significantly expand the methods of numerical optimization of processes in mechanical systems with a «tree» type structure on structures with kinematic constraints [2]. The method of MPL, used in computer optimization [3-6] of manufacturing technologies for various parts and in the assembly of machines and mechanisms, finds its application in various areas of the modern electrical engineering industry and in engineering [7-9].

In [10] modification of methods for calculating the flow velocity field was performed, using the example of solving problems associated with cavitation. In the course of research, existing methods have been improved and new methods of numerical calculation and detection of air bubbles in liquids have been developed from images [11].

The developed algorithms for calculating flow parameters [11,12] are relevant in the numerical optimization of technological schemes of hydraulic installations and electrical installations, when designing in the field of turbine construction, shipbuilding, rocket building, etc.

1. Statement of the research task

The central idea of this work is to develop the theoretical foundations of a universal physical and mathematical model, based on the computer program algorithm (or a set of programs), that allows to perform efficient, with a high degree of accuracy, numerical calculations of parameters of physically interrelated time-evolving nonlinear physical systems under the action various force fields (external, local) and heat fluxes. This type of model system, by its properties and structure, is approximated to the functional elements that are part of the technological schemes of various power plants and systems operating under real production conditions.

The aim of the work is to develop generalized methods of mathematical modeling and numerical optimization of nonlinear physical processes occurring in dissimilar deformable electrically conductive and heat-conducting functional elements (structural and instrumental) of technological circuits of equipment which operate under varying conditions (variable field strengths, temperature).

The methodology of the investigation is based on the MCF method, which, in combination with numerical methods of investigating the properties of functions of many variables [13], establishes the optimal mathematical correspondence between the theoretical (calculated) and experimental values of the characteristic parameters of the physical model. In this article, the special case of a generalized physico-mathematical model of nonlinear processes is considered. This model leads to the polarization of layered dielectric structures (the object of investigation), as an example of crystals with hydrogen bonds (CHB), classified according to electrophysical properties as proton semiconductors and dielectric (SCD) [14].

Theoretical studies of non-linear effects in quantum polarization in SCD in the region of low (70-100 K) and ultralow (1-10 K) temperatures were performed in [15,16]. The mathematical model of nonlinear volume-charge polarization in the region of high (250-550 K) and superhigh (550-1500 K) temperatures is constructed in [17, 18]. However, in [15-18], the theoretical foundations, algorithm and methods of computer programming on the equations of the mathematical model are not affected. In [19-21], the methodology of constructing the program algorithm, with the help of the MCF method, is not considered in detail.

2. Construction and analysis of the comparison function between theory and experiment

A mathematical description of the relaxation polarization in materials of the SCD class (or CHB) makes it possible to construct theoretical temperature spectra of the current density of thermally stimulated depolarization (TSTD) - $J_{TCDP}(T)$ and frequency-temperature spectra of the dielectric loss angle tangent $tg\,\delta(\omega;T)$, due to the contribution of only one type of relaxator [14]. The application of the kinetic theory [14-18, 20] to the calculation of spectra $J_{\mathrm{TCDP}}(\mathrm{T})$ и $\mathrm{tg}\delta(\omega;\mathrm{T})$ is effective only in a neighborhood (on the set of points of the continuum measure) of the experimentally observed maximum. The unity of analytical research and numerical calculations allows one to get an idea of the nature of the course of the relaxation process, the parameters of which are: U_0- the activation energy of particles (protons) on a hydrogen bond (in a given physical model U_0- height of the potential barrier); ν_0- linear frequency of natural oscillations of particles (protons) in a potential well; n_0- equilibrium particle concentration; $a-$ lattice parameter [14,17,18].

Calculations of theoretical spectra $J_{TCDP}(T)$ and $tg\,\delta(\omega;T)$ is performed for a single relaxation time [14,17-19,21]. Position of the maximum of the function $J_{TCDP}(T)$ on the temperature axis of the crystal is

determined by the point $\left(T_{\max};J_{TCDP,\max}\right)$ in the space of characteristics of a monorelaylation process $\left\{\zeta_0=\left(U_0;\nu_0;n_0;a\right);T\right\}$ [21]. Position of function maxima $tg\,\delta^{(\omega_{pol})}(T)$ и $tg\,\delta^{(T_{pol})}(\omega)$ on the temperature axis T (or frequencies ω) is defined by $\left(T_{\max};tg\,\delta_{\max}^{(\omega_{pol})}\right)$, or $\left(\omega_{\max};tg\,\delta_{\max}^{(T_{pol})}\right)$, in space $\{\zeta_0;T\}$, $\{\zeta_0;\omega\}$. Measurements of temperature spectra $tg\,\delta^{(\omega_{pol})}(T)$ are carried out at a constant frequency of the polarizing field ω_{pol}, and the frequency spectra $tg\,\delta^{(T_{pol})}(\omega)$ at a constant temperature T_{pol} [21].

