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Axisymmetric modeling of ultrashort-pulse laser interactions with thin metal film

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Abstract

The hyperbolic two-temperature model is used in order to describe the heat propagation in metal film subjected to an ultrashort-pulse laser heating. An axisymmetric heat source with Gaussian temporal and spatial distributions has been taken into account. At the stage of numerical computations the finite difference method is used. In the final part of the paper the examples of computations are shown.

Keywords: Application of information technology to the foundry industry, Numerical techniques, Micro-scale heat transfer, Finite difference method

1. Introduction

Nowadays in literature the different microscale heat transfer models, among others the microscale two-temperature models (two-step models, phonon-electron interaction models [1, 2, 3, 4]) are formulated. In this paper the hyperbolic two-temperature model is considered. In particular, the thermal processes in axisymmetic metal domain subjected to laser beam are analyzed – Figure 1.

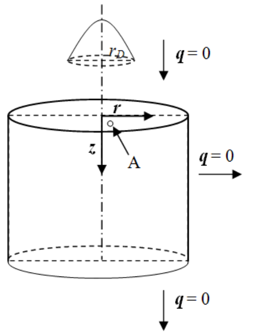

Fig. 1. Axisymmetric domain

2. Mathematical model

The hyperbolic two-temperature model is used to describe the heat propagation in domain subjected to the ultrafast laser heating [1, 2]

$$C_e(T_e)\frac{\partial T_e(r,z,t)}{\partial t} = -\mathrm{div}\,\mathbf{q}_e(r,z,t) - G(T_e)\left[T_e(r,z,t) - T_l(r,z,t)\right] + Q(r,z,t) \tag{1}$$

and

$$C_l(T_l)\frac{\partial T_l(r,z,t)}{\partial t} = -\mathrm{div}\,\mathbf{q}_l(r,z,t) + G(T_e)\left[T_e(r,z,t) - T_l(r,z,t)\right] \tag{2}$$

where T_e, T_l are the electron gas temperature and lattice temperature, respectively, $C_e(T_e)$, $C_l(T_l)$ [J/(m^3 K)] are the thermal capacities, $\mathbf{q}_e$, $\mathbf{q}_l$ are the heat fluxes vectors, $G(T_e)$ [W/(m^3 K)] is the electron-phonon coupling factor, $\{r, z\}$ are the spatial co-ordinates (axisymmetric co-ordinate system is introduced), t is the time, $Q(r, z, t)$ is the laser heating source.

In equations (1), (2) the heat fluxes are defined as follows

$$\mathbf{q}_e(r,z,t)+\tau_e\frac{\partial \mathbf{q}_e(r,z,t)}{\partial t}=-\lambda_e(T_e,T_l)\operatorname{grad}T_e(r,z,t) \tag{3}$$

and

$$\mathbf{q}_l(r,z,t)+\tau_l\frac{\partial \mathbf{q}_l(r,z,t)}{\partial t}=-\lambda_l(T_l)\operatorname{grad}T_l(r,z,t) \tag{4}$$

where $\lambda_e(T_e, T_l)$, $\lambda_l(T_l)$ are the thermal conductivities of electrons and phonons, respectively, τ_e is the relaxation time of free electrons, this means the mean time for electrons to change their states in metals and τ_l is the relaxation time in phonon collisions.

Mathematical formula determining the intensity of internal heat source $Q(r, z, t)$ resulting from laser action can be assumed in the following form

$$Q(r,z,t)=\sqrt{\frac{4\ln 2}{\pi}}(1-R)\frac{I_0}{\delta t_p}\exp\left[-\frac{r^2}{r_D^2}-\frac{z}{\delta}-4\ln 2\frac{(t-2t_p)^2}{t_p^2}\right] \tag{5}$$

where I_0 [J/m^2] is the laser intensity, t_p [s] is the characteristic time of laser pulse, δ [m] is the optical penetration depth, R is the reflectivity of the irradiated surface, r_D [m] is the laser beam radius.

