Numerical study of the optimal control problem for one model of potential distribution in a crystalline semiconductor with the Showalter–Sidorov condition

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Abstract. The paper considers a mathematical model of potentials optimal distribution in a crystalline semiconductor. This model is based on the problem of optimal control of weak generalized solutions of the mathematical model of the potential distribution in a crystalline semiconductor with the Showalter–Sidorov condition. The theoretical results obtained by us earlier made it possible to develop an algorithm for a numerical method for finding an approximate one by solutions of the optimal control problem for the problem under study, based on the methods of decomposition, Ritz, penalty and Galerkin’s projection method. The results of a computational experiment are presented.

At the present stage of development, application, as well as production of electronic computers, the study of the physics of semiconductors does not lose its relevance. Since carrying out field experiments is often difficult, mathematical modeling [1–4] plays an important role in the study of these processes. To study the processes occurring in semiconductor-type substances, analytical and numerical studies of mathematical models of potential distribution in a crystalline semiconductor [2], based on Sobolev type equations

\[(\lambda - \Delta)x_t - a_1 \Delta x - a_2 \text{div}(|\nabla x|^2 \nabla x) = u.\] (1)

The problem of potential distribution in a crystalline semiconductor is considered in [1,2]. This article researches the potential distribution in a semiconductor system. From a mathematical point of view, a semiconductor system is understood as a geometric graph. An important practical problem in numerical modelling of processes is the study of the rational state of the system, as well as finding the optimal control law for these systems [5–7], because such processes can be affected by changes in the parameters of the external environment (for example, the value magnetic field), as well as the internal environment (for example, temperature, chemical composition of a semiconductor). To implement the problem of process control in semiconductors, various mathematical, algorithmic and software tools are being developed. One of the variants of the algorithm of the numerical method for studying the control of such processes is presented in this article. This algorithm is based on the reduction of the initial-boundary value problem for the equation (1) in specially describe functional Banach spaces $\mathcal{X}$ and $\mathcal{U}$ to the Showalter–Sidorov problem

\[L(x(0) - x_0) = 0\] (2)
for a semilinear Sobolev type equation

$$L\dot{x} + Mx + N(x) = u.$$  \hfill (3)

Here $L \in \mathcal{L}(X, X^*)$, $N$ is nonlinear operator. We also note that the use of the initial Showalter–Sidorov condition in numerical studies of applied problems allows us to remove the restrictions on the system in the case of the Cauchy condition. Both problems, depending on the research methods, can be understood in various senses (classical, generalized, weakened, strong, etc.), however, it is obvious that the Showalter–Sidorov problem is more general than Cauchy. In the trivial case (existence of an inverse operator $L$) both problems coincide, which means that their solutions also coincide [8–10].

The purpose of this work is to study a mathematical model of optimal regulation of the potential distribution in a crystalline semiconductor, which is based on the optimal control problem

$$J(x, u) \rightarrow \inf.$$  \hfill (4)

weak generalized solutions of the problem (2), (3). Here $J(x, u)$ is some specially constructed quality target functional; control $u \in U_{ad}$, where $U_{ad}$ is some closed and convex set in the control space $\mathcal{U}$. Optimal control of solutions to the initial-boundary value problem for the equation (1) allows you to adjust the potential difference in the system of crystalline semiconductors with the lowest control costs.

1. Analytical study of the optimal control problem

Let $G = G(V, E)$ is final connected directed graph, $V = \{V_i\}$ are vertex set, but $E = \{E_j\}$ edge set where each edge $E_j$ is of length $l_j \in \mathbb{R}_+$ and and transverse cross-section area $d_j \in \mathbb{R}_+$. On the graph $G$ consider the equations

$$\lambda x_{jt} - x_{jsts} - a_1 x_{jss} - a_2 (|x_{js}|^2 x_{js})_s = u_j, \quad s \in (0, l_j), \quad t \in (0, T).$$  \hfill (5)

