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NUMERICAL SIMULATION OF A JOINT THERMAL-DIFFUSION PROCESS IN SILICON WAFERS

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Abstract. The paper considers the problem of a joint thermal and diffusion process in silicon. The mathematical model of this process is an initial boundary value problem for the system of linear parabolic partial differential equations. In this system, one equation describes the heat transfer process in silicon, and the other describes the process of impurity diffusion in it. Moreover, the equations are not independent, since the diffusion coefficient depends on temperature. The corresponding boundary conditions are set for each equation in this system. The implicit difference scheme and classical sweep method are used to find an approximate solution to the problem. The paper presents a description of the numerical algorithm and exact calculation formulas for solving a discretized parabolic problem.

Keywords: Thermal-diffusion process, sweep method, implicit difference scheme.

Introduction

Physically, diffusion and thermal conductivity processes refer to kinetic processes that bring the body closer to equilibrium. Diffusion processes occur in the presence of different concentrations of substances in a gas or liquid, as well as in solids in the presence of impurities in them or in contact with different solids. Thermal conductivity processes occur in the presence of a temperature gradient in the body [**Error! Reference source not found.**].

The corresponding processes are described by the thermal conductivity and diffusion equations, which are similar to each other [**Error! Reference source not found.**]. With some modifications, this equation also arises in problems of heat transfer, diffusion on the surfaces of different materials and products [3, 4], in problems of heat and moisture exchange in porous structures [**Error! Reference source not found.**]. For the linear diffusion equation and for some initial-boundary conditions, it is possible to write down an explicit formula for solving these problems, but, in most cases, it is not possible to obtain a solution of closed form or even in the form of an infinite series. In this case, various integral expressions of the required function [**Error! Reference source not found.**, 7], methods for approximating the solution by functions from a given set and numerical methods for obtaining an approximate solution are used.

The result of the diffusion process study was the development of a number of mathematical models describing its course for different technological conditions. The basis of all these mathematical models are the equations of mathematical physics describing the first and second Fick's laws [8]. On the basis of mathematical models, computational methods of modeling by diffusion processes [**Error! Reference source not found.**, **Error! Reference source not found.**, 11] have been developed, which are based on different approaches [**Error! Reference source not found.**, 13, 14].

Unfortunately, all these systems are designed for instantaneous temperature measurement, which significantly affects the diffusion coefficient in a solid, and, hence, the final impurity distribution in a semiconductor. In this paper, both processes, that is, thermal and diffusion, are combined in order to take into account the inertia of heat transfer along a semiconductor wafer. It is believed that the temperature conditions can change over time, remaining focused on the semiconductor boundaries. This paper uses the finite difference method to approximate derivatives of the required function and expressions that already contain discretizations of the first-order derivative.

Simulation of a joint thermal-diffusion process

The model problem of the joint thermal conductivity and diffusion process in a solid is considered. This problem arises when removing impurities from a silicon wafer in the production of integrated circuits. The specific feature of the diffusion process in solids is its slowness, compared with diffusion in liquids and gases. However, it is known that the diffusion process depends on the temperature of the substance, where this process is considered, and accelerates with its rise, and the temperature distribution is subject to the linear parabolic equation. In this regard, the paper considers two processes simultaneously, namely thermal and diffusion. This formulation allows to take into account the inertness of the change in the diffusion coefficient depending on the temperature distribution. The change in temperature occurs at the wafer edges (either on one side or on both sides).