Motion of depicting points $\{\zeta_0;T\}$, $\{\zeta_0;\omega\}$ in the space of the characteristics of the process leads to a change in the theoretical value of the relaxation time, and hence to the shift of the maximum points $\left(T_{\max};J_{TCDP,\max}\right)$, $\left(T_{\max};tg\,\delta_{\max}^{(\omega_{pol})}\right)$, $\left(\omega_{\max};tg\,\delta_{\max}^{(T_{pol})}\right)$ along the abscissa axis, and also to changes in the amplitudes of the maxima [21].

The function of comparing theory and experiment can be represented in the form [14]

$$\Psi\left(\vec{\zeta}\right)=\left[\Theta_{th}\left(\vec{\zeta}\right)-\Theta_{\exp}\right]^2, \tag{1}$$

where $\vec{\zeta}=\left\{U_{0,th};\nu_{0,th};n_{0,th};a_{th}\right\}$ — a multidimensional radius vector constructed in the space of theoretical values of the molecular characteristics (parameters) of the process under study [21]; $\Theta_{th}\left(\vec{\zeta}\right)$ — abscissa, corresponding to the position of the theoretical maximum on the graph, which is established by calculation; $\Theta_{\exp}$ — abscissa, corresponding to the position of the experimental maximum in the graph, which is established as a result of precision measurements.

According to (1) comparison function $\Psi\left(\vec{\zeta}\right)$ can not be negative.

Abscissa $\Theta_{\exp}$ is modeled either as the material temperature $T_{\max,\exp}$, or as the frequency of the perturbing alternating external field (electric, magnetic, electromagnetic, etc.) — $\omega_{\max,\exp}$, corresponding to the monorelaxation maximum measured in the experiment of the physical characteristics of the process.

Abscissa $\Theta_{th}\left(\vec{\zeta}\right)$ is established as a result of research on the maximum of the mathematical expression describing the theoretical monorelaxation spectrum. This expression is constructed analytically, by solving the corresponding system of differential equations [15-21], and calculating the abscissa $\Theta_{\text{th}}\left(\vec{\zeta}\right)$, in essence, reduces to the establishment of functional dependencies of the form:

$$\Lambda^{(\omega_{pol})}\left(\vec{\zeta}_{\max}\right)\equiv T_{\max,th}^{\left[tg\,\delta_{\text{th}}^{(\omega_{pol})}\left(T;\vec{\zeta}\right)\right]}\left(U_{0,\text{th},\max};\nu_{0,\text{th},\max};n_{0,\text{th},\max};a_{\text{th},\max}\right); \tag{2.1}$$

$$\Gamma^{(T_{pol})}\left(\vec{\zeta}_{\max}\right)\equiv \omega_{\max,th}^{\left[tg\,\delta_{\text{th}}^{(T_{pol})}\left(\omega;\vec{\zeta}\right)\right]}\left(U_{0,\text{th},\max};\nu_{0,\text{th},\max};n_{0,\text{th},\max};a_{\text{th},\max}\right); \tag{2.2}$$

$$\Omega\left(\vec{\zeta}_{\max}\right)\equiv T_{\max,th}^{\left[J_{\text{TCDP,th}}\left(T;\vec{\zeta}\right)\right]}\left(U_{0,\text{th},\max};\nu_{0,\text{th},\max};n_{0,\text{ th, max}};a_{\text{ th, max}}\right). \tag{2.3}$$

In (2.1)–(2.3) $\Lambda^{(\omega_{pol})}\left(\vec{\zeta}_{\max}\right)$ — calculated in the space of critical parameter values $\vec{\zeta}_{\max}=\left\{U_{0,\text{th},\max};\nu_{0,\text{th},\max};n_{0,\text{th},\max};a_{\text{th},\max}\right\}$ at a constant field frequency ω_{pol} theoretical value of the maximum temperature of the function $tg\delta^{(\omega_{pol})}{}_{th}(\text{T};\vec{\zeta})$, calculated; $\Gamma^{(T_{pol})}\left(\vec{\zeta}_{\max}\right)$ — calculated in the space of critical parameter values $\vec{\zeta}_{\max}$ at a constant temperature T_{pol} theoretical value of the maximum of the function

$tg\delta^{(T_{pol})}{}_{th}(\omega;\vec{\zeta})$; $\Omega\left(\vec{\zeta}_{\max}\right)$ — theoretical value of the maximum temperature of the function $J_{TCDP,TH}(\mathrm{T};\vec{\zeta})$ with the appropriate set of parameters $\vec{\zeta}_{\max}$.