For the equation (5) at each vertex $V_i$ set the conditions

$$\sum_{j: E_j \in E^\alpha(V_i)} d_j x_{js}(0, t) - \sum_{k: E_k \in E^\omega(V_i)} d_k x_{ks}(l_k, t) = 0;$$  \hfill (6)

$$x_n(0, t) = x_j(0, t) = x_k(l_k, t) = x_m(l_m, t),$$  \hfill (7)

for all $E_n, E_j \in E^\alpha(V_i), E_k, E_m \in E^\omega(V_i)$,

which are analogous to Kirchhoff’s laws. Here through $E^{\alpha, \omega}(V_i)$ denotes the set of arcs with the origin (end) at the top $V_i$. The condition (6) means that the stream through each vertex must equal zero, and the condition (7) that the solution at each vertex must be continuous. If we supplement (6), (7) with the initial condition

$$\lambda x_{jt}(s, 0) - x_{jsts}(s, 0) = x_{j0}(s) \text{ for all } s \in (0, l_j),$$  \hfill (8)

then we obtain the Showalter–Sidorov initial-boundary value problem for the equations (5).

To reduce problem (5) – (8) to problem (2) for a semilinear Sobolev type equation (3) in terms of $L_2(G)$ denote the sets

$$L_p(G) = \{g = (g_1, g_2, \ldots, g_j, \ldots) : g_j \in L_p(0, l_j)\}.$$
Space $\mathcal{H} = L_2(G)$ is Hilbert with scalar product

$$\langle g, h \rangle = \sum_{j \in E} d_j \int_0^{l_j} g_j(s)h_j(s) \, ds.$$ 

By $\mathfrak{B}$ we denote the set

$$\mathcal{W}_2^1(G) = \{ x = (x_1, x_2, \ldots, x_j, \ldots) : x_j \in W_2^1(0, l_j) \text{ and done (7)} \}.$$ 

The set $\mathfrak{B}$ is a Banach space in which the norm can be introduced as follows

$$\|x\|_{\mathfrak{B}} = \left( \sum_{j \in E} d_j \int_0^{l_j} (x_j^2 + x_j^2) \, ds \right)^{\frac{1}{2}}.$$ 

By the Sobolev embedding theorem, the space $\mathcal{W}_2^1(G)$ consists of absolutely continuous functions, and so $\mathfrak{B}$ is well-defined, dense, and compactly embedded into $L_2(G)$. Fix $a > 0$ and construct the operator

$$\langle Ag, h \rangle = \sum_{j \in E} d_j \int_0^{l_j} (g_j(s)h_j(s) + ag_j(s)h_j(s)) \, ds, \quad g, h \in \mathfrak{B}.$$ 

By $\mathfrak{N}$ we denote the set

$$\mathcal{W}_4^1(G) = \{ x = (x_1, x_2, \ldots, x_j, \ldots) : x_j \in W_4^1(0, l_j) \text{ and done (7)} \}.$$ 

By $\mathfrak{B}^*$ and $\mathfrak{N}^*$ denote the dual spaces to $\mathfrak{B}$ and $\mathfrak{N}$, with respect to scalar product $\langle \cdot, \cdot \rangle$ in $\mathcal{H}$, respectively. By the Sobolev theorem, there are dense and continuous embedding

$$\mathfrak{N} \hookrightarrow \mathfrak{B} \hookrightarrow \mathcal{H} \hookrightarrow \mathfrak{B}^* \hookrightarrow \mathfrak{N}^*.$$ 

Operators $L, M, N$ are defined as follows:

$$\langle Lx, y \rangle = \sum_{j \in E} d_j \int_0^{l_j} (\lambda xy + x_jy_jds) \, ds, \quad \forall x, y \in \mathfrak{B},$$

$$\langle Mx, y \rangle = a_1 \sum_{j \in E} d_j \int_0^{l_j} x_j y_j ds \, ds, \quad \forall x, y \in \mathfrak{B},$$

$$\langle Nx, y \rangle = a_2 \sum_{j \in E} d_j \int_0^{l_j} |x_jy_j|^2 \, ds, \quad \forall x, y \in \mathfrak{N}.$$ 

