MODELING OF PHASE CHANGES IN MICRO-DOMAIN INDUCED BY AN ULTRASHORT LASER PULSE

Ewa Majchrzak\(^1\), Lukasz Turchan\(^2\), and Jolanta Dzatkiewicz\(^2\)

\(^1\) Silesian University of Technology
44-100 Gliwice, Konarskiego 18A, Poland
e-mail: ewa.majchrzak@polsl.pl

\(^2\) Silesian University of Technology
44-100 Gliwice, Konarskiego 18A, Poland
lukasz.turchan@polsl.pl, jolanta.dzatkiewicz@polsl.pl

**Keywords:** microscale heat transfer, two-temperature model, phase transitions, finite difference method.

**Abstract.** An axisymmetric micro-domain subjected to the ultrashort laser pulse is considered. To describe the process of heat conduction occurring in the analyzed domain, the two-temperature hyperbolic model together with the isothermal solid-liquid and liquid-vapor phase changes is applied. This model, consisting of four equations describing the electrons and lattice temperatures and also the electrons and lattice heat fluxes, is transformed to the model consisting of only two equations describing the electrons and lattice temperatures. Derived equations together with the appropriate boundary and initial conditions, are solved using the finite difference method supplemented by additional numerical procedures which allow to take into account the phase changes. In the final part of the paper the results of computations are shown and the conclusions are formulated.
1 INTRODUCTION

Analysis of thermal processes occurring in the micro-domains subjected to an ultrashort laser pulse is of vital importance in microtechnology applications [1]. It should be noted that taking into account the extreme temperature gradients, extremely short duration of the process and the domain dimensions expressed in nanometers, the macroscopic heat conduction equation basing on the Fourier law cannot be applied [2-5]. So, to analyze the process, various alternative mathematical models can be used, for example the two-temperature hyperbolic model [6-10]. At high power of laser the phase transitions can occur this means melting and evaporation. In this paper the axisymmetric two-temperature hyperbolic model together with the isothermal solid–liquid and liquid-vapor phase changes is discussed. This model, presented in the chapter 2, consists of four equations describing the electrons and lattice temperatures and also the electrons and lattice heat fluxes. In chapter 3, using appropriate mathematical transformations, the model consisting of two equations describing only the electrons and lattice temperatures is proposed. Chapter 4 contains the description of numerical algorithm based on the finite difference method, while in the chapter 5 the results of computations are shown. In the final part of the paper the conclusions are formulated.

2 GOVERNING EQUATIONS

Axisymmetric two-temperature model describing the temporal and spatial evolution of the lattice and electrons temperatures in the irradiated metal together with the isothermal solid–liquid and liquid-vapor phase changes is of the form [6-8]

\[
C_e(T_e) \frac{\partial T_e(r,z,t)}{\partial t} = -\nabla \cdot \mathbf{q}_e(r,z,t) - G(T_e, T_l)[T_e(r,z,t) - T_l(r,z,t)] + Q_e(r,z,t) \tag{1}
\]

\[
C_l \frac{\partial T_l(r,z,t)}{\partial t} = -\nabla \cdot \mathbf{q}_l(r,z,t) + G(T_e, T_l)[T_e(r,z,t) - T_l(r,z,t)] + Q_m(r,z,t) + Q_{ev}(r,z,t) \tag{2}
\]

where \(T_e(r,z,t), T_l(r,z,t), \mathbf{q}_e(r,z,t), \mathbf{q}_l(r,z,t)\) are the temperatures and heat fluxes of the electrons and lattice, respectively, \(C_e, C_l\) are the volumetric specific heats, \(G(T_e, T_l)\) is the electron-phonon coupling factor which characterizes the energy exchange between electrons and phonons, \(Q_e(r,z,t)\) is the source function associated with the irradiation, while \(Q_m(r,z,t)\) and \(Q_{ev}(r,z,t)\) are the source functions associated with the melting and evaporation, respectively.