Large mathematical awkwardness of functions $tg\delta^{(\omega_{pol})}{}_{th}(T;\vec{\zeta})$, $tg\delta^{(T_{pol})}{}_{th}(\omega;\vec{\zeta})$, $J_{TCDP,\mathrm{th}}(\mathrm{T};\vec{\zeta})$ does not allow for an analytical definition of functions $\Lambda^{(\omega_{pol})}\left(\vec{\zeta}_{\max}\right)$, $\Gamma^{(T_{pol})}\left(\vec{\zeta}_{\max}\right)$, $\Omega\left(\vec{\zeta}_{\max}\right)$, they must be obtained as a result of numerical calculations of the dependences (2.1)–(2.3). In this way, $\Theta_{th}\left(\vec{\zeta}\right)$ establishes a correspondence between the temperatures or frequencies at which the maximum in the theory appears and the position of the representative point in the space of characteristics. Neglect of the temperature dependence of the characteristics $\vec{\zeta}=\left\{U_{0,\mathrm{th}};\nu_{0,\mathrm{th}};n_{0,\mathrm{th}};a_{\mathrm{th}}\right\}$ in the vicinity of the experimental maximum, which facilitates the minimization of the function of comparing the theory with experiment. In this case, denoting $\Phi_1\left(T;\vec{\zeta}\right)=tg\,\delta_{th}^{(\omega_{pol})}\left(T;\vec{\zeta}\right)$, $\Phi_2\left(\omega;\vec{\zeta}\right)=tg\,\delta_{th}^{(T_{pol})}\left(\omega;\vec{\zeta}\right)$, $\Phi_3\left(T;\vec{\zeta}\right)=J_{TCDP,th}\left(T;\vec{\zeta}\right)$, write the system of equations

$$\frac{\partial\Phi_1\left(T;\vec{\zeta}\right)}{\partial\vec{\zeta}_i}=0 \;\Leftrightarrow\; \phi_{1i}\left(T_{\max,th};\vec{\zeta}_{\max}\right)=0, \tag{3.1}$$

$$\frac{\partial\Phi_2\left(\omega;\vec{\zeta}\right)}{\partial\vec{\zeta}_{\mathrm{j}}}=0 \;\Leftrightarrow\; \phi_{2\,\mathrm{j}}\left(\omega_{\max,\mathrm{th}};\vec{\zeta}_{\max}\right)=0, \tag{3.2}$$

$$\frac{\partial\Phi_3\left(\mathrm{T};\vec{\zeta}\right)}{\partial\vec{\zeta}_{\mathrm{k}}}=0 \;\Leftrightarrow\; \phi_{3\mathrm{k}}\left(\mathrm{T}_{\max,\mathrm{th}};\vec{\zeta}_{\max}\right)=0, \tag{3.3}$$

where the indices with the corresponding variables $\vec{\zeta}_{\mathrm{i}}$, $\vec{\zeta}_{\mathrm{j}}$, $\vec{\zeta}_{\mathrm{k}}$, take values from 1 to 5. Then, from the systems of equations (3.1)–(3.3) functions that allow one to express each of the parameters from a set of critical values $\vec{\zeta}_{\max}=\left\{\mathrm{U}_{0,\mathrm{th},\max};\nu_{0,\mathrm{th},\max};n_{0,\mathrm{th},\max};a_{\mathrm{th},\max}\right\}$, including T, or ω, can be expressed in terms of all other parameters of the set $\vec{\zeta}_{\max}$ (including T, or ω) at the points of the theoretical maxima of the corresponding functions $\Phi_1\left(\mathrm{T};\vec{\zeta}\right)$, $\Phi_2\left(\omega;\vec{\zeta}\right)$, $\Phi_3\left(\mathrm{T};\vec{\zeta}\right)$. Then, from (3.1)–(3.3) functional dependences

$$\mathrm{T}_{\max,\mathrm{th}}^{\left[\Phi_1\left(\mathrm{T};\vec{\zeta}\right)\right]}=g_{11}\left(\vec{\zeta}_{\max}\right),\ \omega_{\max,\mathrm{th}}^{\left[\Phi_2\left(\omega;\vec{\zeta}\right)\right]}=g_{21}\left(\vec{\zeta}_{\max}\right),\ T_{\max,th}^{\left[\Phi_3\left(T;\vec{\zeta}\right)\right]}=g_{31}\left(\vec{\zeta}_{\max}\right), \tag{4}$$

using numerical methods [13], to calculate the initial dependences (2.1) - (2.3) and, on this basis, proceed to the calculation of the corresponding comparison functions

$$\Psi_1\left(\vec{\zeta}\right)=\left[\mathrm{T}_{\max,\mathrm{th}}^{\left[\Phi_1\left(\mathrm{T};\vec{\zeta}\right)\right]}-\mathrm{T}_{\max,\mathrm{exp}}^{\mathrm{tg}\delta_{\mathrm{exp}}^{(\omega_{pol})}}\right]^2,\ \Psi_2\left(\vec{\zeta}\right)=\left[\omega_{\max,\mathrm{th}}^{\left[\Phi_2\left(\omega;\vec{\zeta}\right)\right]}-\omega_{\max,\mathrm{exp}}^{\mathrm{tg}\delta_{\mathrm{exp}}^{(T_{pol})}}\right]^2,\ \Psi_3\left(\vec{\zeta}\right)=\left[\mathrm{T}_{\max,\mathrm{th}}^{\left[\Phi_3\left(\mathrm{T};\vec{\zeta}\right)\right]}-\mathrm{T}_{\max,\mathrm{exp}}^{J_{\mathrm{TCTД,exp}}}\right]^2. \tag{5}$$