Let's consider the formal formulation of the problem. Note that the one-dimensional case is considered, that is, the case with one spatial coordinate x. Let $\varphi(x,t)$ be the dopant concentration at time t, at point x; $T(x,t)$ is the temperature at time t, at point x. We will assume that $x \in [0;1]$. Let, further, D_0 be the coefficient of thermal conductivity, which is a constant value. Since we consider the diffusion process in a solid, we should consider that atoms in a solid are surrounded by a potential barrier. In order for an atom to leave its place, it must have an activation energy ΔE_1 to overcome a potential barrier. Let $D(T)$ be the diffusion coefficient depending on the temperature T as follows [15]:

$$D(T) = D_1 e^{-\frac{\Delta E_1}{kT}}, \qquad (1)$$

where D_1 is a constant independent of temperature and determined by the substance properties, ΔE_1 is the diffusion activation energy depending on the dopant type, k is the Boltzmann constant. The concentration function satisfies the linear parabolic equation:

$$\frac{\partial \varphi(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(D\big(T(x,t)\big)\frac{\partial \varphi(x,t)}{\partial x}\right) \qquad (2)$$

Due to the retention of impurities in a silicon wafer, the assumption of zero diffusion flux at the edges of the silicon wafer is used, that is, the equation solution (2) satisfies the Neumann boundary conditions (3):

$$\left.\frac{\partial \varphi}{\partial x}\right|_{x=0} = \left.\frac{\partial \varphi}{\partial x}\right|_{x=1} = 0. \quad (3)$$

The initial impurity distribution is considered to be known, that is

$$\varphi(x,0) = f(x). \quad (4)$$

Further, the temperature $T(x,t)$ is a solution of the thermal conductivity equation:

$$\frac{\partial T(x,t)}{\partial t} = D_0 \frac{\partial^2 T(x,t)}{\partial x^2} \qquad (5)$$

At the same time, the specified temperature conditions are maintained at the silicon sample edges:

$$T|_{x=0} = u_1(t), \qquad T|_{x=1} = u_2(t) \qquad (6)$$

The initial temperature of the silicon sample is also given:

$$T(x,0) = T_0(x) \qquad (7)$$

Formally, the considered joint thermal-diffusion process can be written in matrix form:

$$\frac{\partial}{\partial t}\begin{pmatrix}\varphi\\ T\end{pmatrix} = \frac{\partial}{\partial x}\left(\begin{pmatrix}D(T) & 0\\ 0 & D_0\end{pmatrix}\frac{\partial}{\partial x}\begin{pmatrix}\varphi\\ T\end{pmatrix}\right), \qquad (8)$$

boundary conditions:

$$\left.\begin{pmatrix}\frac{\partial}{\partial x} & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\varphi\\ T\end{pmatrix}\right|_{x=0} = \begin{pmatrix}0\\ u_1(t)\end{pmatrix}, \qquad \left.\begin{pmatrix}\frac{\partial}{\partial x} & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\varphi\\ T\end{pmatrix}\right|_{x=1} = \begin{pmatrix}0\\ u_2(t)\end{pmatrix}, \qquad (9)$$

and initial conditions:

$$\left.\begin{pmatrix}\varphi\\ T\end{pmatrix}\right|_{t=0} = \begin{pmatrix}f(x)\\ T_0(x)\end{pmatrix}, \qquad (10)$$

Difference problem

Let's set the step h along the axis x and τ along the time axis, then introduce uniform grids in the interval $[0;1]$ and in the time interval $[0;t_1]$, where $t_1 > 0$. We add the mesh functions $T_i^n = T(ih, \tau n)$ and $\varphi_i^n = \varphi(ih, \tau n)$ at the grid nodes. To discretize partial derivatives with respect to spatial variables, we will use implicit difference schemes:

$$\frac{\partial^2}{\partial x^2} T_i^n = \frac{T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}}{h^2}, \qquad (11)$$

$$\frac{\partial}{\partial x}\varphi_i^n = \frac{\varphi_{i+1}^{n+1} - \varphi_i^{n+1}}{h}. \qquad (12)$$

After discretization of the equation (5), we get:

$$\frac{T_i^{n+1} - T_i^n}{\tau} = D_0 \frac{T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}}{h^2} \qquad (13)$$

Here, the values with indices $n+1$ are unknown and are to be determined. After rearranging the summands, we get:

$$T_{i+1}^{n+1} - \left(2 + \frac{h^2}{\tau D_0}\right) T_i^{n+1} + T_{i-1}^{n+1} = -\frac{h^2 T_i^n}{\tau D_0}, \qquad (14)$$