We denote by $\sigma$ the spectrum of the operator $A$ in terms of $\{\lambda_i\}$ set of eigenvalues numbered nonincreasing and $\{\varphi_i\}$ is a family of corresponding own functions [11].
Lemma 1 (i) For all $\lambda \geq -\lambda_1$ operator $L \in \mathcal{L}(\mathcal{B}, \mathcal{B}^*)$ is self-adjoint, Fredholm and non-negative defined.

(ii) For all $a_1 \in \mathbb{R}_+$ operator $M \in \mathcal{L}(\mathcal{B}, \mathcal{B}^*)$ $s$-monotone 2-coercive.

(iii) For all $a_2 \in \mathbb{R}_+$ operator $N \in \mathcal{C}^\infty (\mathcal{N}, \mathcal{N}^*)$ $s$-monotone 4-coercive.

Proof. Equation (1) belongs to the class of semilinear Sobolev type equations with $p$-coercive and $s$-monotone operator. An equation of this type was first considered in [12]. The main ideas of the proof are based on the reduction of the problem we are researching to the generalproblem (2), (3). The conceptual proof of this Lemma is similar to the proof of Lemma 1 in [15].

We are looking for approximate solutions to problem (5) – (8) in form

$$x^m(s, t) = \sum_{i=1}^m a_i(t)\varphi_i(s), \quad m > \dim \ker L,$$

where the coefficients $a_i = a_i(t)$, $i = 1, ..., m$, are determined by the system of equations

$$\sum_{j:E_j \in \mathcal{E}} d_j \int_0^{l_j} \left( \lambda x_j \varphi_{ji} + x_j s \cdot \varphi_{ji} \right) ds + \sum_{j:E_j \in \mathcal{E}} d_j \int_0^{l_j} \left( a_1 x_j s \cdot \varphi_{jis} + a_2 |x_j|^2 x_j s \cdot \varphi_{jis} \right) ds = \sum_{j:E_j \in \mathcal{E}} d_j \int_0^{l_j} u_j \varphi_{ji} ds$$

and conditions

$$\sum_{j:E_j \in \mathcal{E}} d_j \int_0^{l_j} [\lambda (x_j(s, 0) - x_0(s)) \varphi_{ji}(s)] ds = - \sum_{j:E_j \in \mathcal{E}} d_j \int_0^{l_j} [(x_j(s, 0) - x_0(s)) s \cdot \varphi_{jis}(s)] ds.$$

Let’s construct the set

$$\text{coim} L = \{ x \in \mathcal{B} : \quad < x, \varphi > = 0 \quad \forall \varphi \in \ker L \setminus \{0\} \}$$

and consider the space

$$\mathfrak{X} = \{ x \mid x \in L_\infty(0, T; \text{coim} L) \cap L_4(0, T; \mathfrak{N}) \}.$$

Definition 1 A vector-function $x \in \mathfrak{X}$ for $T \in \mathbb{R}_+$ is a weak generalized solution to Showalter–Sidorov problem (5) – (8), if it satisfies

$$\int_0^T \left( < L \frac{dx}{dt}, \zeta > + < M + N(x), \zeta > \right) dt = 0, \quad \zeta \in \mathfrak{N},$$

$$< L(x(0) - u), \zeta > = 0.$$

Let $T_m \in \mathbb{R}_+$, $T_m = T_m(u)$, $\mathfrak{N}^m = \text{span}\{ \varphi_1, \varphi_2, ..., \varphi_m \}$.

Theorem 1 Let $\lambda \geq -\lambda_1$, $a_1, a_2 \in \mathbb{R}_+$, then for $u \in L_4^2(0, T; \mathfrak{N}^*)$ there exists a unique solution $x \in \mathfrak{X}$ to problem (5) – (8).
**Proof.** The main ideas of the proof are based on the reduction of the problem we are researching to the general problem (2), (3). The conceptual proof of this Theorem is similar to the proof of Theorem 1 in [15]. Thus the theorem is proved.