In a place of classical Fourier law the following formulas are introduced

\[
\mathbf{q}_e(r,z,t) + \tau_e \frac{\partial \mathbf{q}_e(r,z,t)}{\partial t} = -\lambda_e(T_e, T_l) \nabla T_e(r,z,t) \tag{3}
\]

\[
\mathbf{q}_l(r,z,t) + \tau_l \frac{\partial \mathbf{q}_l(r,z,t)}{\partial t} = -\lambda_l \nabla T_l(r,z,t) \tag{4}
\]

where \(\lambda_e(T_e, T_l), \lambda_l\) are the thermal conductivities of the electrons and lattice, respectively, \(\tau_e\) is the relaxation time of free electrons in metals (the mean time for electrons to change their states), \(\tau_l\) is the relaxation time in phonon collisions and \(\nabla (\cdot)\) denotes the gradient.

The laser irradiation is described by a source term introduced in equation (1) [11, 12]

\[
Q(r,z,t) = \sqrt{\frac{4 \ln 2}{\pi}} \frac{I_0}{\delta t_p} \exp \left[ -\frac{r^2}{r_p^2} - \frac{z}{\delta} - 4 \ln 2 \frac{(t - 2t_p)^2}{t_p^2} \right] \tag{5}
\]
where $I_0$ is the laser intensity, $t_p$ is the characteristic time of laser pulse, $\delta$ is the optical penetration depth, $R$ is the reflectivity of the irradiated surface and $r_D$ is the laser beam radius.

The internal heat sources resulting from the phase changes (melting and evaporation) take a form [13-15]

$$Q_{m}(r,z,t) = -L_m \frac{\partial S_m(r,z,t)}{\partial t}$$
$$Q_{ev}(r,z,t) = -L_{ev} \frac{\partial S_{ev}(r,z,t)}{\partial t}$$

(6)

where $L_m$ is the volumetric heat of fusion, $L_{ev}$ is the volumetric heat of evaporation, $S_m$ and $S_{ev}$ are the volumetric molten and gaseous state fractions in the surroundings of the point considered. Both $S_m$ and $S_{ev}$ are equal to zero at the beginning of heating process and increase from 0 to 1 when the local temperature achieves the melting $T_m$ and boiling $T_{ev}$ temperatures, respectively.

The above presented mathematical model is supplemented by the boundary conditions (no-flux conditions), it means

$$q_{be}(r,z,t) = -\lambda_e(T_e,T_t) \mathbf{n} \cdot \nabla T_e(r,z,t) = 0$$
$$q_{bt}(r,z,t) = -\lambda_l \mathbf{n} \cdot \nabla T_l(r,z,t) = 0$$

(7)

where $\mathbf{n}$ is the outward unit normal vector.

The initial temperature distribution is also known

$$t = 0: \quad T_e(r,z,t) = T_l(r,z,t) = T_0$$

(8)

where $T_0$ is constant.

For high laser intensity the following dependencies are used [6, 8, 16]

$$C_e(T_e) = \begin{cases} 
AT_e, & T_e < T_F/\pi^2 \\
AT_F/\pi^2 + \frac{N k_B - AT_F/\pi^2}{2T_F/\pi^2} (T_e - T_F/\pi^2), & T_F/\pi^2 \leq T_e < 3T_F/\pi^2 \\
N k_B + \frac{N k_B/2}{T_e - 3T_F/\pi^2} (T_e - 3T_F/\pi^2), & 3T_F/\pi^2 \leq T_e < T_F \\
3N k_B/2, & T_e \geq T_F 
\end{cases}$$

(9)

where $T_F$ is the Fermi temperature, $N$ is the density of electrons, $k_B$ is the Boltzmann constant, $A = \pi^2 N k_B / (2 T_F)$, $\chi, \eta, A_e, B_l$ are the constants and $G_{rt}$ is the coupling factor at room temperature. Other parameters: $\lambda_l, C_l, \tau_e, \tau_l$ are assumed to be constant.
3 MATHEMATICAL MANIPULATIONS

In this chapter, another form of the two-temperature model will be presented. Introducing (3) into (1) and (4) into (2), respectively, one has

\[ C_e(T_e) \frac{\partial T_e(r, z, t)}{\partial t} = \nabla \cdot \left[ \tau_e \frac{\partial q_e(r, z, t)}{\partial t} + \lambda_e(T_e, T_i) \nabla T_e(r, z, t) \right] - \]

\[ G(T_e, T_i) \left[ T_e(r, z, t) - T_i(r, z, t) \right] + Q(r, z, t) \]

