Mathematical modeling diffusion systems with delay applied to estimation of temperature distribution for heating materials under electron irradiation

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Abstract. The paper presents the design and implementation of mathematical model of diffusion process with time delay applied to the simulation of temperature heating for materials exposed to electron irradiation at diagnostics with scanning electron microscope techniques. The computational scheme based on alternating direction method was proposed to solve a parabolic partial differential equation with delay. Program implementation of simulation algorithm was performed in Matlab application package. The results of computational experiments were also described in terms of the electron probe thermal impact on the irradiated solids taking into account delay effect.

1. Introduction
Recently, “reaction-convection-diffusion” systems have a wide range of applications for modeling processes and the phenomena in chemistry, physics, hydrodynamics, biology, the theory mass- and heat transfer and other scientific areas. The one type of numerous systems can be specified by models formalized with use of the partial differential equations in consideration of delay effect or heredity phenomenon [1-3]. Also such type of equations is named functional differential equations.

The physical sense of delay is usually associated with the finite speed of perturbance distribution or the inertial nature of the physical system. External exposure on this system results in forming response not instantly, but with time lag. Mathematical models described by initial-boundary problems for parabolic partial equations with delay in diffusion, reaction components, boundary conditions or in components specified time-derivative, internal source have been reported elsewhere [1-8].

Note that rather limited class of problems defined as delay parabolic partial differential equation enables us to find analytical solution [3]. Numerous studies have been devoted to the analysis of solution properties as stability, asymptotic nature, periodic behavior, oscillations appearance. On the other hand, using computer simulation and technique of computational experiment requires us to construct the flexible and effective computational scheme in many practical applications. Consequently, numerical methods, in particular, finite difference method, have become commonly used [4-8].

As an example of a physical system and a model of diffusion process one can consider mathematical model of time-dependent process of heating solids under electron irradiation at diagnostics with scanning electron microscope (SEM) techniques [9-15]. The analysis of the thermal fields resulting from electron beam interaction with material has become increasingly important for interpretation of experimental data in scanning electron microscopy, cathodoluminescence, Auger- and the X-ray spectral
microanalysis. The high spatial concentration of energy in the electron beam can cause unnecessary sample heating even at insignificant power of the source.

For the first time the estimation of heating temperature for sample irradiated with SEM has been proposed in [9], where the source size has been attributed to diameter of the electron probe. Further the Castaing formula [9] has been repeatedly modified. The previous study [10] has suggested the analytical relation for maximum value of heating temperature to estimate the time of transformation to steady state. The area of heat generation has been identified with the characteristic size of electron energy loss area. Then the density of heat generation has been calculated in [11] using simulation of electron energy loss process by Monte-Carlo method and approximation of heat generation area by a semi-ellipsoid. The solution of multidimensional heat-transfer steady equation using the Green function for this problem has been reported in [12]. The estimation of heating temperature induced by electron beam also has been noted in experimental study [13]. The similar approach combined with Monte-Carlo and molecular dynamics hybrid method has been demonstrated in [14].

The general feature of previous studies is estimation the temperature maximum level using expressions or constructing solutions for stationary models for the accepted approximation of heat source depending (or not depending) on distribution of electron energy. However there are high-velocity modes of SEM and also unconventional techniques when exposure time can be less than the time of transformation to stationary temperature distribution in a sample. Our previous study has devoted to numerical simulation of non-stationary heat conductivity processes in materials irradiated by electron bunches in SEM [15]. In view of the importance of physical mechanisms defining the diffusion nature of heat conductivity process we can suppose that the delay effect of system reaction to external exposure can be considered in the corresponding equation in mathematical statement of the model [15].

The so-called “non-Fourier model” has been described in [7]. The authors have proposed the model based on transformation of the Fourier law expression in consideration of time delay effect. In addition, the previous work [5] has demonstrated the approach to numerical implementing model of delayed physical system in one-dimensional case (with respect to spatial variables). This approach assumes division of diffusion term into two components – without delay and taking into account delay respectively. Moreover, the heat conductivity model transformed to the hyperbolic equation has been examined in previous work [8] using COMSOL Multiphysics to investigate thermal waves distribution in biological tissues.