As a result of the reduction of the problem (5) − (8) to the problem (2), (3), this theorem is a consequence of Theorem 1 [13]. Theorem 1 shows the convergence of the Galerkin approximations (10) to the weak generalization solution to problem (5) − (8). We construct the control space \( U = \mathbb{R} \) and we choose \( U_{ad} \subset U \) is nonempty, closed, convex set. Let’s set the quality functional

\[
J(x, u) = \vartheta \int_0^T \| x - x_f \|_{2q}^4 dt + (1 - \vartheta) \int_0^T \| u \|_{2q}^4 \|_{3} \|_N^2 dt \rightarrow \inf, \quad \vartheta \in (0, 1),
\]

(11)

here \( x_f \) is the required state of the system, for example, the state in which the system was before exposure to the magnetic field.

**Definition 2** A pair \((\tilde{x}, \tilde{u}) \in \mathbb{R} \times U_{ad}\) is called a solution to the problem (4) − (8), if

\[
J_\theta(\tilde{x}, \tilde{u}) = \inf_{(x, u)} J_\theta(x, u),
\]

where the pairs \((\tilde{x}, \tilde{u}) \in \mathbb{X} \times U_{ad}\) satisfy to the problem (5) − (8) in the weak generalized case.

**Theorem 2** Let \( \lambda \geq -\lambda_1, a_1, a_2 \in \mathbb{R}_+ \), then for any \( x_0 \in \mathbb{R} \) there is a solution \((\tilde{x}, \tilde{u})\) problem (4) − (8).

**Proof.** The main ideas of the proof are based on the reduction of the problem we are researching to the general problem (2), (3). The conceptual proof of this Theorem is similar to the proof of Theorem 2 in [15]. Thus the theorem is proved.

Some physical processes are described by complex mathematical models and it is not always possible to find analytical solutions. Therefore, the construction numerical algorithms for solving problems is becoming increasingly relevant. Theorem 1 and Theorem 2 establish the existence of a solution, but do not describe the method for finding it. In order to linearize the equation (5) we need to introduce and to find an additional vector-function \( x(s, t) = v(s, t) \) for a numerical study of the mathematical model of process distribution potential in a semicrystalline semiconductor. Then problem (4) − (8) is equivalent to the following problem

\[
L\dot{x} + Mx + N(v) = u, \quad x(u, v) = v,
\]

(12)

\[
x(0) = x_0,
\]

(13)

\[
J_\theta(x, u, v) = \vartheta \int_0^T \| x - x_f \|_{2q}^4 dt + (1 - \vartheta) \int_0^T \| u \|_{2q}^4 \|_{3} \|_N^2 dt \rightarrow \inf, \quad \vartheta, \vartheta \in (0, 1).
\]

(14)

**Theorem 3** Let \( \lambda \geq -\lambda_1, a_1, a_2 \in \mathbb{R}_+ \), then for any \( x_0 \in \mathbb{R} \) is a solution to problem (12) − (14).

**Proof.** The main ideas of the proof are based on the reduction of the problem we are researching to the general problem (2), (3). The conceptual proof of this Theorem is similar to the proof of Theorem 3 in [15]. Thus the theorem is proved.
Applying the penalty method, we find that the problem (12) – (14) is equivalent to the following problem:

\[ L\dot{x} + Mx + N(v) = u, x(u, v) = v, \]  
\[ x(0) = x_0, \]  
\[ J_\theta^e(x, v, u) = \theta \cdot \vartheta \int_0^T \|x - x_f\|_N^2 dt + \]  
\[ +(1 - \theta) \cdot \vartheta \int_0^T \|v - f\|_V^2 dt + (1 - \vartheta) \int_0^T \|u\|_A^4 dt + r_\varepsilon \int_0^T \|x - v\|_N^2 dt \rightarrow \inf, \; \theta, \vartheta \in (0, 1), \]  

where the penalty parameter \( r_\varepsilon \rightarrow +\infty \) at \( \varepsilon \rightarrow +0 \).