(12)

and

\[ C_i \frac{\partial T_i(r, z, t)}{\partial t} = \nabla \cdot \left[ \tau_i \frac{\partial q_i(r, z, t)}{\partial t} + \lambda_i \nabla T_i(r, z, t) \right] + \]

\[ G(T_e, T_i) \left[ T_e(r, z, t) - T_i(r, z, t) \right] + Q(r, z, t) \]

(13)

Assuming that \( \tau_e \) and \( \tau_i \) are the constant values, the equations (12), (13) can be written in the form

\[ C_e(T_e) \frac{\partial T_e(r, z, t)}{\partial t} = \tau_e \frac{\partial}{\partial t} \left[ \nabla \cdot q_e(r, z, t) \right] + \nabla \left[ \lambda_e(T_e, T_i) \nabla T_e(r, z, t) \right] - \]

\[ G(T_e, T_i) \left[ T_e(r, z, t) - T_i(r, z, t) \right] + Q(r, z, t) \]

(14)

and

\[ C_i \frac{\partial T_i(r, z, t)}{\partial t} = \tau_i \frac{\partial}{\partial t} \left[ \nabla \cdot q_i(r, z, t) \right] + \nabla \left[ \lambda_i \nabla T_i(r, z, t) \right] + \]

\[ G(T_e, T_i) \left[ T_e(r, z, t) - T_i(r, z, t) \right] + Q_m(r, z, t) + Q_{ev}(r, z, t) \]

(15)

From equations (1), (2) results that

\[ -\nabla \cdot q_e(r, z, t) = C_e(T_e) \frac{\partial T_e(r, z, t)}{\partial t} + G(T_e, T_i) \left[ T_e(r, z, t) - T_i(r, z, t) \right] - Q(r, z, t) \]

(16)

and

\[ -\nabla \cdot q_i(r, z, t) = C_i \frac{\partial T_i(r, z, t)}{\partial t} - G(T_e, T_i) \left[ T_e(r, z, t) - T_i(r, z, t) \right] - \]

\[ Q_m(r, z, t) - Q_{ev}(r, z, t) \]

(17)

Introducing (16) into (14) and (17) into (15), respectively, the equations (14), (15) have a form

\[ C_e(T_e) \frac{\partial T_e(r, z, t)}{\partial t} + \tau_e \frac{\partial C_e(T_e)}{\partial t} \frac{\partial T_e(r, z, t)}{\partial t} + \tau_e C_e(T_e) \frac{\partial^2 T_e(r, z, t)}{\partial t^2} = \]

\[ \nabla \left[ \lambda_e(T_e, T_i) \nabla T_e(r, z, t) \right] - \left[ G(T_e, T_i) + \tau_e \frac{\partial G(T_e, T_i)}{\partial t} \right] \left[ T_e(r, z, t) - T_i(r, z, t) \right] - \]

\[ \tau_e G(T_e, T_i) \left[ \frac{\partial T_e(r, z, t)}{\partial t} - \frac{\partial T_i(r, z, t)}{\partial t} \right] + Q(r, z, t) + \tau_e \frac{\partial Q(r, z, t)}{\partial t} \]

(18)
and
\[
C_l \frac{\partial T_i(r, z, t)}{\partial t} + \tau_i C_l \frac{\partial^2 T_i(r, z, t)}{\partial t^2} = \nabla [\lambda_i \nabla T_i(r, z, t)] + \\
\left[ G(T_e, T_i) + \tau_e \frac{\partial G(T_e, T_i)}{\partial t} \right] [T_e(r, z, t) - T_i(r, z, t)] + \tau_i G(T_e, T_i) \left[ \frac{\partial T_e(r, z, t)}{\partial t} - \frac{\partial T_i(r, z, t)}{\partial t} \right]
\]
(19)

\[
Q_m(r, z, t) + \tau_i \frac{\partial Q_m(r, z, t)}{\partial t} + Q_{ev}(r, z, t) + \tau_i \frac{\partial Q_{ev}(r, z, t)}{\partial t}
\]