The above presented mathematical model is supplemented by boundary conditions

$$(r,z)\in\Gamma:\quad q_e(r,z,t)=q_l(r,z,t)=0 \tag{6}$$

and initial ones

$$t=0:\quad T_e(r,z,t)=T_l(r,z,t)=T_p \tag{7}$$

where T_p is the initial temperature of electrons and lattice.

To solve the problem formulated, the certain mathematical manipulations will be done [5]. At first, introducing dependence (3) into equation (1) one obtains

$$\begin{gathered}C_e(T_e)\frac{\partial T_e}{\partial t}=\operatorname{div}\left[\lambda_e(T_e,T_l)\operatorname{grad}T_e+\tau_e\frac{\partial \mathbf{q}_e}{\partial t}\right]-\\ G(T_e)\left(T_e-T\right)+Q\end{gathered} \tag{8}$$

or using the Schwarz theorem

$$\begin{gathered}C_e(T_e)\frac{\partial T_e}{\partial t}=\operatorname{div}\left[\lambda_e(T_e,T_l)\operatorname{grad}T_e\right]+\\ \tau_e\frac{\partial}{\partial t}\left(\operatorname{div}\mathbf{q}_e\right)-G(T_e)\left(T_e-T_l\right)+Q\end{gathered} \tag{9}$$

From equation (1) results

$$\operatorname{div}\mathbf{q}_e=-C_e(T_e)\frac{\partial T_e}{\partial t}-G(T_e)\left(T_e-T\right)+Q \tag{10}$$

Introducing (10) into (9) one has

$$\begin{gathered}C_e(T_e)\frac{\partial T_e}{\partial t}+\tau_e\frac{\partial}{\partial t}\left[C_e(T_e)\frac{\partial T_e}{\partial t}\right]=\operatorname{div}\left[\lambda_e(T_e,T_l)\operatorname{grad}T_e\right]-\\ G(T_e)\left(T_e-T_l\right)-\tau_e\frac{\partial}{\partial t}\left[G(T_e)\left(T_e-T_l\right)\right]+Q+\tau_e\frac{\partial Q}{\partial t}\end{gathered} \tag{11}$$

Because

$$\frac{\partial G(T_e)}{\partial t}=\frac{\mathrm{d}G(T_e)}{\mathrm{d}T_e}\frac{\partial T_e}{\partial t}=G'(T_e)\frac{\partial T_e}{\partial t} \tag{12}$$

and

$$\frac{\partial C_e(T_e)}{\partial t}=\frac{\mathrm{d}C_e(T_e)}{\mathrm{d}T_e}\frac{\partial T_e}{\partial t}=C_e'(T_e)\frac{\partial T_e}{\partial t} \tag{13}$$

then the equation (11) can be written in the form

$$\begin{gathered}C_e(T_e)\frac{\partial T_e}{\partial t}+\tau_e C_e'(T_e)\left(\frac{\partial T_e}{\partial t}\right)^2+\tau_e C_e(T_e)\frac{\partial^2 T_e}{\partial t^2}=\\ \operatorname{div}\left[\lambda_e(T_e,T_l)\operatorname{grad}T_e\right]-G(T_e)\left(T_e-T_l\right)-\\ \tau_e G'(T_e)\frac{\partial T_e}{\partial t}\left(T_e-T_l\right)-\tau_e G(T_e)\left(\frac{\partial T_e}{\partial t}-\frac{\partial T_l}{\partial t}\right)+Q+\tau_e\frac{\partial Q}{\partial t}\end{gathered} \tag{14}$$

or

$$\begin{gathered}C_e(T_e)\left(\frac{\partial T_e}{\partial t}+\tau_e\frac{\partial^2 T_e}{\partial t^2}\right)=\operatorname{div}\left[\lambda_e(T_e,T_l)\operatorname{grad}T_e\right]-\\ \left[G(T_e)+\tau_e G'(T_e)\frac{\partial T_e}{\partial t}\right]\left(T_e-T_l\right)-\tau_e G(T_e)\left(\frac{\partial T_e}{\partial t}-\frac{\partial T_l}{\partial t}\right)-\\ \tau_e C_e'(T_e)\left(\frac{\partial T_e}{\partial t}\right)^2+Q+\tau_e\frac{\partial Q}{\partial t}\end{gathered} \tag{15}$$