**Definition 3** A triple \((\tilde{x}, \tilde{v}, \tilde{u}) \in R \times R \times \Omega_{ad}\) is called a solution to the problem of start control and final observation (15) – (17), if

\[ J_\theta^e(\tilde{x}, \tilde{v}, \tilde{u}) = \inf_{(x, v, u)} J_\theta^e(x, v, u), \]

where the triple \((x, v, u) \in X \times X \times \Omega_{ad}\) satisfies (15), (16) in the weak generalized case.

**Theorem 4** Let \( \lambda \geq -\lambda_1, a_1, a_2 \in R_+ \), then for any \( x_0 \in H \) there is a solution \((x_\varepsilon, v_\varepsilon, u_\varepsilon)\) to problem (15) – (17), moreover \( u_\varepsilon \rightarrow \bar{u}, x_\varepsilon \rightarrow \bar{x} \) for \( \varepsilon \rightarrow +0 \).

**Proof.** The main ideas of the proof are based on the reduction of the problem we are researching to the general problem (2), (3). The conceptual proof of this Theorem is similar to the proof of Theorem 4 in [15]. Thus the theorem is proved.

2. Numerical Algorithm

Based on the theoretical results obtained in the article, an algorithm was developed for the approximate solution of the optimal control problem (4) – (8) based on modified decomposition, Galerkin and Ritz methods [16–18]. Having applied the penalty method, we proceed to consider the control problem (15) – (17), where the proximity of the approximate solutions \( \tilde{x} \) and \( \tilde{v} \) achieved by introducing a new functional in the form (17), where the penalty parameter \( r_\varepsilon \rightarrow +\infty \) at \( \varepsilon \rightarrow +0 \). Using the method Galerkin, approximate solution \( \tilde{x}, \tilde{v}, \tilde{u} \) optimal problems (15) – (17) we search in the form

\[ \tilde{x}(s, t) = \sum_{i=1}^m a_i(t) \varphi_i(s), \quad \tilde{u} = \sum_{i=1}^m u_i(t) \varphi_i(s), \quad \tilde{v}(s, t) = \sum_{i=1}^m v_i(t) \varphi_i(s), \]

here \( m \in N \), to take into account the effects of the degenerate equation, it is necessary to take such that \( m > l \), here \( l = \dim \ker L \).

To find the unknown coefficients, we compose a system of differential equations

\[ < (\lambda - \Delta)x_t, \varphi_i > - a_1 < \Delta x, \varphi_{is} > - a_2 < |v_s|^2v_s, \varphi_{is} > = < u, \varphi_{is} > \]  
(18)

with the terms of Showalter–Sidorov

\[ < x(s, 0) - x_0(s), \varphi_i > = 0, \quad i = 1, m. \]  
(19)

Solve the problem (18), (19) relatively the unknown \( a_i(t) \). Note that depending on parameter \( \lambda \), equations in the system can be either differential or algebraic. Consider these cases in more details:
If \( \lambda \notin \sigma \), then all equations of the system (18) are ordinary differential equations of the first order. In order to solve this system relatively \( a_i(t) \), \( i = 1, \ldots, m \), we find \( m \) initial conditions \( a_i(0) = u_i \), \( i = 1, \ldots, m \), from the initial conditions (19). Further, we solve the obtained system of the linear differential equations of the first order with the initial conditions, and express unknown coefficients \( a_i(t) \) of the approximate solution \( \tilde{x}(s, t) \) by \( v_i(t) \), \( u_i \), \( i = 1, \ldots, m \).

