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Numerical Modeling of Short-Pulse Laser Interactions with Multi-Layered Thin Metal Films

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Abstract: Multi-layered thin metal film subjected to a short-pulse laser heating is considered. Mathematical description of the process discussed bases on the equation in which there appear the relaxation time and the thermalization time (dual-phase-lag-model). In this study we develop a three level implicit finite difference scheme for numerical modelling of heat transfer in non-homogeneous metal film. At the interfaces an ideal contact between successive layers is assumed. At the stage of computations a solution of only one three-diagonal linear system corresponds to transition from time t to $t + \Delta t$. The mathematical model, numerical algorithm and examples of computations are presented in the paper.

Keywords: microscale heat transfer, multi-layered metal films, laser pulse, numerical simulation

1 Introduction

Heat transfer through thin films subjected to an ultrafast laser pulse is of vital importance in microtechnology applications and it is a reason that the problems connected with fast heating of solids has become a very active research area. Generally speaking, the differences between the macroscopic heat conduction equation basing on the Fourier law and the models describing the ultrafast laser pulse interactions with metal films appear because of extremely short duration, extreme temperature gradients and geometrical features of domain considered [Özişik and Tzou (1994); Tamma and Zhou (1998); Al-Nimr (1997)].

From the mathematical point of view, nowadays there exist different models describing the mechanism of process discussed. The first approach leads to the so-called continuum models. In this place the well known Cattaneo equation can be

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mentioned. Modification of Fourier law depending on the assumption of finite speed of thermal energy propagation leads to the hyperbolic equation describing the transient temperature field in domain considered [Chen, Borca-Tasciuc and Yang (2004)]. In this equation the parameter τ_q called the relaxation time of heat carriers appears.

The microscopic two-step parabolic model belongs also to the continuum ones [Chen and Beraun (2001); Kaba and Dai (2005); Lin and Zhigilei (2008)].The two-step parabolic model involves two energy equations determining the thermal processes in the electron gas and the metal lattice. It is also possible to transform this model to the equation containing a second order time derivative and higher order mixed derivative in both time and space. Two positive constants τ_q, τ_T appear in this equation. They correspond to the relaxation time, which is the mean time for electrons to change their energy states and the thermalization time, which is the mean time required for electrons and lattice to reach equilibrium [Orlande and Özişik (1995)].

The same energy equation can be obtained on the basis of classical Fourier-Kirchhoff equation in which the vector of heat flux $\mathbf{q}$ is defined in a special way (both relaxation and thermalization times are taken into account – see: chapter 2).

A second group of models bases on the Boltzmann transport equation (BTE). It is a conservation equation where the conserved quantity is the number of particles [Tian and Yang (2008)]. The general form of BTE is rather complex but it can be modified to analyse the special cases, for instance the systems created by phonons, electrons etc.

Microscale heat transfer processes can be also considered using the molecular approaches [Smith and Norris (2003); Theodosiou and Saravanos (2007); Liu and Tsai (2009); Chen, Cheng and Hsu (2007)]. Here the lattice dynamic approach, molecular dynamic approach and Monte Carlo simulations can be mentioned.

In this paper we consider the mathematical model created by the system of microscopic heat transfer equations which is supplemented by ideal thermal contact conditions at the interfaces, non-flux conditions on the external surfaces of thin film and initial ones corresponding to initial temperature and initial heating rate. The short-pulse laser interaction with the film is taken into account by introduction of internal volumetric heat sources to the microscopic heat transfer equations. The 1D problem is analyzed. For most short laser pulse interactions with thin films, the laser spot size is much larger than film thickness. Therefore, it is reasonable to treat the interactions as a one-dimensional heat transfer process [Chen and Beraun (2001)], although the method proposed can be easily generalized on the 2D or 3D tasks and also nonhomogeneous materials can be considered, e.g. [Sladek , Sladek

and Alturi (2004)].

To solve the problem formulated the three level implicit finite difference method is developed. In particular, the version close to the control volume method approach is discussed [Mochnacki and Suchy (1995)]. Both the ideal contact conditions and the adiabatic ones are introduced to the FDM equations by the appropriate definitions of thermal resistances between the nodes. This approach corresponds to conventional homogenization of multi-layered domain. The transition from time t to $t+\Delta t$ reduces to the solution of one three-diagonal system of equations (the Thomas algorithm has been applied).

To verify the algorithm proposed, the results of simulation have been compared with the analytical solution concerning the homogeneous domain. The comparison allowed to analyze the influence of time and space discretization on the errors distribution. The results have been also verified by the comparison with the experimental results for 0.1 μm gold film obtained in [Tang and Araki (1999)] and with the solution concerning double layered gold-chromium film [Dai and Nassar (2000)]. It should be pointed out that the transient temperature field measurements are possible only in indirect way. In particular the variation of reflectivity is shown to be proportional to variation of the electron temperature and the measurements of this parameter changes can be re-calculated on the changes of temperature [Orlande, Özişik and Tzou (1995)].

The last example presented in this paper shows the possibilities of method application in the case of non-homogeneous domain created by parallel layers gold-chromium-gold-chromium.