Because
\[
\frac{\partial C_e(T_e)}{\partial t} = \frac{dC_e(T_e)}{dT_e} \frac{\partial T_e}{\partial t}
\]
\[
\frac{\partial G(T_e, T_i)}{\partial t} = \frac{\partial G(T_e, T_i)}{\partial T_e} \frac{\partial T_e}{\partial t} + \frac{\partial G(T_e, T_i)}{\partial T_i} \frac{\partial T_i}{\partial t}
\]

(20)

therefore
\[
C_e(T_e) \left[ \frac{\partial T_e(r, z, t)}{\partial t} + \tau_e \frac{\partial^2 T_e(r, z, t)}{\partial t^2} \right] + \tau_e G(T_e, T_i) \frac{\partial T_e(r, z, t)}{\partial t} = \\
\nabla [\lambda_e(T_e, T_i) \nabla T_e(r, z, t)] - \tau_e \frac{dC_e(T_e)}{dT_e} \left[ \frac{\partial T_e(r, z, t)}{\partial t} \right]^2 - \\
\left\{ G(T_e, T_i) + \tau_e \left[ \frac{\partial G(T_e, T_i)}{\partial T_e} \frac{\partial T_e(r, z, t)}{\partial t} + \frac{\partial G(T_e, T_i)}{\partial T_i} \frac{\partial T_i(r, z, t)}{\partial t} \right] \right\} [T_e(r, z, t) - T_i(r, z, t)] + \\
\tau_e G(T_e, T_i) \frac{\partial T_i(r, z, t)}{\partial t} + Q(r, z, t) + \tau_e \frac{\partial Q(r, z, t)}{\partial t}
\]
(21)

and
\[
C_l \left[ \frac{\partial T_i(r, z, t)}{\partial t} + \tau_i \frac{\partial^2 T_i(r, z, t)}{\partial t^2} \right] + \tau_i G(T_e, T_i) \frac{\partial T_i(r, z, t)}{\partial t} = \nabla [\lambda_i \nabla T_i(r, z, t)] + \\
\left\{ G(T_e, T_i) + \tau_i \left[ \frac{\partial G(T_e, T_i)}{\partial T_e} \frac{\partial T_e(r, z, t)}{\partial t} + \frac{\partial G(T_e, T_i)}{\partial T_i} \frac{\partial T_i(r, z, t)}{\partial t} \right] \right\} [T_e(r, z, t) - T_i(r, z, t)] + \\
\tau_i G(T_e, T_i) \frac{\partial T_i(r, z, t)}{\partial t} + Q_m(r, z, t) + \tau_i \frac{\partial Q_m(r, z, t)}{\partial t} + Q_{ev}(r, z, t) + \tau_i \frac{\partial Q_{ev}(r, z, t)}{\partial t}
\]
(22)

Finally
\[ C_e(T_e) + \tau_e G(T_e, T_l) \frac{\partial T_e(r, z, t)}{\partial t} + \frac{\partial^2 T_e(r, z, t)}{\partial t^2} = 0 \]
\[ \nabla \left[ \lambda_e(T_e, T_l) \nabla T_e(r, z, t) \right] - \tau_e \left( \frac{\partial C_e(T_e)}{\partial T_e} \right)^2 \]
\[ \left\{ G(T_e, T_l) + \tau_e \left[ \frac{\partial G(T_e, T_l)}{\partial T_e} \frac{\partial T_e(r, z, t)}{\partial t} + \frac{\partial G(T_e, T_l)}{\partial T_l} \frac{\partial T_l(r, z, t)}{\partial t} \right] \right\} \left[ T_e(r, z, t) - T_l(r, z, t) \right] + \]
\[ \tau_e G(T_e, T_l) \frac{\partial T_l(r, z, t)}{\partial t} + Q(r, z, t) + \tau_e \frac{\partial Q(r, z, t)}{\partial t} \]