The current study was aimed to developing and program implementing mathematical model of heat conductivity process in solids in consideration of time delay. Also the purpose of the study was focused on mathematical model application to computer simulation of temperature heating processes in solids irradiated by electron beam of SEM.

2. Mathematical model

2.1. Problem formulation

Modeling diffusion processes with time delay was performed on the example of applied problem described by functional partial differential equation of parabolic type. To be precise let us consider the heat conductivity process arising in solid specimen exposed to electron bunches with average energies (1-40 keV). This effect occurs when analyzing materials by SEM techniques [9-15]. It is well known that the object responds to changes in temperature gradient not instantly, but with some time delay. As previously indicated in [8-9] the time estimations [8-9] is over the range of $10^{-15}$ to $10^{-8}$ s depending on thermal properties of material and exposure peculiarities.

Hence we can formulate the problem definition as follows: it is required to express mathematical model of dynamics heating objects by electron probe of SEM under the conditions of time delay, develop the numerical scheme for the solving several-dimensional problem, perform algorithmization, program implementation and computational experiments, analyse simulation results.

The mathematical model of heat conductivity process with time delay under the conditions of Fourier law modification has been proposed before in [7]:
\[ q(r, t + \tau_q) = -k_T \nabla T(r, t + \tau_T), \quad (1) \]

where \( q \) is heat flux; \( T \) is temperature in the space point determined by \( r \) in time point of \( t \); \( k_T \) is heat conductivity coefficient of material; \( \tau_q, \tau_T \) are time lags of heat flux and temperature field respectively.

As long as we neglect the delay \( \tau_q = \tau_T = 0 \) in the equation (1), Fourier law becomes true and the physical system is described by the classical equation of heat conductivity. The model corresponds to single-phase delay model (SPL model) provided delay takes place in the flux term \( \tau_q > 0, \tau_T = 0 \). In general case the expressions \( \tau_q > 0, \tau_T > 0 \) correspond to double phase delay model (DPL model).

We have previously reported (in particular, in [15]) the approaches to development and implementation of mathematical model of heat conductivity process in dielectrics irradiated by electron beam in the SEM. The mathematical statement of the problem is given by the heat conductivity equation, where a source function is determined with use of electron trajectories spatial distributions simulated by means of Monte-Carlo method [16-19]. We can observe the dynamic heat conductivity process while the order of time magnitude is given by microseconds. This indicates that time delay can become relevant factor when analyzing thermal impact of electron irradiation on a sample in SEM.

### 2.2. Governing equations

Let us consider the heat conductivity process in certain area \( G_1 \). Also assume that a sample is modelled by the isotropic continuous environment and internal heat source starts action instantly. The linear temperature mode is under consideration and thermalphysic characteristics of the material do not depend on temperature. In order to reduce the number of space coordinates we use cylindrical symmetry of a problem as shown in figure 1. Geometrical parameters of the sample correspond to the linear sizes \( R \) and \( Z \). The internal source is defined by function of position and approximated geometrically by means of a quarter of ellipsoid \( G_2 \) with parameters \( B_1 \) and \( B_2 \).

![Figure 1. The geometrical scheme of an object and internal heat source related to cylindrical symmetry of the problem.](image)