In similar way the equation describing lattice temperature can be derived and then

$$\begin{gathered}C_l(T_l)\left(\frac{\partial T_l}{\partial t}+\tau_l\frac{\partial^2 T_l}{\partial t^2}\right)=\operatorname{div}\left[\lambda_l(T_l)\operatorname{grad}T_l\right]+\\ \left[G(T_e)+\tau_l G'(T_e)\frac{\partial T_e}{\partial t}\right]\left(T_e-T_l\right)+\\ \tau_l G(T_e)\left(\frac{\partial T_e}{\partial t}-\frac{\partial T_l}{\partial t}\right)-\tau_l C_l'(T_l)\left(\frac{\partial T_l}{\partial t}\right)^2\end{gathered} \tag{16}$$

Using the approach above presented, only two equations (15), (16) instead of equations (1), (2), (3), (4) should be solved. These equations are supplemented by boundary conditions (6) and the initial ones

$$\begin{gathered}t=0:\quad T_e(r,z,t)=T_l(r,z,t)=T_p\\ \left.\frac{\partial T_e(r,z,t)}{\partial t}\right|_{t=0}=\left.\frac{\partial T_l(r,z,t)}{\partial t}\right|_{t=0}=0\end{gathered} \tag{17}$$

It should be pointed out that in cylindrical co-ordinate system:

$$\begin{gathered}\operatorname{div}\left[\lambda_e(T_e,T_l)\operatorname{grad}T_e\right]=\frac{1}{r}\frac{\partial}{\partial r}\left[r\lambda_e(T_e,T_l)\frac{\partial T_e}{\partial r}\right]+\\ \frac{\partial}{\partial z}\left[\lambda_e(T_e,T_l)\frac{\partial T_e}{\partial z}\right]\end{gathered} \tag{18}$$

and

$$\operatorname{div}\left[\lambda_l(T_l)\operatorname{grad}T_l\right]=\frac{1}{r}\frac{\partial}{\partial r}\left[r\lambda_l(T_l)\frac{\partial T_l}{\partial r}\right]+\frac{\partial}{\partial z}\left[\lambda_l(T_l)\frac{\partial T_l}{\partial z}\right] \tag{19}$$

3. Finite difference method

The problem formulated has been solved using finite difference method [7]. The regular mesh created by $n\times n$ nodes with constant step h has been introduced. In Figure 2 the central node i,j and adjacent nodes i-1,j , i+1,j, i,j-1 , i,j+1 are shown. These nodes form so-called 5-points star.

For internal node $i\ j$ the following approximation of equation (15) is proposed

$$
\begin{aligned}
&C_{e\,i\,j}^{f-1}\left[\frac{T_{e\,i\,j}^{f}-T_{e\,i\,j}^{f-1}}{\Delta t}+\tau_e\frac{T_{e\,i\,j}^{f}-2T_{e\,i\,j}^{f-1}+T_{e\,i\,j}^{f-2}}{(\Delta t)^2}\right]=\\
&\operatorname{div}\left(\lambda_e\operatorname{grad}T_e\right)_{i\,j}^{f-1}-\\
&\left[G_{i\,j}^{f-1}+\frac{\tau_e}{\Delta t}G'^{\,f-1}_{i\,j}\left(T_{e\,i\,j}^{f-1}-T_{e\,i\,j}^{f-2}\right)\right]\left(T_{e\,i\,j}^{f-1}-T_{l\,i\,j}^{f-1}\right)-\\
&\tau_e G_{i\,j}^{f-1}\left(\frac{T_{e\,i\,j}^{f-1}-T_{e\,i\,j}^{f-2}}{\Delta t}-\frac{T_{l\,i\,j}^{f-1}-T_{l\,i\,j}^{f-2}}{\Delta t}\right)-\\
&\tau_e C'^{\,f-1}_{e\,i\,j}\left(\frac{T_{e\,i\,j}^{f-1}-T_{e\,i\,j}^{f-2}}{\Delta t}\right)^2+Q_{i\,j}^{f-1}+\tau_e\left(\frac{\partial Q}{\partial t}\right)_{i\,j}^{f-1}
\end{aligned}
\tag{20}
$$