and
\[ C_l \left[ \frac{\partial T_l(r, z, t)}{\partial t} + \frac{\partial^2 T_l(r, z, t)}{\partial t^2} \right] + \tau_i G(T_e, T_l) \frac{\partial T_l(r, z, t)}{\partial t} = \nabla \left[ \lambda_i \nabla T_l(r, z, t) \right] + \]
\[ \left\{ G(T_e, T_l) + \tau_i \left[ \frac{\partial G(T_e, T_l)}{\partial T_e} \frac{\partial T_e(r, z, t)}{\partial t} + \frac{\partial G(T_e, T_l)}{\partial T_l} \frac{\partial T_l(r, z, t)}{\partial t} \right] \right\} \left[ T_e(r, z, t) - T_l(r, z, t) \right] + \]
\[ \tau_i G(T_e, T_l) \frac{\partial T_l(r, z, t)}{\partial t} + Q_m(r, z, t) + \tau_i \frac{\partial Q_m(r, z, t)}{\partial t} + Q_{er}(r, z, t) + \tau_i \frac{\partial Q_{er}(r, z, t)}{\partial t} \]

Summarizing, the equations (23) and (24) supplemented by boundary conditions (7) and initial condition (8) create an equivalent two-temperature model described in the chapter 2. It should be noted that in this model the second time derivatives appear and therefore the additional initial condition should be introduced
\[ t = 0: \quad \frac{\partial T(r, z, t)}{\partial t} \bigg|_{t=0} = 0 \]

The phase transitions are modeled using the autorial version of the algorithm called ‘a temperature recovery method’ [17]. When the local temperature at the node \((i, j)\) achieves the value of melting point \(T_m\) then the source function \(Q_m(r, z, t)\) starts, at the same time, because the melting process proceeds at the constant temperature the derivatives of lattice temperature with respect to time (equation (24)) are equal to 0. So, one has (c.f. equation (24))
\[ 0 = \nabla \left[ \lambda_i \nabla T_l(r, z, t) \right] + \left\{ G(T_e, T_l) + \tau_i \frac{\partial G(T_e, T_l)}{\partial T_e} \frac{\partial T_e(r, z, t)}{\partial t} \right\} \left[ T_e(r, z, t) - T_m \right] + \]
\[ \tau_i G(T_e, T_l) \frac{\partial T_e(r, z, t)}{\partial t} - L_m \frac{\partial S_m(r, z, t)}{\partial t} - \tau_j L_m \frac{\partial^2 S_m(r, z, t)}{\partial t^2} \]

it means
\[ L_m \frac{\partial^2 S_m(r, z, t)}{\partial t^2} + \tau_i L_m \frac{\partial^2 S_m(r, z, t)}{\partial t^2} = \nabla \left[ \lambda_i \nabla T_l(r, z, t) \right] + \]
\[ \left\{ G(T_e, T_l) + \tau_i \frac{\partial G(T_e, T_l)}{\partial T_e} \frac{\partial T_e(r, z, t)}{\partial t} \right\} \left[ T_e(r, z, t) - T_m \right] + \tau_i G(T_e, T_l) \frac{\partial T_e(r, z, t)}{\partial t} \]
The similar equation describes the evaporation process

\[
L_{ev} \frac{\partial S_{ev}(r,z,t)}{\partial t} + \tau_e L_{ev} \frac{\partial^2 S_{ev}(r,z,t)}{\partial t^2} = \nabla [\lambda_e \nabla T_e(r,z,t)] + \left[G(T_e,T_i) + \tau_e G(T_e,T_i) \frac{\partial T_e(r,z,t)}{\partial t}\right]
\]

\[
\left[T_e(r,z,t) - T_{ev}\right] + \tau_e G(T_e,T_i) \frac{\partial T_e(r,z,t)}{\partial t}
\]

(28)

4 METHOD OF SOLUTION

To solve the problem formulated in the chapter 3, the finite difference method is used [18, 19]. The geometrical mesh with dimensions \(n \times n\) is introduced and the temperatures for time \(t_f = f \Delta t (f \geq 2, \Delta t\) is the constant time step) at the node \((i, j)\) are denoted as \(T_f^{i,j} = T_e(r_j,z_i,t_f)\) and \(T_i^{f,i,j} = T_i(r_j,z_i,t_f)\), respectively.