Mathematical statement of the problem can be expressed by initial-boundary value problem for the functional differential equation of parabolic type with division diffusion term on two components:

\[
\frac{\partial T}{\partial t} = \alpha^2 \left( \frac{\partial^2 T(r,z,t)}{\partial r^2} + \frac{1}{r} \frac{\partial T(r,z,t)}{\partial r} + \frac{\partial^2 T(r,z,t)}{\partial z^2} \right) + \\
+ \alpha^2 \left( \frac{\partial^2 T(r,z,t-t^*)}{\partial r^2} + \frac{1}{r} \frac{\partial T(r,z,t-t^*)}{\partial r} + \frac{\partial^2 T(r,z,t-t^*)}{\partial z^2} \right) + \frac{f(r,z)}{\rho c}, \quad (2)
\]
where \(0 \leq r \leq R, \ 0 \leq z \leq Z, \ t \geq 0\), \(T(r, y, t)\) is temperature distribution in K; \(a^2 = k_r / \rho c\) is thermal diffusion coefficient in \(m^2/s\); \(c\) is specific heat capacity in \(J/(kg \cdot K)\); \(\rho\) is density in \(kg/m^3\), \(\gamma = \alpha^2\); \(\gamma \in [0, 1]\) is constant, \(0 \leq \gamma \leq 1\); \(f(r, z)\) is source function in units of volume density of source power \(-W/m^3\); \(t^*\) is time lag in s.

In order to close the mathematical problem statement we introduce the prehistory of the process as follows:

\[
T(x, y, t_0) = T_0, \quad t \in [-t^*, 0].
\]

(3)

In addition we need to specify the boundary conditions. Let us set boundary conditions at \(t \geq 0\) on boundaries \(\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4\) of area \(G_1\) attributed to the physical sense. The Dirichlet boundary conditions on boundaries \(\Gamma_3\) and \(\Gamma_4\) mean considerable distance from a heat source when boundaries cannot lead to changes in temperature field in gradient area. Also, Neumann boundary conditions on the \(\Gamma_1\) and \(\Gamma_2\) boundaries correspond to zero heat flux through these boundaries:

\[
T \bigg|_{\Gamma_3} = T_0, \quad T \bigg|_{\Gamma_4} = T_0, \quad \frac{\partial T}{\partial r} \bigg|_{\Gamma_2} = 0, \quad \frac{\partial T}{\partial z} \bigg|_{\Gamma_1} = 0.
\]

(4)

Notice that to formulate the governing equations of the model we used here the concept of the SPL model proposed in [7] and also we applied the idea of diffusion operator division into two components (where first component includes time delay whereas the second, respectively, does not include time delay), which was reported in [5] for one-dimensional case.

2.3. Computational scheme

In order to solve the delay diffusion equation we will design the computational scheme for the problem (2) – (4) based on modification of the alternating direction method of Peacan-Rachford [20]. Introduce \(\omega_{h_1, h_2}\) to be rectangular space-time mesh for three coordinates:

\[
\omega_{h_1, h_2} = \{r_i = ih_1, \ i = 1, N; \ z_j = jh_2, \ j = 1, M; \ t^k = k \tau, \ k = 1, 2, \ldots\},
\]

where \(h_1, h_2\) are spatial step sizes related to spatial variables \(r\) and \(z\) respectively; \(\tau\) is time step size.

Using this mesh we approximate the equation on the top time layer \(t^{k+1} = (k + 1) \tau\). The finite difference scheme is designed in two stages with introduction of approximation for the equation and boundary conditions on two time layers corresponding \(\tau/2\) and \(\tau\). So that the numerical scheme can be formally written in following form

\[
\frac{T_y^{k+1/2} - T_y^k}{\tau} = \frac{a^2}{2h_1^2} \left( T_{y+1/2}^{k+1/2} - 2T_y^{k+1/2} + T_{y-1/2}^{k+1/2} \right) + \frac{a^2}{4h_1 r_y^2} \left( T_{y+1/2}^{k+1/2} - T_{y-1/2}^{k+1/2} \right) + \frac{a^2}{2h_2^2} \left( T_{y+1}^{k+1/2} - 2T_y^{k+1/2} + T_{y-1}^{k+1/2} \right) + \frac{f_y}{2c \rho},\quad (5)
\]

\[
\frac{T_y^{k+1} - T_y^k}{\tau} = \frac{a^2}{2h_1^2} \left( T_{y+1}^{k+1} - 2T_y^{k+1} + T_{y-1}^{k+1} \right) + \frac{a^2}{4h_1 r_y^2} \left( T_{y+1}^{k+1} - T_{y-1}^{k+1} \right) + \frac{a^2}{2h_2^2} \left( T_{y+1}^{k+1/2} - 2T_y^{k+1/2} + T_{y-1}^{k+1/2} \right) + \frac{f_y}{2c \rho}.
\]