If \( \lambda \in \sigma \), then the first equation is algebraic, and the rest ones are differential. Separately, consider the system of differential equations having first order and the algebraic equation. Using the Showalter–Sidorov conditions, we find \( (m-1) \) initial conditions. Solve the system of the algebraic and differential equations, and express the unknown coefficients \( a_i(t) \), \( i = 2, \ldots, m \) of the approximate solution \( \tilde{x}(s, t) \) by \( v_i(t) \), \( u_i \), \( i = 1, \ldots, m \). Turn to search for the minimum of functional. Substitute the obtained decompositions in the functional.

Based on the Ritz method, we search for unknowns \( v_i(t) \), \( u_i(t) \), \( i = 1, \ldots, m \) in the form
\[
v_i(t, N) = \sum_{i=1}^{N} b_i t^i, \quad u_i(t, N) = \sum_{i=1}^{N} c_i t^i,
\]
such that \( v_i(0, N) = x_i(0) \), \( i = 1, \ldots, m \). Let’s move on to finding minimum functional, we substitute the obtained decompositions into the functional. We will be take the coefficients \( b_n \) so that the functions \( v_i(t, N) \) and \( u_i(t, N) \) deliver a minimum functional (17). Thus, the problem reduces to finding the extremum of the function of several variables.

**Example.** Consider problem (4) – (8) on the graph \( G \) (see figure 1) consisting of three consecutively joined edges and four vertices and \( d_1 = d_2 = 1, l_1 = l_2 = \pi \) in the case of \( m = 2 \), \( n = 2 \), \( a_1 = 6 \), \( a_2 = 5 \), \( T = 1 \), \( \lambda = \frac{1}{4} \), \( \theta = \frac{1}{2} \), \( \vartheta = \frac{99}{100} \), \( \varepsilon = \frac{1}{100} \), \( \lambda_{11} = \sqrt{\frac{t}{\pi}} \cos \frac{s}{2} \), \( \lambda_{12} = \sqrt{\frac{t}{\pi}} \sin \frac{s}{2} \) and the initial functions
\[
x_{011}(s) = \frac{2}{\pi} (1 + \cos 0, 5s + \cos s), \quad x_{012}(s) = \frac{2}{\pi} (1 - \cos 0, 5s - \cos s).
\]
The eigenfunctions of the Sturm–Liouville problem

**Figure 1. The graph G**

\[
X_1'' = \lambda X_1, \quad X_2'' = \lambda X_2, \\
X_1'(\pi) = X_2'(0) = 0, \quad X_1(\pi) = X_2(0), \\
X_1'(0) = 0, \quad X_2'(\pi) = 0
\]
on the graph \( G \) have the form:
\[
\varphi_1 = (\varphi_1^1, \varphi_1^2) = \left( \sqrt{\frac{1}{\pi}}, \sqrt{\frac{1}{\pi}} \right), \\
\varphi_2 = (\varphi_2^1, \varphi_2^2) = \left( \frac{1}{\pi} \cos \frac{s}{2}, \frac{1}{\pi} \cos \frac{s}{2} \right).
\]
Figure 2. Graphs of the optimal control $u_j$, $j = 1, 2$

Figure 3. Graphs of $x_j, x_d^f_j$, $j = 1, 2$

Figure 4. Graphs of $v_j, x_d^f_j$, $j = 1, 2$

The control coefficients (to within $10^{-8}$)

|       | $b_{1,1}$ | $b_{1,2}$ | $b_{2,1}$ | $b_{2,2}$ | $c_{1,0}$ | $c_{1,1}$ | $c_{1,2}$ | $c_{2,0}$ | $c_{2,1}$ | $c_{2,2}$ |
|-------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
|       | -5.65182657 | -4.70758690 | -0.01640803 | -0.00891264 | 0.00000514 | -0.00370847 | 0.00460690 | 0.00004497 | 0.00671085 | -0.00900376 |
As a result of the calculations, the control coefficients shown in the Table were found, for which the value of the functional $J = 1,091645262$ (accurate to $10^{-8}$), the solution of the problem is shown in figures 2-4.

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