The following approximation of equation (23) is proposed

\[
\left(C_{ei,j}^{-1} + \tau_e G_{ei,j}^{-1}\right) \frac{T_f^{i,j} - T_{ei,j}^{-1}}{\Delta t} + \tau_e C_{ei,j}^{-1} \frac{T_i^{f,i,j} - 2T_{ei,j}^{-1} + T_{ei,j}^{-2}}{(\Delta t)^2}
\]

\[
\nabla (\lambda_e \nabla T_e)_{i,j}^{-1} - \tau_e \left(\frac{d C_e}{d T_e}\right)_{i,j}^{-1} \left(\frac{T_f^{i,j} - T_{ei,j}^{-1}}{(\Delta t)^2}\right) -
\]

\[
\left\{G_{i,j}^{-1} + \tau_e \left[\frac{\partial G}{\partial T_e}\right]_{i,j}^{-1} \frac{T_f^{i,j} - T_{ei,j}^{-1}}{\Delta t} + \left(\frac{\partial G}{\partial T_l}\right)_{i,j}^{-1} \frac{T_{li,j}^{-1} - T_{ei,j}^{-2}}{\Delta t}\right\} \left(\frac{T_f^{i,j} - T_{ei,j}^{-1}}{\Delta t}\right) +
\]

\[
\tau_e G_{i,j}^{-1} \frac{T_{li,j}^{-1} - T_{ei,j}^{-2}}{\Delta t} + Q_f^{i,j} + \tau_e \left(\frac{\partial Q}{\partial t}\right)_{i,j}^{-1}
\]

where

\[
\nabla (\lambda_e \nabla T_e)_{i,j}^{-1} = \Phi_1 \frac{T_{ei,j}^{-1} - T_{ei,j}^{-1}}{R_{f,i,j}^{-1}} + \Phi_2 \frac{T_{ei,j}^{-1} - T_{ei,j}^{-1}}{R_{i,i,j}^{-1}} +
\]

\[
\Phi_3 \frac{T_{ei,j}^{-1} - T_{ei,j}^{-1}}{R_{f,i,j}^{-1}} + \Phi_4 \frac{T_{ei,j}^{-1} - T_{ei,j}^{-1}}{R_{f,i,j}^{-1}}
\]

(30)

while

\[
R_{f,i,j}^{-1} = \frac{h}{2} \left(\frac{1}{\lambda_{ei,i}^{-1}} + \frac{1}{\lambda_{ei,j}^{-1}}\right), \quad R_{i,i,j}^{-2} = \frac{h}{2} \left(\frac{1}{\lambda_{ei,i}^{-1}} + \frac{1}{\lambda_{ei,j}^{-1}}\right)
\]

(31)
are the thermal resistances between adjacent nodes \([18, 19]\) and

\[
\Phi_i = \left( r_{i,j} - 0.5h \right) / \left( h r_{i,j} \right), \quad \Phi_2 = \left( r_{i,j} + 0.5h \right) / \left( h r_{i,j} \right), \quad \Phi_3 = \Phi_4 = 1 / h
\]

are the shape functions of differential mesh for the axially-symmetrical task.

After mathematical manipulations one has

\[
T_{e,i,j}^{f-1} = \frac{(\Delta t)^2 \nabla (\lambda_e \nabla T_e)}{\Delta t (C_{e,i,j} + \tau_e G_{e,i,j}^{f-1}) + \tau_e C_{e,i,j}^{f-1}} + \frac{\Delta t (C_{e,i,j} + \tau_e G_{e,i,j}^{f-1}) + 2\tau_e C_{e,i,j}^{f-1}}{\Delta t (C_{e,i,j} + \tau_e G_{e,i,j}^{f-1}) + \tau_e C_{e,i,j}^{f-1}} T_{e,i,j}^{f-1} - \frac{\tau_e C_{e,i,j}^{f-1} T_{e,i,j}^{f-2}}{\Delta t (C_{e,i,j} + \tau_e G_{e,i,j}^{f-1}) + \tau_e C_{e,i,j}^{f-1}} - \frac{\tau_e T_{e,i,j}^{f-1} - T_{e,i,j}^{f-2}}{\Delta t (C_{e,i,j} + \tau_e G_{e,i,j}^{f-1}) + \tau_e C_{e,i,j}^{f-1}} \left( \frac{\partial G}{\partial T_e} \right)_{i,j}^{f-1} + \left( \frac{\partial G}{\partial T_i} \right)_{i,j}^{f-1} T_{i,i,j}^{f-1} - T_{i,i,j}^{f-2} \right]
\]