The equation (14) is true for each $i-th$ node, and, consequently, a system of linear algebraic equations with a tridiagonal matrix arises. This system can be solved by the standard sweep method. For this purpose, we suppose that there is a set of parameters a_i, b_i, which are called sweep coefficients, with the equality:

$$T_{i-1}^{n+1} = a_i T_i^{n+1} + b_i, \qquad (15)$$

$$T_0^{n+1} = u_1\big((n+1)\tau\big), \qquad T_N^{n+1} = u_2\big((n+1)\tau\big), \qquad (16)$$

where N is the point number along the axis x such that $x_N = 1$.

Next, we obtain recurrence equations for the sweep coefficients. To do this, we substitute the expression from (15) into the formula (14):

$$T_{i+1}^{n+1} - \left(2 + \frac{h^2}{\tau D_0}\right) T_i^{n+1} + a_i T_i^{n+1} + b_i = -\frac{h^2 T_i^n}{\tau D_0}, \qquad (17)$$

and express the value T_i^{n+1}:

$$T_i^{n+1} = \frac{1}{2 + \frac{h^2}{\tau D_0} - a_i} T_{i+1}^{n+1} + \frac{b_i + \frac{h^2 T_i^n}{\tau D_0}}{2 + \frac{h^2}{\tau D_0} - a_i}, \qquad (18)$$

If we compare the expression (18) with the formula (15), then it is easy to see that the sweep coefficients should satisfy the recurrence equations

$$a_{i+1} = \frac{1}{2 + \frac{h^2}{\tau D_0} - a_i}, \qquad b_{i+1} = \frac{b_i + \frac{h^2 T_i^n}{\tau D_0}}{2 + \frac{h^2}{\tau D_0} - a_i} \qquad (19)$$

To calculate the starting values in the formula (15), we set $i = 0$ and get $T_0^{n+1} = a_1 T_1^{n+1} + b_1$. To satisfy the first boundary condition (16), it is necessary to set

$$a_1 = 0, \qquad b_1 = u_1\big((n+1)\tau\big), \qquad (20)$$

From (16), the value of T_N^{n+1} and the found sweep coefficients allow, using the formula (15), to calculate the values of the grid function T_i^{n+1} for all i.

Next, we write down the difference equation for the concentration function $\varphi(x,t)$:

$$\frac{\varphi_i^{n+1} - \varphi_i^n}{\tau} = \frac{1}{h}\left(D_{i+\frac{1}{2}} \frac{\varphi_{i+1}^{n+1} - \varphi_i^{n+1}}{h} - D_{i-\frac{1}{2}} \frac{\varphi_i^{n+1} - \varphi_{i-1}^{n+1}}{h}\right), \qquad (21)$$

here $D_{i+\frac{1}{2}} = D\left(\frac{T_{i+1}^{n+1} - T_i^{n+1}}{2}\right)$ and $D_{i-\frac{1}{2}} = D\left(\frac{T_i^{n+1} - T_{i-1}^{n+1}}{2}\right)$. Note that the formula (12) is used to approximate the derivatives of the function $\varphi(x,t)$ with respect to the spatial variable x. We denote $\frac{\tau}{h^2} = r$ and group the summands so that, on the right, there is an expression depending on the index $n+1$:

$$-rD_{i+\frac{1}{2}} \varphi_{i+1}^{n+1} + \left(1 + r\left(D_{i+\frac{1}{2}} + D_{i-\frac{1}{2}}\right)\right) \varphi_i^{n+1} - rD_{i-\frac{1}{2}} \varphi_{i-1}^{n+1} = \varphi_i^n. \qquad (22)$$