where Δt is the time step and [6, 7]

$$
\begin{aligned}
&\operatorname{div}\left(\lambda_e\operatorname{grad}T_e\right)_{i\,j}^{f-1}=\frac{1}{h\,r_{i\,j}}\left[r_{i\,j+0.5}\,\lambda_{e\,i\,j+0.5}^{f-1}\left(\frac{\partial T_e}{\partial r}\right)_{i\,j+0.5}^{f-1}-\right.\\
&\left.r_{i\,j-0.5}\,\lambda_{e\,i\,j-0.5}^{f-1}\left(\frac{\partial T_e}{\partial r}\right)_{i\,j-0.5}^{f-1}\right]+\\
&\frac{1}{h}\left[\lambda_{e\,i+0.5\,j}^{f-1}\left(\frac{\partial T_e}{\partial z}\right)_{i+0.5\,j}^{f-1}-\lambda_{e\,i-0.5\,j}^{f-1}\left(\frac{\partial T_e}{\partial z}\right)_{i-0.5\,j}^{f-1}\right]
\end{aligned}
\tag{21}
$$

or

$$
\begin{aligned}
&\operatorname{div}\left(\lambda_e\operatorname{grad}T_e\right)_{i\,j}^{f-1}=\frac{1}{h\,r_{i\,j}}\left[\left(r_{i\,j}+\frac{h}{2}\right)\lambda_{e\,i\,j+0.5}^{f-1}\frac{T_{e\,i\,j+1}^{f-1}-T_{e\,i\,j}^{f-1}}{h}-\right.\\
&\left.\left(r_{i\,j}-\frac{h}{2}\right)\lambda_{e\,i\,j-0.5}^{f-1}\frac{T_{e\,i\,j}^{f-1}-T_{e\,i\,j-1}^{f-1}}{h}\right]+\\
&\frac{1}{h}\left[\lambda_{e\,i+0.5\,j}^{f-1}\frac{T_{e\,i+1\,j}^{f-1}-T_{e\,i\,j}^{f-1}}{h}-\lambda_{e\,i-0.5\,j}^{f-1}\frac{T_{e\,i\,j}^{f-1}-T_{e\,i-1\,j}^{f-1}}{h}\right]
\end{aligned}
\tag{22}
$$

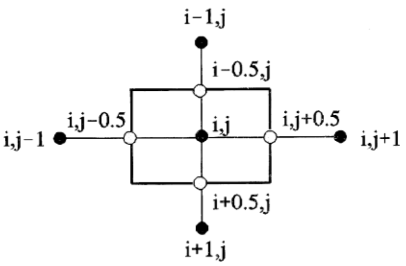

Fig. 2. 5-points star

The following formulas concerning the calculations of thermal conductivities are introduced [7]

$$
\lambda_{e\,i-0.5\,j}^{f-1}=\frac{2\lambda_{e\,i\,j}^{f-1}\lambda_{e\,i-1\,j}^{f-1}}{\lambda_{e\,i\,j}^{f-1}+\lambda_{e\,i-1\,j}^{f-1}}\,,\quad
\lambda_{e\,i+0.5\,j}^{f-1}=\frac{2\lambda_{e\,i\,j}^{f-1}\lambda_{e\,i+1\,j}^{f-1}}{\lambda_{e\,i\,j}^{f-1}+\lambda_{e\,i+1\,j}^{f-1}}
\tag{23}
$$