(6)
Here the form of Laplace operator is taken to be
\[ \Delta = \frac{\partial^2 r}{\partial t^2} + \frac{\partial^2 z}{\partial t^2} \] at \( r = 0 \). The above expressed finite difference equations are defined for internal mesh points. For the general numerical scheme we can re-write the initial condition in discrete form as \( T(r_i, z_j, t_0) = T_{i,j}^0 \). Furthermore the first computational subscheme (5) is constructed by adding the finite difference approximation of first-type boundary conditions, which require that \( T_{S_{i,j}}^{k+1/2} = T_{i,j}^{k+1/2} = 0 \). Similarly, we can define \( T_{S_{i,j}}^{k+1} = 0, \ T_{i,j}^{k+1} = 0 \) for the second computational subscheme (6).

In addition, second-type boundary conditions are included on default in modified difference equations using additional layers on spatial variables with fictitious mesh points and second order approximations:
\[ \frac{T_{S_{i,j}}^{k+1/2} - T_{S_{i,j}}^{k+1/2}}{2h_r} = 0, \quad \frac{T_{i,j}^{k+1} - T_{i,j}^{k+1}}{2h_z} = 0. \] (7)

The systems of linear algebraic equations for each time layer are solved by sweep method to approximate the solution of the partial differential equation.

The constructed splitting scheme can be characterized as space-efficient due to application of sweep method. The scheme has the second order of approximation on coordinates and time \( O(h_r^2 + h_z^2 + \tau^2) \) and it is unconditionally stable. Note that the algorithmic feature of numerical solution of the delay equation consists in using values of function on a time layer \( k - q \) to calculate the values of this function on \( k + 1 \) layer. This causes requirement storing values of function on \( q \) previous time layers in dynamic structure of “delay window”. The dynamic structure is need to be re-written on each time layer. Generally, such process results in resource intensity of the numerical solution of a partial differential equation with time delay.

3. Results of numerical experiments and discussions
The constructed numerical scheme (5)-(6) was implemented as computer program using Matlab application package. The program allows one to solve the initial-boundary value problem for delay parabolic partial differential equation according to problem statement (2)-(4). Also we designed a software application which enables performing computational experiments at given model parameters and simulating time-depended heat process of solids under electron beam exposure. In this case an electron probe of SEM effects on a sample as internal heat source causing changes in temperature of this sample.

Since the heat source is related to irradiation dose we should specify the electron trajectories distribution in the irradiated sample and corresponding function of electron energy loss. Hence the program module was integrated into general software application to calculate electron transport in irradiated target by means of Monte-Carlo simulation [19]. Using the normal function of electron energy loss distribution heat source function can be initialized as Gauss function in the form
\[ f(r, z) = f_0 \exp \left\{ -\frac{(\sqrt{r^2 + z^2} - \delta_1)^2}{2 \cdot \delta_2^2} \right\}, \] (8)

where \( \delta_1, \delta_2 \) are approximating parameters determined by least squares procedure employed to function of electron energy loss distribution in m; \( f_0 = W/V \) is volume density of source power in W/m³; \( W = I \cdot U \) is the source power in W; \( I \) is probe current in A; \( U \) is the accelerating voltages in V; \( V \) is volume of an internal source in m³.
3.1. Verification of simulation model

In order to verify of the model data obtained with authoring software application we also performed simulation using COMSOL Multiphysics finite element analysis system. We compared the results of simulation for test example with normalized quantities (parameters $a^2$, $c$, $\rho$, $f_0$ are set to be unities). Here the mode without delay (at delay parameter $\gamma$ equals zero) was under consideration. The sample has cube form with linear sizes of 5 arb. units. The internal source is approximated to be a half of sphere with radius equal 2 arb. units. The figure 2 shows the temperature distribution calculated with both of application program and COMSOL package at time moment $t=1$ arb. units, and initial temperature $T_0=0$ arb. units.