The equation (22) is similar to (14), so we use the sweep method again. Let there be a set of parameters A_i, B_i such that

$$\varphi_{i-1}^{n+1} = A_i \varphi_i^{n+1} + B_i, \qquad (23)$$

and it is necessary to determine the recurrence equations for these parameters. To do this, we substitute (23) into the formula (22):

$$-rD_{i+\frac{1}{2}} \varphi_{i+1}^{n+1} + \left(1 + r\left(D_{i+\frac{1}{2}} + D_{i-\frac{1}{2}}\right)\right) \varphi_i^{n+1} - rD_{i-\frac{1}{2}} (A_i \varphi_i^{n+1} + B_i) = \varphi_i^n, \qquad (24)$$

here, after elementary transformations, we get the expression:

$$\varphi_i^{n+1} = \frac{rD_{i+\frac{1}{2}}}{1 + r\left(D_{i+\frac{1}{2}} + D_{i-\frac{1}{2}}(1 - A_i)\right)}\varphi_{i+1}^{n+1} + \frac{rD_{i-\frac{1}{2}}B_i + \varphi_i^n}{1 + r\left(D_{i+\frac{1}{2}} + D_{i-\frac{1}{2}}(1 - A_i)\right)}. \quad (25)$$

Whence it follows that the required recurrence equations will be as follows (26):

$$A_{i+1} = \frac{rD_{i+\frac{1}{2}}}{1 + r\left(D_{i+\frac{1}{2}} + D_{i-\frac{1}{2}}(1 - A_i)\right)}, B_{i+1} = \frac{rD_{i-\frac{1}{2}}B_i + \varphi_i^n}{1 + r\left(D_{i+\frac{1}{2}} + D_{i-\frac{1}{2}}(1 - A_i)\right)}, (26)$$

To calculate the sweep coefficients using the formulas (26), it is necessary to set the starting values. To do this, we use the boundary condition at point x=0. So, by the condition (3), by approximating the first derivative to the central point and introducing a dummy point with a negative index, we get

$$\frac{\varphi_1^{n+1} - \varphi_{-1}^{n+1}}{2h} = 0. \quad (27)$$

Further, in the formula (22), we set $i = 0$:

$$-rD_{\frac{1}{2}}\varphi_1^{n+1} + \left(1 + r\left(D_{\frac{1}{2}} + D_{-\frac{1}{2}}\right)\right)\varphi_0^{n+1} - rD_{-\frac{1}{2}}\varphi_{-1}^{n+1} = \varphi_0^n, \quad (28)$$

where $D_{\frac{1}{2}} = D\left(\frac{T_0^{n+1} + T_1^{n+1}}{2}\right), D_{-\frac{1}{2}} = D(T_0^{n+1})$. Now we take into account (27) and express from (28) φ_0^{n+1}:

$$\varphi_0^{n+1} = \frac{r\left(D_{\frac{1}{2}} + D_{-\frac{1}{2}}\right)}{1 + r\left(D_{\frac{1}{2}} + D_{-\frac{1}{2}}\right)}\varphi_1^{n+1} + \frac{\varphi_0^n}{1 + r\left(D_{\frac{1}{2}} + D_{-\frac{1}{2}}\right)},$$

which gives the expressions for A_1 and B_1:

$$A_1 = \frac{r\left(D_{\frac{1}{2}} + D_{-\frac{1}{2}}\right)}{1 + r\left(D_{\frac{1}{2}} + D_{-\frac{1}{2}}\right)}, \quad B_1 = \frac{\varphi_0^n}{1 + r\left(D_{\frac{1}{2}} + D_{-\frac{1}{2}}\right)}. \quad (29)$$

To calculate unknown values of φ_i^{n+1} , it is necessary to determine φ_N^{n+1}. However, in this case, the situation differs from the case for determining T_i^{n+1}. The difficulty lies in the fact that the boundary condition gives a constraint on the first derivative.