The procedure for minimizing the functions (5), using formulas

$$\frac{\partial\Psi_1\left(\vec{\zeta}\right)}{\partial\left(\vec{\zeta}_{\mathrm{i,max}}\right)}=\frac{\partial}{\partial\left(\vec{\zeta}_{\mathrm{i,max}}\right)}\left[g_{11}\left(\vec{\zeta}_{\max}\right)-\mathrm{T}_{\max,\mathrm{exp}}\right]^2=2\left[g_{11}\left(\vec{\zeta}_{\max}\right)-\mathrm{T}_{\max,\mathrm{exp}}\right]\cdot\frac{\partial g_{11}\left(\vec{\zeta}_{\max}\right)}{\partial\left(\vec{\zeta}_{\mathrm{i,max}}\right)}=0, \tag{6.1}$$

$$\frac{\partial\Psi_2\left(\vec{\zeta}\right)}{\partial\left(\vec{\zeta}_{\mathrm{i,max}}\right)}=\frac{\partial}{\partial\left(\vec{\zeta}_{\mathrm{i,max}}\right)}\left[g_{21}\left(\vec{\zeta}_{\max}\right)-\omega_{\max,\mathrm{exp}}\right]^2=2\left[g_{21}\left(\vec{\zeta}_{\max}\right)-\omega_{\max,\mathrm{exp}}\right]\cdot\frac{\partial g_{21}\left(\vec{\zeta}_{\max}\right)}{\partial\left(\vec{\zeta}_{\mathrm{i,max}}\right)}=0, \tag{6.2}$$

$$\frac{\partial\Psi_3\left(\vec{\zeta}\right)}{\partial\left(\vec{\zeta}_{\mathrm{i,max}}\right)}=\frac{\partial}{\partial\left(\vec{\zeta}_{\mathrm{i,max}}\right)}\left[g_{31}\left(\vec{\zeta}_{\max}\right)-\mathrm{T}_{\max,\mathrm{exp}}\right]^2=2\left[g_{31}\left(\vec{\zeta}_{\max}\right)-\mathrm{T}_{\max,\mathrm{exp}}\right]\cdot\frac{\partial g_{31}\left(\vec{\zeta}_{\max}\right)}{\partial\left(\vec{\zeta}_{\mathrm{i,max}}\right)}=0, \tag{6.3}$$

allows us to write down the optimized values of the parameters (4), each of which corresponds to certain sets *l,m,n* corresponding points $\left(\vec{\zeta}_{\max;\mathrm{opt},l}\right)$, $\left(\vec{\zeta}_{\max;\mathrm{opt},m}\right)$, $\left(\vec{\zeta}_{\max;\mathrm{opt},n}\right)$, one of which $\vec{\zeta}_{\max;\mathrm{opt,l}}=\left\{\mathrm{U}_{0,\mathrm{th},\max;\mathrm{opt,l}};\nu_{0,\mathrm{th},\max;\mathrm{opt,l}};n_{0,\mathrm{th},\max;\mathrm{opt,l}};a_{\mathrm{th},\max;\mathrm{opt,l}}\right\}$, for each function (4), is the experimental max-

imum point $T^{\left[\Phi_1\left(T;\vec{\zeta}\right)\right]}_{(\max,th);opt,1} = g_{11}\left(\vec{\zeta}_{\max;opt,1}\right) = T^{tg\delta\left(\omega_{pol}\right)}_{exp}_{max,exp}$, $\omega^{\left[\Phi_2\left(\omega;\vec{\zeta}\right)\right]}_{(\max,th);opt,1} = g_{21}\left(\vec{\zeta}_{\max;opt,1}\right) = \omega^{tg\delta\left(T_{pol}\right)}_{exp}_{max,exp}$, $T^{\left[\Phi_3\left(T;\vec{\zeta}\right)\right]}_{(\max,th);opt,1} = g_{31}\left(\vec{\zeta}_{\max;opt,1}\right) = T^{J_{TCDP,exp}}_{max,exp}$, and all other points correspond to all possible ones distributed near the experimental values $T^{tg\delta\left(\omega_{pol}\right)}_{exp}_{max,exp}$, $\omega^{tg\delta\left(T_{pol}\right)}_{exp}_{max,exp}$, $T^{J_{TCDP,exp}}_{max,exp}$ optimized theoretical values of the parameters $T^{\left[\Phi_1\left(T;\vec{\zeta}\right)\right]}_{(\max,th);opt,l} = g_{11}\left(\vec{\zeta}_{\max;opt,l}\right)$, $\omega^{\left[\Phi_2\left(\omega;\vec{\zeta}\right)\right]}_{(\max,th);opt,m} = g_{21}\left(\vec{\zeta}_{\max;opt,m}\right)$, $T^{\left[\Phi_3\left(T;\vec{\zeta}\right)\right]}_{(\max,th);opt,n} = g_{31}\left(\vec{\zeta}_{\max;opt,n}\right)$. These values are calculated from equations

$$\frac{\partial g_{11}\left(\vec{\zeta}_{\max;opt,l}\right)}{\partial\left(\vec{\zeta}_{i,\max}\right)} = 0,\ \frac{\partial g_{21}\left(\vec{\zeta}_{\max;opt,m}\right)}{\partial\left(\vec{\zeta}_{i,\max}\right)} = 0,\ \frac{\partial g_{31}\left(\vec{\zeta}_{\max;opt,n}\right)}{\partial\left(\vec{\zeta}_{i,\max}\right)} = 0.$$