In a similar way the equation (24) can be approximated and for the temperatures below the melting point one obtains

\[
T_{i,i,j}^{f-1} = \frac{(\Delta t)^2 \nabla (\lambda_j \nabla T_j)}{\Delta t (C_j + \tau_j G_{j,i,j}^{f-1}) + \tau_j C_j} + \frac{\Delta t (C_j + \tau_j G_{j,i,j}^{f-1}) + 2\tau_j C_j}{\Delta t (C_j + \tau_j G_{j,i,j}^{f-1}) + \tau_j C_j} T_{i,i,j}^{f-1} - \frac{\tau_j C_j^{f-1} T_{i,i,j}^{f-2}}{\Delta t (C_j + \tau_j G_{j,i,j}^{f-1}) + \tau_j C_j^{f-1}} - \frac{\tau_j T_{i,i,j}^{f-1} - T_{i,i,j}^{f-2}}{\Delta t (C_j + \tau_j G_{j,i,j}^{f-1}) + \tau_j C_j^{f-1}} \left( \frac{\partial G}{\partial T_i} \right)_{i,j}^{f-1} + \left( \frac{\partial G}{\partial T_j} \right)_{i,j}^{f-1} T_{i,i,j}^{f-1} - T_{i,i,j}^{f-2} \right]
\]

In turn, the finite difference approximation of equation (27) is of the form

\[
L_m S_{mi,j}^{f-1} \frac{S_{mi,j}^{f-1} - S_{mi,j}^{f-2}}{(\Delta t)} + \tau_i L_m S_{mi,j}^{f-1} \frac{S_{mi,j}^{f-1} - 2S_{mi,j}^{f-1} + S_{mi,j}^{f-2}}{(\Delta t)^2} = \nabla [\lambda_i \nabla T_i(r, z, t)]_{i,j}^{f-1} + \left( \frac{\partial G}{\partial T_i} \right)_{i,j}^{f-1} \left( T_{i,i,j}^{f-1} - T_{i,i,j}^{f-2} \right) + \tau_i G_{i,j}^{f-1} \frac{T_{e,i,j}^{f-1} - T_{i,i,j}^{f-2}}{\Delta t} + \tau_i G_{i,j}^{f-1} \frac{T_{e,i,j}^{f-1} - T_{i,i,j}^{f-2}}{\Delta t}
\]

and next

\[
S_{mi,j}^{f} = \frac{(\Delta t) + \tau_i S_{mi,j}^{f-1} - \frac{\tau_i S_{mi,j}^{f-2}}{\Delta t + \tau_i} + \left( \frac{\partial G}{\partial T_i} \right)_{i,j}^{f-1} \frac{T_{i,i,j}^{f-1} - T_{i,i,j}^{f-2}}{\Delta t} + \tau_i G_{i,j}^{f-1} \frac{T_{e,i,j}^{f-1} - T_{i,i,j}^{f-2}}{\Delta t}}{L_m (\Delta t + \tau_i)} + \left( \frac{\partial G}{\partial T_i} \right)_{i,j}^{f-1} \frac{T_{i,i,j}^{f-1} - T_{i,i,j}^{f-2}}{\Delta t} + \left( \frac{\partial G}{\partial T_i} \right)_{i,j}^{f-1} \frac{T_{i,i,j}^{f-1} - T_{i,i,j}^{f-2}}{\Delta t}
\]
In a similar way one obtains (c.f. equation (28))

\[ S_{ev,i,j}^f = \frac{\Delta t + 2\tau_l}{\Delta t + \tau_l} S_{ev,i,j}^{f-1} - \frac{\tau_l}{\Delta t + \tau_l} S_{ev,i,j}^{f-2} + \frac{(\Delta t)^2}{L_{ev}(\Delta t + \tau_l)} \nabla \left[ \lambda_l \nabla T_i(r, z, t) \right]_{i,j}^{f-1} + \]

\[ \frac{(\Delta t)^2}{L_{ev}(\Delta t + \tau_l)} \left[ G_{i,j}^{f-1} + \tau_l \left( \frac{\partial G_f}{\partial T_e} \right)_{i,j}^{f-1} \right] \left( T_{ei,j}^{f-1} - T_{ei,j}^{f-2} \right) \left( T_{ei,j}^{f-1} - T_{ei,j}^{f-2} \right) \]