Based on the boundary condition (3), we obtain a difference expression approximating the first derivative with respect to the spatial variable on the right edge:

$$\frac{\varphi_{N+1}^{n+1} - \varphi_{N-1}^{n+1}}{2h} = 0, \quad (30)$$

Further, in the formulas (22) and (23), we set $i = N$:

$$-rD_{N+\frac{1}{2}}\varphi_{N+1}^{n+1} + \left(1 + r\left(D_{N+\frac{1}{2}} + D_{N-\frac{1}{2}}\right)\right)\varphi_N^{n+1} - rD_{N-\frac{1}{2}}\varphi_{N-1}^{n+1} = \varphi_N^n, \quad (31)$$

$$\varphi_{N-1}^{n+1} = A_N\varphi_N^{n+1} + B_N, \quad (32)$$

here $D_{N-\frac{1}{2}} = D\left(\frac{T_N^{n+1} + T_{N-1}^{n+1}}{2}\right), D_{N+\frac{1}{2}} = D(T_N^{n+1})$. The equations (30), (31), (32) can be solved with respect to φ_N^{n+1} and we get the expression (33):

$$\varphi_N^{n+1} = \frac{B_N r\left(D_{N+\frac{1}{2}} + D_{N-\frac{1}{2}}\right) + \varphi_N^n}{1 + r\left(D_{N+\frac{1}{2}} + D_{N-\frac{1}{2}}\right)(1 - A_N)}. \quad (33)$$

Note that the calculation of grid functions for thermal conductivity and diffusion processes should be carried out simultaneously. On each time layer, to calculate new values of the concentration function, it is necessary to use the just obtained temperature values. When calculating separately, it is necessary to store all intermediate calculation results, which can lead to the use of large amounts of memory.

We give an explicit algorithm for the numerical method of calculating the approximate solution of the problem (8) - (10). We will introduce the necessary variables:

a, b are one-dimensional arrays of real numbers, where the current values of the sweep coefficients will be stored;

d0 is a diffusion constant;

D is a one-dimensional array that stores the current diffusion coefficient values;

$U1, U2$ are given one-dimensional arrays of real numbers that contain the temperatures at the left and right ends of silicon;

$r, par, Di15, Di05$ are scalar real variables.

Next, we introduce the value r:

$r = d0 * {}^{tau}/_{(h * h)}$.

Step 1. Based on the formula (6), we will initialize the first and last elements in the temperature array:

Temperature[0] = U1[n]

Temperature[Temperature.Length - 1] = U2[n].

Here, the parameter n denotes the number of the corresponding time layer. Then, based on the formula (20), we initialize the starting values of the sweep coefficients:

n=n+1

a[0] = 0

b[0] = U1[n].

Step 2. After that, we calculate the sweep coefficients using the formula (19) and calculate all temperature array values by the following formula (15):

```
for (i=1; i < a.Length; i++)
{
par = 1 / (1 - r * a[i - 1] + 2 * r);
a[i] = r * par;
b[i] = (r * b[i - 1] + Temperature[i - 1]) * par;
}
```

```
for (i = Temperature.Length - 1; i > 1; i--)
Temperature[i - 1] = a[i] * Temperature[i] + b[i];
```

Now it is possible to immediately calculate the approximate value of the impurity concentration in silicon on the current time layer. To do this, we will initialize the parameters that are necessary for the numerical solution of the equation (2):

$r = {}^{r}/_{d0}$;

$par = 2 * r * D(Temperature[0])$.

To save memory, we will use the same arrays of sweep coefficients.

Step 3. Using the formula (29), we initialize the starting values:

```
a[1] = par / (1 + par);
b[1] = Profile[0] / (1 + par);
```

Step 4. Next, using the formula (26), we fill in all values of the sweep coefficients:

```
for (i = 1; i < a.Length - 1; i++)
{
    Di05 = D((Temperature[i - 1] + Temperature[i]) * 0.5);
    Di15 = D((Temperature[i] + Temperature[i + 1]) * 0.5);
    par = 1.0 / (1 + r * (Di15 + Di05 * (1 - a[i])));
    a[i + 1] = r * Di15 * par;
    b[i + 1] = (r * Di05 * b[i] + Profile[i]) * par;
}
```

Step 5. The last step here is to calculate the approximate value of the impurity concentration at the right end using the following formula (33)

```
par = 2 * r * D(Temperature[Temperature.Length - 1]);
Profile[Profile.Length - 1] = (b[b.Length - 1] + Profile[Profile.Length - 1] / par) / (1.0 / par + 1 - a[a.Length - 1]);
```

and a typical calculation of all array values by the following formula (32):

```
for (i = Profile.Length - 1; i > 0; i--)
    Profile[i - 1] = a[i] * Profile[i] + b[i];
```

By this moment, on the current time layer, we have approximate values of temperature and impurity concentration in silicon. To move to the next time layer, we should return to Step 1 and repeat all calculations.