The comparison functions (5) have in the space of characteristics $\vec{\zeta}_{\max}$ complex relief. Some characteristics vary in small limits, for example, the activation energy is selected from the interval (0.05, 0.7) eV, while the equilibrium concentration of relaxators during the motion of the theoretical maximum along the temperature axis can vary by several orders of magnitude. This leads to the fact that the relief of the comparison function is a multidimensional complex tortuous and very narrow ravine containing a large number of minima. Computationally simple methods have been developed in computational mathematics that allow one to pass along a ravine and to leave in a hollow of a minimum, but these methods of calculation are capricious, and the algorithm for passing along the ravine contains a number of non-formalizable corrections that must be introduced into the program straight down the course of calculations [13, 22, 23]. The speed of movement along the ravine is very small. The effectiveness of the search for a minimum of the comparison function with such a relief depends very much on how successfully the zero approximation for the characteristics was selected. It is convenient to change the scale using double logarithms for different reasons. Successful selection of the bases of logarithms reduces the computation time. The selection of the bases is influenced by the selection of the zeroth approximation. Great help is provided by an exact experiment.

Conclusions

1. The scientific and practical importance of methods for numerical optimization of nonlinear physical processes occurring in technological circuits of power equipment which operates under extreme conditions (strong fields, ultra-low temperatures, ultra-low and superhigh frequencies, etc.) is substantiated. Conceptual bases of the universal physical and mathematical model of nonlinear processes of various nature are formulated.

2. As an example, the algorithm for minimizing the comparison function (MCF) is described for comparing the results of the theory and experiment at the study of nonlinear relaxation polarization in proton semiconductors and dielectrics (SCD). On this basis had elaborated scheme of a numerical optimization for the parameters of the relaxation process (including temperature and frequency of an alternating electric field) in the SCD is carried out.

3. The peculiarities of the work of the numerical calculation program based on the algorithm of the MCF method with respect to the analysis of the parameters of the current spectra and dielectric losses in the CHB are revealed. The possibilities of extending the range of variation of variable parameters (frequency and amplitude of the field, temperature) of the process at the application of the MCF method for numerical study of a wider range of nonlinear processes (magnetic, optical, mechanical, thermal, etc.) in dissimilar functional elements of process units and systems are defined.

References

1 Тихомиров П.О. Минимизация времени простоя процессов при их миграции в облачном хостинге / П.О. Тихомиров, П.В. Емельянов, Н.С. Плотник, А.В. Зырянов // Вестн. НГУ. Сер. Информационные технологии. — 2014. — Т. 12. — № 4. — С. 112–120.

2 Иванов В.Н. Численные методы исследования механических систем с дополнительными связями / В.Н. Иванов // Вестн. Пермского ун-та. Сер. Математика. Механика. Информатика. — 2015. — Т. 31. — № 4. — С. 16–27.

3 Shabana A.A. Computational Dynamics / A.A. Shabana. — New-York: Wiley, 2001.

4 Wittenburg J. Dynamics of Multibody Systems / J. Wittenburg. — Berlin: Springer – Verlag, 2008.

5 Nocedal J. Numerical Optimization / J. Nocedal, S.J. Wright. — Berlin: Springer, 2006.

6 Солодушкин А.И. Модифицированный алгоритм расчета поля векторов смещений для оценки деформации / А.И. Солодушкин, В.В. Кибиткин, В.С. Плешанов // Известия Томского политехн. ун-та. Сер. Управление, вычислительная техника и информатика. — 2011. — Т. 318. — № 5. — С. 48–51.

7 Хуснулина А.Л. Автоматизированная система сбора и визуализации технологических данных в производстве полупроводниковых приборов / А.Л. Хуснулина, О.Б. Воскобойникова // Вестн. НГУ. Сер. Информационные технологии. — 2017. — Т. 15. — Вып. № 3. — С. 100–110. — DOI 10.25205/1818–7900–2017–15–3–100–110. – ISSN 1818–7900.

8 Кротов К.В. Градиентный метод формирования динамических расписаний обработки данных в конвейерной системе при различных моментах времени их поступления / К.В. Кротов // Вестн. НГУ. Сер. Информационные технологии. — 2016. — Т. 14. — Вып. № 1. — С. 39–60.

9 Аймагамбетова Р.Ж. Оценка качества процессов напыления слоев полупроводниковых материалов в производстве электронных изделий с помощью кластеризации методом k-средних / Р.Ж. Аймагамбетова, О.В. Стукач // Современные методы оценки и оборудование в металловедении: тр. Междунар. науч.-практ. конф. — Караганда: Изд. КарГТУ, 2015. — С. 50–51.

10 Карчевский М.Н. Алгоритмы распознавания и слежения за пузырями для измерения параметров кавитации на гидрокрыле / М.Н. Карчевский, И.Е. Полетаев, Г.С. Сухоруков // Вестн. НГУ. Сер. Информационные технологии. — 2016. — Т. 14. — Вып. № 1. — С. 23–38.