$$
\lambda_{e\,i\,j-0.5}^{f-1}=\frac{2\lambda_{e\,i\,j}^{f-1}\lambda_{e\,i\,j-1}^{f-1}}{\lambda_{e\,i\,j}^{f-1}+\lambda_{e\,i\,j-1}^{f-1}}\,,\quad
\lambda_{e\,i\,j+0.5}^{f-1}=\frac{2\lambda_{e\,i\,j}^{f-1}\lambda_{e\,i\,j+1}^{f-1}}{\lambda_{e\,i\,j}^{f-1}+\lambda_{e\,i\,j+1}^{f-1}}
\tag{24}
$$

and then the dependence (22) can be written in the form

$$
\begin{aligned}
&\operatorname{div}\left(\lambda_e\operatorname{grad}T_e\right)_{i\,j}^{f-1}=\Phi_1\frac{T_{e\,i\,j-1}^{f-1}-T_{e\,i\,j}^{f-1}}{R_{e\,i\,j1}^{f-1}}+\Phi_2\frac{T_{e\,i\,j+1}^{f-1}-T_{e\,i\,j}^{f-1}}{R_{e\,i\,j2}^{f-1}}+\\
&\Phi_3\frac{T_{e\,i-1\,j}^{f-1}-T_{e\,i\,j}^{f-1}}{R_{e\,i\,j3}^{f-1}}+\Phi_4\frac{T_{e\,i+1\,j}^{f-1}-T_{e\,i\,j}^{f-1}}{R_{e\,i\,j4}^{f-1}}
\end{aligned}
\tag{25}
$$

where

$$
R_{e\,i\,j1}^{f-1}=\frac{h}{2}\left(\frac{1}{\lambda_{e\,i\,j}^{f-1}}+\frac{1}{\lambda_{e\,i\,j-1}^{f-1}}\right),\quad
R_{e\,i\,j2}^{f-1}=\frac{h}{2}\left(\frac{1}{\lambda_{e\,i\,j}^{f-1}}+\frac{1}{\lambda_{e\,i\,j+1}^{f-1}}\right)
\tag{26}
$$

$$
R_{e\,i\,j3}^{f-1}=\frac{h}{2}\left(\frac{1}{\lambda_{e\,i\,j}^{f-1}}+\frac{1}{\lambda_{e\,i-1\,j}^{f-1}}\right),\quad
R_{e\,i\,j4}^{f-1}=\frac{h}{2}\left(\frac{1}{\lambda_{e\,i\,j}^{f-1}}+\frac{1}{\lambda_{e\,i+1\,j}^{f-1}}\right)
\tag{27}
$$

and

$$
\Phi_1=\frac{r_{i\,j}-0.5h}{h\,r_{i\,j}}\,,\quad \Phi_2=\frac{r_{i\,j}+0.5h}{h\,r_{i\,j}}\,,\quad \Phi_3=\Phi_4=\frac{1}{h}
\tag{28}
$$

On the basis of equation (20) the temperature $T_{ei\,j}^{f}$ is calculated, this means