Let's consider an example of the problem (2)-(7). Let in (4) the initial distribution of the impurity concentration be determined by the following law:

$$f(x) = \begin{cases} 20, x \in [0; 0.15] \cup [0.3; 0.62] \cup [0.82; 1] \\ 0, in\ other\ cases \end{cases}.$$

Figure 1 shows the plot $f(x)$.

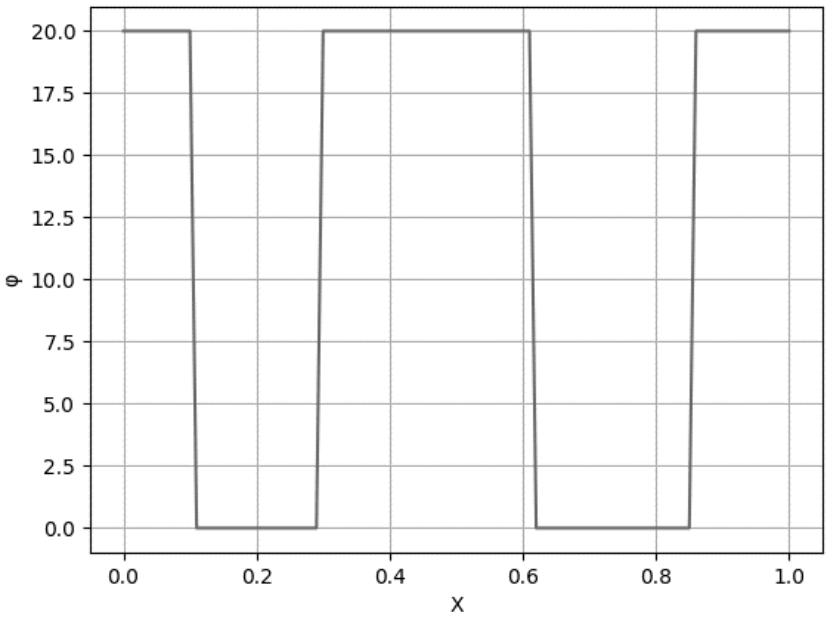

Figure 1. Initial impurity distribution.

In (7), we define the linear temperature distribution

$$T_0(x) = 100(8 - 7x),$$

we leave conditions (3) for the function φ unchanged, and we will determine boundary conditions in the formula (6) by the following formulas:

$$u_1(t) = 800 + 3t, \qquad u_2(t) = 700 + 25t^2,$$

which corresponds to uneven heating on the left and right edges, respectively. Figure (2) shows a plot of the temperature distribution $T(x,t)$ on the 300th time layer, that is, $t = 300\tau$.