These findings demonstrate acceptable qualitative agreement of the simulation results based on both approaches. The temperature has maximum at incident point of heat source. The maximum value of temperature is calculated to be $T_{\text{max}} = 0.28928$ arb. units with use software application whereas computation with COMSOL results in magnitude of $T_{\text{max}} = 0.289348$ arb. units. The ratio error is equal to 0.023%.

Note also that error of simulation result is commonly specified by three components. Firstly, this is error of model representation of physical process. In certain cases one can estimate this error by comparing the simulation results with experimental data. However direct measurement of temperature sample heating in column of SEM meets experimental difficulties. Secondly, error of numerical solving partial differential equation appears. This error depends on spatial and time steps sizes as shown above. Particularly, the error value has order of $10^{-4}$ for our problem solved in normalized units. Finally, we have error due to numerical solving linear equations system. The accuracy of numerical solution of linear equations system by sweep method yields $10^{-13}$ for considerable example.

![Figure 2. The result of model verification as thermal distribution simulation (in the mode which is not taking into account delay effect) performed with: developed program – a and COMSOL Multiphysics – b in arbitrary units.](image)

3.2. Simulation results

The performance of the model is illustrated as applied to the estimation of temperature heating silicon oxide ($\text{SiO}_2$) exposed to electron beam of the SEM. This semiconductor material is used in making glass, ceramics, abrasives, concrete products, fiber-optic cables and also the silicon. Films of this oxide can be also used as an insulator in production of microchips and other components of microelectronics. In addition $\text{SiO}_2$ becomes frequently a research object in SEM techniques.

In order to realize the computational experiments the simulation parameters need to be initialize. Simulation of electron trajectories by mean of Monte-Carlo method was performed using the following...
parameters: start beam energy $E_0=8$ keV, number of electron histories $N=5000$ and electron beam diameter $d=1$ μm. The normalized depth distribution of electron energy loss in SiO$_2$ (as current energy value divided by maximum value of energy) simulated by Monte-Carlo method is shown in figure 3.

Figure 3. The normalized depth profile of the electron energy loss function in sample SiO$_2$ (calculated data as a result of Monte-Carlo simulation and Gauss function approximation obtained by the least squares method).

The Monte-Carlo simulation of electron trajectories in irradiated sample allows us to estimate the volume of internal source. The volume of internal source is determined by the parameters $B_1$ and $B_2$ and approximately equals to $V = \frac{2}{3} \pi \cdot B_1^2 \cdot B_2 = 1.53 \cdot 10^{-18}$ m$^3$. Also using these findings we can specify the parameters of approximation by Gauss function (8) $\delta_1, \delta_2$ followed by heat source function $f(r,z)$. Source power is estimated to be $W = 8 \cdot 10^{-6}$ W when probe current $I=10^{-6}$ A and accelerating voltages $U=8$ kV.

The Table 1 contains the variables, model and computational parameters as well as the values used in simulation.

Table 1. Variables and parameters in model (2)-(4) with values used in simulation.