$$
\begin{aligned}
&T_{e\,i\,j}^{f}=\frac{(\Delta t)^2}{C_{e\,i\,j}^{f-1}\left(\Delta t+\tau_e\right)}\operatorname{div}\left(\lambda_e\operatorname{grad}T_e\right)_{i\,j}^{f-1}-\\
&\frac{(\Delta t)^2}{C_{e\,i\,j}^{f-1}\left(\Delta t+\tau_e\right)}\left[G_{i\,j}^{f-1}+\frac{\tau_e}{\Delta t}G'^{\,f-1}_{i\,j}\left(T_{e\,i\,j}^{f-1}-T_{e\,i\,j}^{f-2}\right)\right]\left(T_{e\,i\,j}^{f-1}-T_{l\,i\,j}^{f-1}\right)-\\
&\frac{\tau_e(\Delta t)^2G_{i\,j}^{f-1}}{C_{e\,i\,j}^{f-1}\left(\Delta t+\tau_e\right)}\left(\frac{T_{e\,i\,j}^{f-1}-T_{e\,i\,j}^{f-2}}{\Delta t}-\frac{T_{l\,i\,j}^{f-1}-T_{l\,i\,j}^{f-2}}{\Delta t}\right)-\\
&\frac{\tau_e(\Delta t)^2C'^{\,f-1}_{e\,i\,j}}{C_{e\,i\,j}^{f-1}\left(\Delta t+\tau_e\right)}\left(\frac{T_{e\,i\,j}^{f-1}-T_{e\,i\,j}^{f-2}}{\Delta t}\right)^2+\frac{\Delta t+2\tau_e}{\Delta t+\tau_e}T_{e\,i\,j}^{f-1}-\frac{\tau_e}{\Delta t+\tau_e}T_{e\,i\,j}^{f-2}+\\
&\frac{(\Delta t)^2}{C_{e\,i\,j}^{f-1}\left(\Delta t+\tau_e\right)}\left[Q_{i\,j}^{f-1}+\tau_e\left(\frac{\partial Q}{\partial t}\right)_{i\,j}^{f-1}\right]
\end{aligned}
\tag{29}
$$

In similar way the difference equation for internal node i, j and lattice temperature (c.f. equation (21) can be derived and then

$$
\begin{aligned}
&T_{l\,i\,j}^{f}=\frac{(\Delta t)^2}{C_{l\,i\,j}^{f-1}\left(\Delta t+\tau_l\right)}\operatorname{div}\left(\lambda_l\operatorname{grad}T_l\right)_{i\,j}^{f-1}+\\
&\frac{(\Delta t)^2}{C_{l\,i\,j}^{f-1}\left(\Delta t+\tau_l\right)}\left[G_{i\,j}^{f-1}+\frac{\tau_l}{\Delta t}G'^{\,f-1}_{i\,j}\left(T_{l\,i\,j}^{f-1}-T_{l\,i\,j}^{f-2}\right)\right]\left(T_{e\,i\,j}^{f-1}-T_{l\,i\,j}^{f-1}\right)+\\
&\frac{\tau_l(\Delta t)^2G_{i\,j}^{f-1}}{C_{l\,i\,j}^{f-1}\left(\Delta t+\tau_l\right)}\left(\frac{T_{e\,i\,j}^{f-1}-T_{e\,i\,j}^{f-2}}{\Delta t}-\frac{T_{l\,i\,j}^{f-1}-T_{l\,i\,j}^{f-2}}{\Delta t}\right)-\\
&\frac{\tau_l(\Delta t)^2C'^{\,f-1}_{l\,i\,j}}{C_{l\,i\,j}^{f-1}\left(\Delta t+\tau_l\right)}\left(\frac{T_{l\,i\,j}^{f-1}-T_{l\,i\,j}^{f-2}}{\Delta t}\right)^2+\frac{\Delta t+2\tau_l}{\Delta t+\tau_l}T_{l\,i\,j}^{f-1}-\frac{\tau_l}{\Delta t+\tau_l}T_{l\,i\,j}^{f-2}
\end{aligned}
\tag{30}
$$

Summing up, for each transition $t^{f-1}\rightarrow t^{f}$ the electrons temperatures T_e and lattice temperatures T_l can be determined using the equations (29) and (30).

4. Examples of computations

In hyperbolic two-temperature model the thermophysical parameters appear: C_e, C_l, λ_e, λ_l, G, τ_e and τ_l. To define the thermal conductivity λ_e and heat capacity C_e of electrons the following relationships are widely used [1, 2, 3]