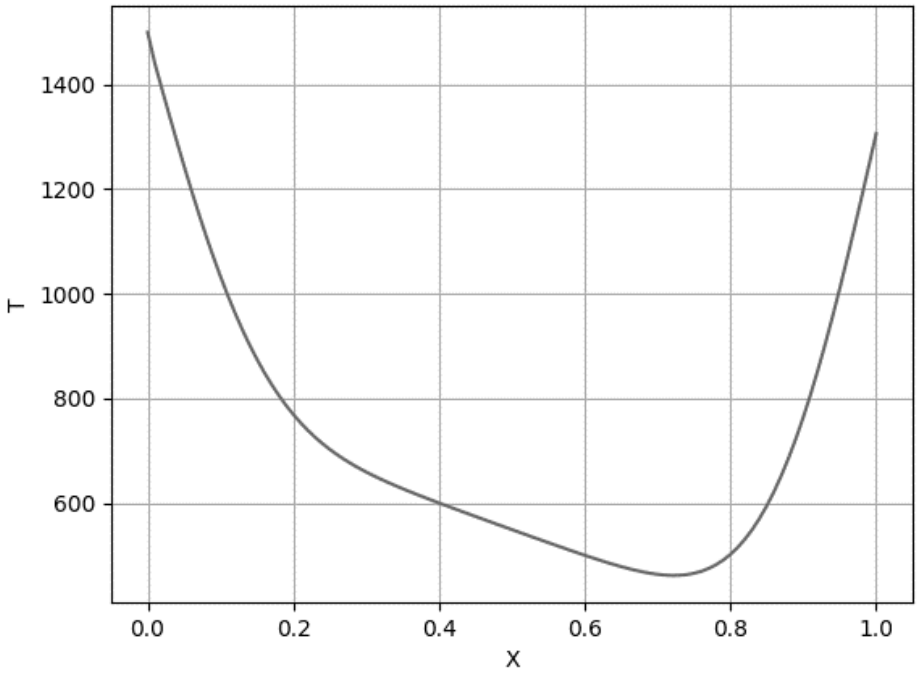

Figure 2. Temperature distribution $T(x, 300\tau)$.

Figure 3 shows a plot of the impurity distribution at the same time.

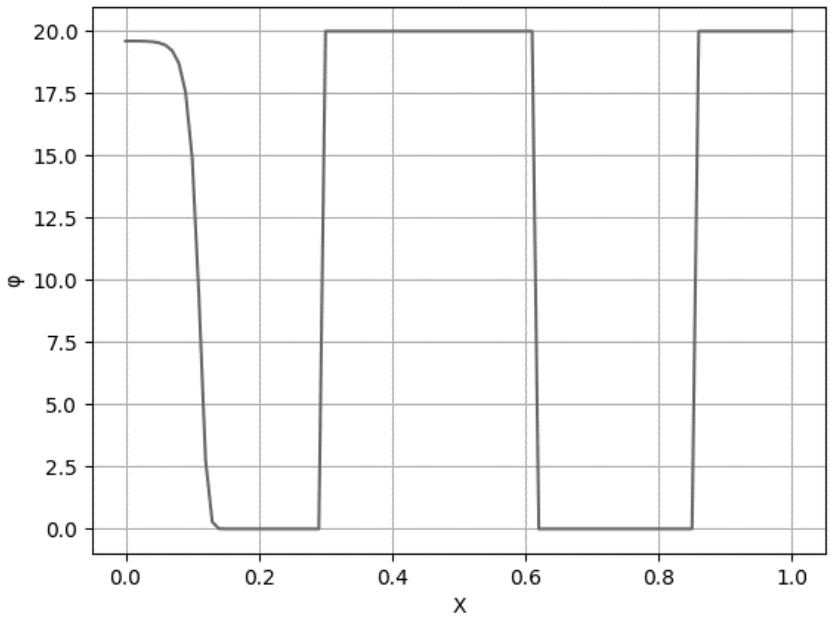

Figure 3. Concentration plot $\varphi(x, 300\tau)$.

Due to the selected boundary conditions for the thermal conductivity equation, the entire silicon sample is heated, which naturally leads to an acceleration of the impurity diffusion process. As an example, let's consider temperature distribution (Fig. 4) and impurity concentrations (Fig. 5) at $t = 4500\tau$.