11 Панин М.П. Моделирование переноса излучения / М.П. Панин. — М.: МИФИ, 2008. — 212 с.

12 Скарано Ф. Обзор PIV в сверхзвуковых потоках / Ф. Скарано // PIV. — Берлин: Гейельберг: Спрингер, 2008.

13 Калиткин Н.Н. Численные методы / Н.Н. Калиткин. — М.: Наука. 1978. — 512 с.

14 Калытка В.А. Протонная проводимость: монография [Электронный ресурс] / В.А. Калытка, М.В. Коровкин. — Germany. Издат. дом: LAP LAMBERT Academic Publishing, 2015. — 180 с. — Режим доступа: http://www.lap–publishing.com.

15 Kalytka V.A. Quantum effects at a proton relaxation at low temperatures / V.A. Kalytka, M.V. Korovkin // Russian Physics Journal. — 2016, November. — Vol. 59. — No. 7. — P. 994–1001. DOI: 10.1007/s11182–016–0865–x.

16 Калытка В.А. Зонная структура энергетического спектра и волновые функции протона в диэлектриках с протонной проводимостью / В.А. Калытка, А.И. Алиферов, З.К. Баймуханов, А.Д. Мехтиев // Доклады Академии наук высш. шк. Российской Федерации. — 2017. — № 2 (35). — С. 18–31. DOI: 10.17212/1727–2769–2017–2–18–31.

17 Kalytka V.A. Dispersion relations for proton relaxation in solid dielectrics / V.A. Kalytka, M.V. Korovkin // Russian Physics Journal. — April, 2017. — Vol. 59. — No. 12. — P. 2151–2161. DOI: 10.1007/s11182–017–1027–5.

18 Калытка В.А. Нелинейные эффекты при поляризации диэлектриков со сложной кристаллической структурой / В.А.Калытка, З.К. Баймуханов, А.Д. Мехтиев // Доклады Академии наук высш. шк. Российской Федерации. — 2016. — № 3(32). — С. 7–21. DOI: 10.17212/1727–2769–2016–3–7–21.

19 Калытка В.А., Никонова Т.Ю. Нелинейные электрофизические свойства протонных полупроводников и диэлектриков // Актуальные проблемы электронного приборостроения: тр. XIII Междунар. науч.-практ. конф. (АПЭП – 2016) (3–6 октября 2016 г.). — Т. 2. Электронно-физическая секция. — Новосибирск, 2016. — С. 57–65.

20 Тонконогов М.П. Термодеполяризационный способ определения параметров и концентрации дефектов структуры в кристаллах с водородными связями / М.П. Тонконогов, Ж.Т. Исмаилов, К.К. Фазылов // Предпатент № 36703. 7 G01N 27/00. - Промышленная собственность. Официальный бюллетень: Минюст РК. — 2003. — № 6. — С. 87.

21 Annenkov Yu. M. Quantum effects under migratory polarization in nanometer layers of proton semiconductors and dielectrics at ultralow temperatures / Yu.M. Annenkov, V.A. Kalytka, M.V. Korovkin // Russian Physics Journal. — 2015. — Vol. 58. — No. 1. — P. 35–41. DOI: 10.1007/s11182–015–0459–z.

22 Сырямкин В.И. Автоматическое программное обеспечение для автоматизации расчёта микротвёрдости материалов / В.И. Сырямкин, А.В. Чесноков, Д.В. Коваль // Известия высших учебных заведений. Физика. — 2001. — № 11. — С. 78–82.

23 Сырямкин В.И. Метод измерения рельефа поверхности для исследования процессов деформации и оценки состояния нагруженных материалов / В.И. Сырямкин, С.В. Панин, Н.А. Зуев, А.В. Чесноков // Известия высших учебных заведений. Физика. — 2001. — № 11. — С. 83–88.

В.А. Калытка, М.В. Коровкин, А.И. Алиферов, А.В. Баширов, Д.Р. Таласпеков

Әртүрлі қатты денелі элементтердің электрфизикалық процестері сандық көрсеткіштерінің оңтайлы сұлбасы

Сызықты емес физикалық процестердің өріс және температура әсеріне ұшыраған әртүрлі жүйелердегі (денелердегі) әмбебап математикалық моделінің тұжырымдамалық негіздері сипатталған. Бағдарламалық және аппараттық қамтамасыз етудің осы моделіне негізделген практикалық қолданудың басты бағыттары анықталды. Мысал ретінде теория мен эксперименттің нәтижесін салыстыру функциясын азайту (СФА) әдісімен сандық есептеу алгоритмі мен күрделі кристалды торлы жартылай өткізгіштерді поляризациялау барысында релаксациондық процестердің параметрлерін оңтайландыру сипатталған. Атап айтқанда, протонды жартылайөткізгіштердің және диэлектриктердің СФА әдісінің негізінде протон релаксациясының қолданыстағы теориясының формулалары бойынша есептелген және экспериментте өлшенген максималды нүктелерді сандық салыстыру болып табылады.

Кілт сөздер: сызықтық емес процестердің математикалық моделі, технологиялық схемалардың элементтері, протон жартылайөткізгіштер және диэлектриктер, салыстыру функциясын азайту әдісі.