$$\lambda_e(T_e, T_l) = \lambda_0 T_e / T_l \tag{31}$$

and

$$C_e(T_e) = A_e T_e \tag{32}$$

where λ_0, A_e are the material constants. The remaining parameters, this means λ_l, C_l, G, τ_e, τ_l usually are assumed to be constant ones The domain of dimensions 200 nm $\times$ 200 nm made of gold is considered. The radius of laser beam is equal to r_D =50 nm. The following thermal parameters of gold have been taken into account [1, 2, 8, 9, 10]: lattice thermal conductivity $\lambda_l = \lambda_0 = 315$ W/(mK), electron thermal conductivity $\lambda_e = \lambda_0 T_e / T_l$, electrons volumetric specific heat $C_e = 70 T_e$ J/(m^3 K), lattice volumetric specific heat $C_l = 2.5$ MJ/(m^3 K), electron-phonon coupling factor $G = 2.6 \cdot 10^{16}$ W/(m^3 K), relaxation time of electrons $\tau_e = 0.04$ ps, relaxation time of phonons $\tau_l = 0.8$ ps.

Initial temperature is equal to T_p =300 K . The domain is subjected to a ultrashort-pulse laser irradiation (R =0.93, I_0 =13.4 J/m^2, t_p=0.1 ps, δ=15.3 nm).

The problem has been solved using finite difference method under the assumption that Δt=0.0001 ps and h = 4 nm.

In Figure 3 the calculated electrons temperature history at the point A marked in Figure 1 is shown. In Figure 4 the lattice temperature distribution for time 0.6 ps is presented. It is visible that the lattice temperature is very close to the initial temperature.

Figures 5 and 6 illustrate temperature distribution of electrons for selected moments of times.