(37)

5 RESULTS OF COMPUTATIONS

Numerical simulation of a thermal process taking place in the cylindrical domain with dimensions \( Z = 100 \cdot 10^{-9} [m] \) and \( R = 100 \cdot 10^{-9} [m] \) subjected to the short-pulse laser heating has been done. The initial temperature is equal to \( T_p = 300 K \). Thermophysical parameters of material are equal to (gold): thermal conductivity of lattice \( \lambda_l = 315 W/(mK) \), volumetric specific heat of lattice \( C_l = 2.5 MJ/(m^3 K) \), electrons relaxation time \( \tau_e = 0.04 \text{ ps} \), phonons relaxation time \( \tau_l = 0.8 \text{ ps} \) [20], reflectivity \( R = 0.93 \), optical penetration depth \( \delta = 15.3 \text{ nm} \). The Fermi temperature is equal to \( T_F = 64 200 K \) and the density of electrons is equal to \( N = 5.9 \cdot 10^{28} 1/m \) (c.f. equation (9)) [6]. The constants in equations (10), (11) are the following: \( \chi = 353 W/(mK) \), \( \eta = 0.16 \), \( A_e = 1.2 \cdot 10^7 1/(K^2 s) \), \( B_l = 1.23 \cdot 10^{11} 1/(Ks) \) and \( G_{rt} = 2.2 \cdot 10^{16} W/(m^3 K) \) [6]. The melting point is equal to \( T_m = 1336 K \), the boiling point: \( T_e = 3127 K \), the volumetric heat of fusion: \( L_m = 1.23 \cdot 10^3 MJ/m^3 \) and the volumetric heat of evaporation: \( L_{ev} = 3.277 \cdot 10^4 MJ/m^3 \).

The laser beam radius is equal to \( r_D = R/8 \). The calculations were performed for five values of the laser intensity: \( I_0 = 2 \cdot 10^5 J/m^2 \), \( I_0 = 4 \cdot 10^5 J/m^2 \), \( I_0 = 6 \cdot 10^5 J/m^2 \), \( I_0 = 8 \cdot 10^5 J/m^2 \) and \( I_0 = 10^6 J/m^2 \) under the assumption that the characteristic time of laser pulse is equal to \( t_p = 100 \text{ ps} \) (c.f. formula (5)). The problem is solved using the finite difference method. Number of nodes is equal to \( 50 \times 50 = 2500 \) (\( h = 2 \text{ nm} \)) and time step is equal to 0.0005 ps.

In Figures 1 and 2 the heating curves at the point (2nm, 2nm) are shown. As can be seen, for the lowest laser intensity only the heating process is observed, while for the higher laser intensity the melting process appears (‘stop’ corresponding to the melting process). In the case of the largest laser intensity (Figure 2) the isothermal liquid-vapour phase change starts. Figures 3 and 4 illustrate the courses of electrons and lattice temperatures at the same point.
Figure 2: Lattice temperature history at the point (2 nm, 2nm).

Figure 3: Temperature history at the point (2nm, 2nm) for $I_0 = 6 \times 10^5$ J/m$^2$.

Figure 4: Temperature history at point (2nm, 2nm) for $I_0 = 10^6$ J/m$^2$. 
In Figure 5 the electrons and phonons temperature distribution after 150 ps for laser intensity $I_0 = 8 \times 10^5 \text{ J/m}^2$ is shown.

![Figure 5: Temperature distribution after 150 ps, A) electrons, B) lattice.](image)

6 FINAL REMARKS

The thermal processes occurring in the axisymmetric micro-domain subjected to the ultra-short laser pulse are analyzed. The problem is described by two equations for electrons and lattice temperatures supplemented by appropriate boundary and initial conditions. At the stage of numerical computations the finite difference method together with the procedures modeling the phase transitions is used. In the future, the algorithm will be supplemented by a procedure modeling the ablation process.

ACKNOWLEDGEMENT

This work is supported by the project BK-255/RMT4/2016.

REFERENCES