В.А. Калытка, М.В. Коровкин, А.И. Алиферов, А.В. Баширов, Д.Р. Таласпеков

Схема численной оптимизации параметров электрофизических процессов в разнородных твердотельных элементах

В статье описаны концептуальные основы универсальной математической модели нелинейных физических процессов в разнородных системах (телах), возмущенных полевыми и температурными воздействиями. Определены основные направления практического применения построенного (в перспективе) на основе данной модели программно-аппаратного обеспечения. В качестве примера описывается алгоритм численного расчета и оптимизации параметров релаксационных процессов при поляризации диэлектриков со сложной структурой кристаллической решетки (в частности, в протонных полупроводниках и диэлектриках (ППД)) методом минимизации функции сравнения (МФС) результатов теории и эксперимента. В основу метода МФС положено численное сопоставление точек максимумов, рассчитанных по формулам существующей теории протонной релаксации и измеренных в эксперименте.

Ключевые слова: математическая модель нелинейных процессов, элементы технологических схем, протонные полупроводники и диэлектрики (ППД), метод минимизации функции сравнения (МФС - метод).

References

1 Tikhomirov, P.O., Emelyanov, P.V., Plotnik, N.S., & Zyryanov, V. (2014). Minimizatsiia vremeni prostoia protsessov pri ikh mihratsii v oblachnom hostinhe [Minimization of downtime of processes during their migration in cloud hosting]. *Vestnik Novosibirskoho hosudarstvennoho universiteta. Seriia Informatsionnye tekhnolohii – Bulletin of Novosibirsk State University. Series: Information technology, Vol. 12,* 4, 112–120 [in Russian].

2 Ivanov, V.N. (2015). Chislennye metody issledovaniia mekhanicheskikh system s dopolnitelnymi sviaziami [Numerical methods for investigating of mechanical systems with additional constraints]. *Vestnik Permskoho universiteta. Seriia: Matematika. Mekhanika. Informatika – Bulletin of Perm University. Series: Mathematics. Mechanics. Computer science, Vol. 31,* 4, 16–27 [in Russian].

3 Shabana, A.A. (2001). *Computational Dynamics.* New-York: Wiley.

4 Wittenburg, J. (2008). Dynamics of Multibody Systems. Berlin: Springer – Verlag.

5 Nocedal, J., & Wright, S.J. (2006). Numerical Optimization. Berlin: Springer.

6 Solodushkin, A.I., Kibitkin, V.V., & Pleshanov, V.S. (2016). Modifitsirovannyi alhoritm rascheta polia vektorov smeshchenii dlia otsenki deformatsii [A modified algorithm for calculating the displacement field for deformation estimation]. *Izvestiia Tomskoho politekhnicheskoho universiteta. Seriia: Upravlenie, vychislitelnaia tekhnika i informatika – Proceedings of Tomsk Polytechnic University. Series: Management, Computer Science and Informatics, Vol. 318,* 5, 48–51 [in Russian].

7 Khusnulina, A.L., & Voskobovnikova, O.B., (2017). Avtomatizirovannaia sistema sbora i vizualizatsii tekhnolohicheskikh dannykh v proizvodstve poluprovodnikovykh priborov [Automated system of data acquisition and visualization in semiconductor devices production]. *Vestnik Novosibirskoho hosudarstvennoho universiteta. Seriia: Informatsionnye tekhnolohii – Bulletin of Novosibirsk State University. Series: Information technology, Volume 15*, 3, 100–110. DOI 10.25205 / 1818-7900-2017-15-3-100-110. - ISSN 1818-7900. [in Russian].

8 Krotov, K.V. (2016). Hradientnyi metod formirovaniia dinamicheskikh raspisanii obrabotki dannykh v konveernoi sisteme pri razlichnykh momentakh vremeni ikh postupleniia [Gradient method for the formation of dynamic schedules of data processing in the conveyor system at various times of their arrival]. *Vestnik Novosibirskoho hosudarstvennoho universiteta. Seriia: Informatsionnye tekhnolohii – Bulletin of Novosibirsk State University. Series: Information technology, Vol. 14,* 1, 39–60 [in Russian].

9 Aimagambetova, R.Zh., & Stukach, O.V. (2015). Otsenka kachestva protsessov napyleniia sloev poluprovodnikovykh materialov v proizvodstve elektronnykh izdelii s pomoshchiu klasterizatsii metodom k-srednikh [Evaluation of the quality of the processes of deposition of layers of semiconductor materials in the production of electronic products using k-means clustering]. Proceedings from Modern methods of assessment and equipment in metallurgy: *Mezhdunarodnaia nauchno-prakticheskaia konferentsiia – Proceedings of the International Scientific and Practical Conference* (pp. 50–51). Karaganda: Izdatelstvo KarHTU [in Russian].