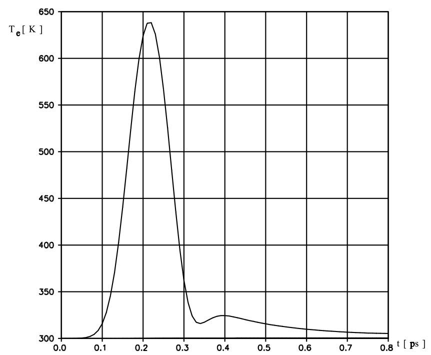

Fig. 3. Electrons temperature history at the point A

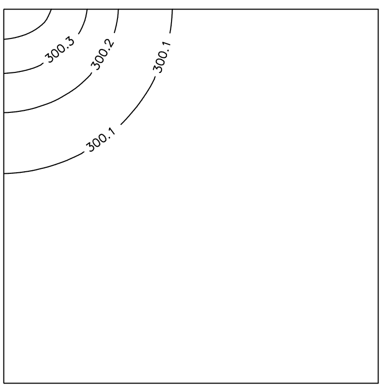

Fig. 4. Lattice temperature distribution for time 0.6 ps

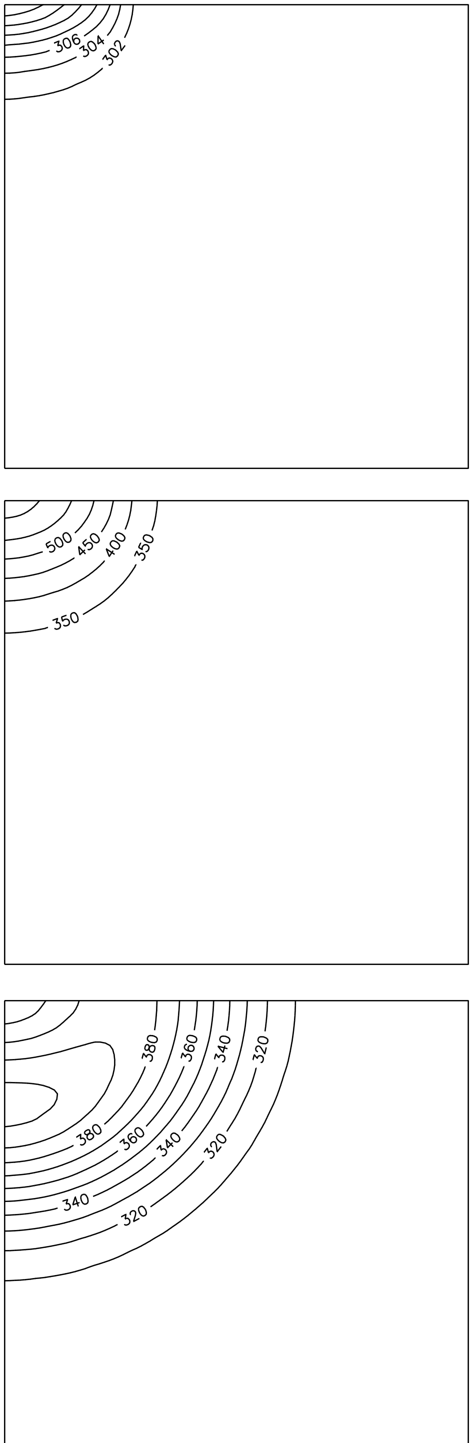

Fig. 5. Electrons temperature distribution for times 0.1, 0.2 and 0.3 ps

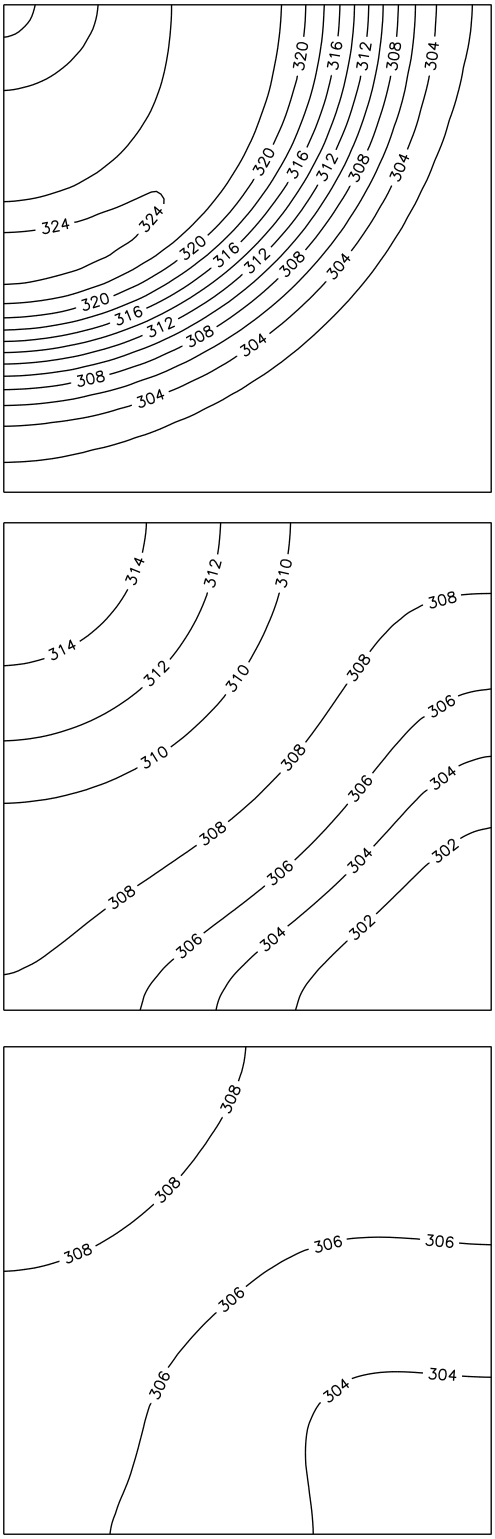

Fig. 6. Electrons temperature distribution
for times 0.4, 0.5 and 0.6 ps

5. Conclusions

Heat transfer proceeding in metal film subjected to an ultrashort-pulse laser heating is discussed. To describe the process the two-temperature model is applied. The problem has been solved using the explicit scheme of finite difference method. The approach presented here can be used for analysis of heat transfer proceeding in the multi-layered domains being a composition of optional number of thin films with different parameters. The FDM algorithm proposed here allows one to treat such a domain as a conventionally homogeneous one.

The problems discussed in this paper concern only the heating process proceeding in metal film subjected to the laser pulse. The phase changes (e.g. melting or ablation) are not taken into account. The investigations in this range are at present realized.

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