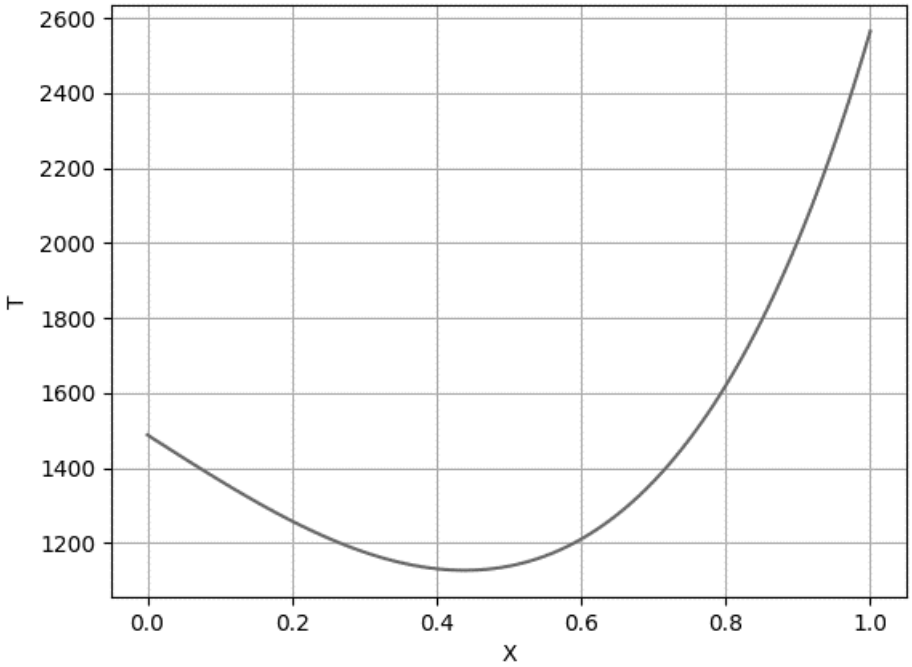

Figure 4. Temperature distribution $T(x, 4500\tau)$.

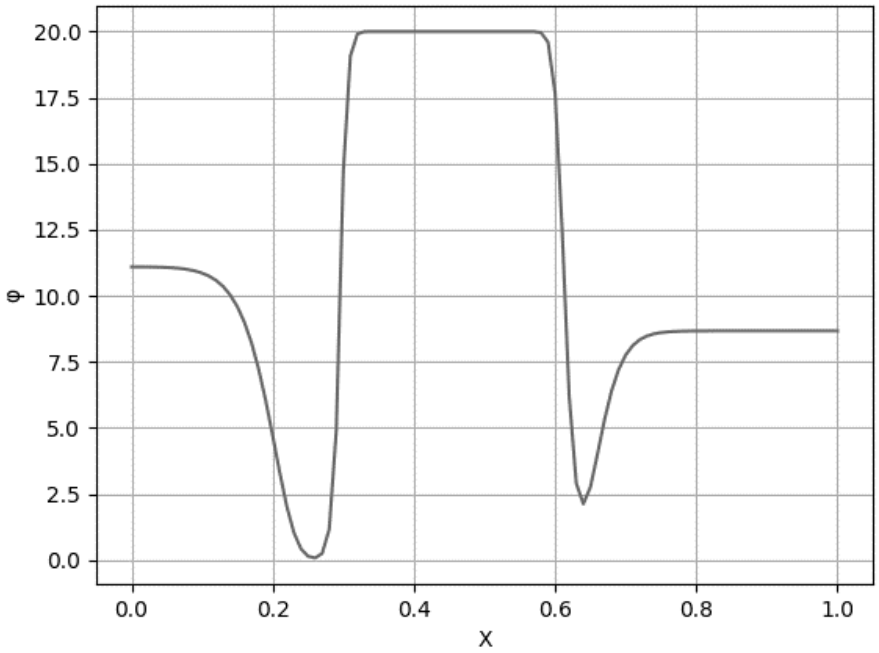

Figure 5. Concentration plot $\varphi(x, 4500\tau)$.

Conclusion

The paper considers a mathematical model of the joint thermal-diffusion process. The initial boundary value problem for a parabolic system of partial differential equations is set. Using the discretization of this differential problem, a numerical algorithm for finding an approximate solution is developed, which is based on the sweep method. This algorithm has been formally described.

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