| Symbol | Name / Description | Units | Value |
|--------|--------------------|-------|-------|
| $T$    | temperature as difference with initial value $T_0$ | K     |       |
| $r, z$ | space variables    | m     |       |
| $t$    | time               | s     |       |
| $h_1, h_2$ | spatial step sizes | μm    | 0.1-1 |
| $\tau$ | time step size     | μs    | 0.05-0.2 |
| $It$   | number of time layers (observation period is $It \cdot \tau$ in s) | unit less | 50-500 |
| $R, Z$ | spatial sizes of calculation area | μm | 100 |
| $B_1, B_2$ | spatial sizes of internal heat source | μm | 0.9 |
| Symbol | Name / Description                  | Units        | Value           |
|--------|-------------------------------------|--------------|-----------------|
| δ₁, δ₂ | approximating parameters of heat source | µm           | δ₁=0.355, δ₂=0.298 |
| ρ      | material density                    | kg·m⁻³       | 2200            |
| c      | heat capacity of material           | J·(kg·K)⁻¹  | 730             |
| a²     | heat diffusion coefficient of material | m²·s⁻¹    | 8.72·10⁻⁷      |
| f(r,z) | source function as volume density of source power | W·m⁻³     | Equation (8)    |
| T₀     | initial temperature                 | K            | 295             |
| γ      | “delay constant”                    | unit less    | [0-1]           |
| ℓ      | time lag                            | µs           | [0-2]           |

The figure 4 presents the computational experiment results. The thermal distribution for silicon oxide crystal exposed to electron beam was simulated at time point \( t=5 \) µs (\( I=50, \tau=0.1 \) µs). The calculation data are provided for mode taking into account effect of delay as well as the mode without delay.

Data of computing experiment indicate that the value of heating temperature in the mode with delay is much less than the same value in the mode without delay. The constant \( \gamma \) in mathematical model is attributed to “degree” of delay. Provided the value of this constant is closer to zero, the heating temperature is higher and, respectively, in delay is considered less.

In addition, we performed a computing experiment at variation of time delay value. These computations suggest increase threefold in delay time leads to decrease in temperature level approximately of 10 %.

\[ t_{Fo} = \frac{L^2}{a^2} \approx 5 \text{ µs}, \]

where \( L \) is character distance scale in m (such as gradient zone size).

Thus, to reach steady state it takes time \( t_{Fo} \approx 5 \) µs according to analytical analysis. In this way we can find out this result with numerical model. The dynamics of changes in maximum value of heating temperature for SiO₂ is presented in figure 5. The delay parameter \( \gamma \) is set to be unit and time of delay
is equal to $t^* = 2 \mu s$. Notice inductively that the system transforms to the state corresponding to the stationary mode after $50 \mu s$. The temperature value is calculated to be at the level of 0.47 K.

![Figure 5](image.png)

**Figure 5.** Dynamics of changes in maximum value of heating temperature in SiO\textsubscript{2} during transition to steady state.

4. Conclusions

Thus, the time-dependent mathematical model of heat conductivity process in solids in view of importance of time delay effects was proposed. The model was formalized by functional partial differential equation of parabolic type. The model belongs to the class of systems with single-phase delay and allows one to estimate of heating temperature in materials analyzing with SEM techniques. The numerical scheme was constructed using altering direction method. The scheme is space-efficient and unconditional stable. The scheme has the second order approximation on time and spatial variables.

Program implementation was assumed for solving considered class of problems. The relevant feature of numerical solution of the delay equation consists in necessity of storing values of function on previous time layers in dynamic structure, which results in resource intensity of the numerical solution. The results of computer simulation were verified by means of numerical accuracy estimation as well as comparison of the simulated temperature distribution with results obtained with COMSOL Multiphysics.

Also we described the results of computational experiments on estimation of temperature distribution in solids induced by electron beam of SEM. The parameters of the electron irradiation doze and heat source function were specified by 3D Monte-Carlo simulation of electron trajectories in the solid specimen. The computation was associated with promising material like SiO\textsubscript{2} crystal exposed to electron bunches of SEM with average energy (2-40 keV). The time-depended thermal distributions were calculated taking into account effect of time delay. Our data indicates time delay decreases half as much the level of thermal heating. According to parameters of simulation in this case we conclude that the time equal to $50 \mu s$ is specified as time to reach steady state for this material and considering conditions of experiment.

Generally, the proposed mathematical model and program application allow performing simulation of non-stationary temperature distribution in sample electron beam irradiated in SEM and identifying characteristics of heating level depending on a variation of control scanning parameters such as probe current and accelerating voltages.
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