10 Karchevsky, M.N., Poletaev, I.E., & Sukhorukov, G.S. (2016). Alhoritmy raspoznavaniia i slezheniia za puzyriami dlia izmereniia parametrov kavitatsii na hidrokryle [Algorithms for recognition and tracking of bubbles for measuring the parameters of cavitation at the hydrofoil]. *Vestnik Novosibirskoho hosudarstvennoho universiteta. Seriia: Informatsionnye tekhnolohii – Bulletin of Novosibirsk State University. Series: Information technology, Vol. 14,* 1, 23–38 [in Russian].

11 Panin, M.P. (2008). *Modelirovanie perenosa izlucheniia [Simulation of radiation transfer]*. Moscow: MIFI [in Russian].

12 Scarano, F. Obzor PIV v sverkhzvukovykh potokakh [Overview of PIV in supersonic flow]. PIV. Berlin: Heyelberg: Springer, 2008.

13 Kalitkin, N.N. (1978). *Chislennye metody [Numerical methods]*. Moscow: Nauka [in Russian].

14 Kalytka, V.A., & Korovkin, M.V. (2015). Protonnaia provodimost [Proton conductivity]. Germany: Izdatelskii dom «LAP LAMBERT Academic Publishing» Retrieved from http://www.lap-publishing.com [in Russian].

15 Kalytka, V.A., Korovkin, M.V. (2016). Quantum effects at a proton relaxation at low temperatures. *Russian Physics Journal, Vol. 59,* 7, November, 994–1001.

16 Kalytka, V.A., Aliferov, A.I., Baimukhanov, Z. K., & Mekhtiev, A.D. (2017). Zonnaia struktura enerheticheskoho spektra i volnovye funktsii protona v dielektrikakh s protonnoi provodimostiu [Zone structure of the energy spectrum and wave functions of proton in proton conductivity dielectrics]. *Doklady Akademii nauk vysshei shkoly Rossiiskoi Federatsii – Proceedings the Russian High School Academy of Sciences, 2 (35),*18–31. DOI: 10.17212/1727-2769-2017-2-18-31 [in Russian].

17 Kalytka, V.A., & Korovkin, M.V. (2017). Dispersion relations for proton relaxation in solid dielectrics. *Russian Physics Journal, Vol. 59,* 12, April, 2017, 2151–2161. DOI: 10.1007/s11182-017-1027-5.

18 Kalytka, V.A., Baimukhanov, Z.K., & Mekhtiev, A.D. (2016). Nelineinye effekty pri poliarizatsii dielektrikov so slozhnoi kristtallicheskoi strukturoi [Nonlinear effects under polarization of dielectrics with compound crystalline structure]. *Doklady Akademii nauk vysshei shkoly Rossiiskoi Federatsii – Proceedings the Russian High School Academy of Sciences, 3(32),* 7–21. DOI: 10.17212 / 1727-2769-2016-3-7-21 [in Russian].

19 Kalytka, V.A. & Nikonova, T.Yu. (2016). Nelineinye elektrofizicheskie svoistva protonnykh poluprovodnikov i dielektrikov [Nonlinear electrophysical properties of proton semiconductors and dielectrics]. Proceedings from On Actual Problems of Electronic Instrument Engineering (APEIE-2016): (APEP-2016): *XIII Mezhdunarodnaia nauchno-tekhnicheskaia konferentsiia (3–6 oktiabria, 2016 hoda) – XIII-th International Scientific-Technical Conference.* (pp. 57–65). Vol. 2. The electronic physical section. Novosibirsk [in Russian].

20 Tonkonogov, M.P., Ismailov, Zh.T., & Fazylov, K.K. (2003). Termodepoliarizatsionnyi sposob opredeleniia parametrov i kontsentratsii defektov struktury v kristallakh s vodorodnymi sviaziami [The thermodepolarization method for determining the parameters and concentration of structure defects in crystals with hydrogen bonds]. Predpatent No. 36703. 7 G01N 27/00. — Industrial property. Official Bulletin: Ministry of Justice of the Republic of Kazakhstan. No. 6, 87.

21 Annenkov, Yu. M., Kalytka, V.A., & Korovkin, M.V. (2015). Quantum effects under migratory polarization in nanometer layers of proton semiconductors and dielectrics at ultralow temperatures. *Russian Physics Journal, Vol. 58,* 1, May, 2015, 35–41. DOI: 10.1007/s11182-015-0459-z.

22 Syryamkin, V.I., Chesnokov, A.V., & Koval, D.V. (2001). Avtomaticheskoe prohrammnoe obespechenie dlia avtomatizatsii rascheta mikrotverdosti materialov [Automatic software for automation of calculation of microhardness of materials]. *Izvestiia vysshikh uchebnykh zavedenii. Fizika – Proceedings of Higher Educational Institutions. Physics, 11,* 78–82 [in Russian].

23 Syryamkin, V.I., Panin, S.V., Zuev, N.A., & Chesnokov, A.V. (2001). Metod izmereniia relefa poverkhnosti dlia issledovaniia protsessov deformatsii i otsenki sostoianiia nahruzhennykh materialov [Method for measuring the surface of the relief for studying of deformation processes and estimating of the state of loaded materials]. *Izvestiia vysshikh uchebnykh zavedenii. Fizika – Proceedings of Higher Educational Institutions. Physics, 11,* 83–88 [in Russian].