2 Heat transport at the microscale

At first, the microscopic two-step model presented among others in [Al-Nimr (1997); Lin and Zhigilei (2008)] will be discussed. The two-step model involves two energy equations determining the heat exchange in the electron gas and the metal lattice. The equations creating the model discussed can be written in the form

$$c_e(T_e)\frac{\partial T_e}{\partial t} = \nabla\left[\lambda_e(T_e)\nabla T_e\right] - G(T_e - T_l) \tag{1}$$

$$c_l(T_l)\frac{\partial T_l}{\partial t} = \nabla\left[\lambda_l(T_l)\nabla T_l\right] + G(T_e - T_l) \tag{2}$$

where $T_e = T_e(x,t)$, $T_l = T_l(x,t)$ are the temperatures of electrons and lattice, respectively, $c_e(T_e)$, $c_l(T_l)$ are the volumetric specific heats, $\lambda_e(T_e)$, $\lambda_l(T_l)$ are the thermal conductivities, G is the coupling factor [Al-Nimr (1997)]. which characterizes the energy exchange between phonon and electrons [Tian and Yang (2008)]. In the case

of pure metals the system of equations (1), (2) under the assumption that volumetric specific heats c_e and c_l are the constant values, is reduced to

$$c_e \frac{\partial T_e}{\partial t} = \nabla (\lambda_e \nabla T_e) - G(T_e - T_l) \tag{3}$$

$$c_l \frac{\partial T_l}{\partial t} = G(T_e - T_l) \tag{4}$$

This simplification, according to [Al-Nimr (1997)], results from the fact that the incident radiation and conductional heat flux are absorbed and diffused mainly by electrons.

The equations (3), (4) using a certain elimination technique can be substituted by a single equation containing a higher-order mixed derivative in both time and space. From equation (4) it results that

$$T_e = T_l + \frac{c_l}{G} \frac{\partial T_l}{\partial t} \tag{5}$$

Putting (5) into (3) one has

$$c_e \left(\frac{\partial T_l}{\partial t} + \frac{c_l}{G} \frac{\partial^2 T_l}{\partial t^2} \right) = \nabla (\lambda_e \nabla T_l) + \frac{c_l}{G} \nabla \left[\lambda_e \frac{\partial}{\partial t} (\nabla T_l) \right] - c_l \frac{\partial T_l}{\partial t} \tag{6}$$

this means

$$(c_e + c_l) \frac{\partial T_l}{\partial t} + \frac{c_e c_l}{G} \frac{\partial^2 T_l}{\partial t^2} = \nabla (\lambda_e \nabla T_l) + \frac{c_l}{G} \frac{\partial}{\partial t} [\nabla (\lambda_e \nabla T_l)] \tag{7}$$

or

$$(c_e + c_l) \left[\frac{\partial T_l}{\partial t} + \frac{c_e c_l}{G(c_e + c_l)} \frac{\partial^2 T_l}{\partial t^2} \right] = \nabla (\lambda_e \nabla T_l) + \frac{c_l}{G} \frac{\partial}{\partial t} [\nabla \lambda_e (\nabla T_l)] \tag{8}$$

Denoting

$$\tau_T = \frac{c_l}{G}, \quad \tau_q = \frac{1}{G} \left(\frac{1}{c_e} + \frac{1}{c_l} \right)^{-1} \tag{9}$$

finally one obtains

$$c \left[\frac{\partial T(x,t)}{\partial t} + \tau_q \frac{\partial^2 T(x,t)}{\partial t^2} \right] = \nabla [\lambda \nabla T(x,t)] + \tau_T \nabla \left[\lambda \frac{\partial \nabla T(x,t)}{\partial t} \right] \tag{10}$$

where $T(x, t) = T_l(x, t)$ is the macroscopic lattice temperature [Özişik and Tzou (1994)], $c = c_l + c_e$ is the effective volumetric specific heat resulting from the serial assembly of electrons and phonons and $\lambda = \lambda_e$ [Tzou and Chiu (2001)].

The positive constants τ_q, τ_T correspond to relaxation time and thermalization time, respectively and they are characteristic for the so-called dual-phase-lag model. The relaxation time τ_q is the mean time for electrons to change their energy states, while the thermalization time τ_T is the mean time required for electrons and lattice to reach equilibrium [Orlande and Özişik (1995)].

The well known macroscopic energy equation

$$c\frac{\partial T(x,t)}{\partial t} = -\nabla \cdot \mathbf{q}(x,t) \tag{11}$$

can be transformed to the microscale when in the place of classical Fourier law $\mathbf{q}(x,t) = -\lambda \nabla T(x,t)$ one introduces the following formula

$$\mathbf{q}(x,t+\tau_q) = -\lambda \nabla T(x,t+\tau_T) \tag{12}$$

Using the Taylor series expansions the following first-order approximation of equation (12) can be taken into account

$$\mathbf{q}(x,t) + \tau_q \frac{\partial \mathbf{q}(x,t)}{\partial t} = -\lambda \left[\nabla T(x,t) + \tau_T \frac{\partial \nabla T(x,t)}{\partial t} \right] \tag{13}$$

or

$$-\mathbf{q}(x,t) = \tau_q \frac{\partial \mathbf{q}(x,t)}{\partial t} + \lambda \nabla T(x,t) + \tau_T \lambda \frac{\partial \nabla T(x,t)}{\partial t} \tag{14}$$

This formula should be introduced to equation (11) and then

$$c\frac{\partial T(x,t)}{\partial t} = \tau_q \frac{\partial}{\partial t} \left[\nabla \mathbf{q}(x,t) \right] + \nabla \left[\lambda \nabla T(x,t) \right] + \tau_T \nabla \left[\lambda \frac{\partial \nabla T(x,t)}{\partial t} \right] \tag{15}$$

Substituting $-\nabla \mathbf{q}$ by $c(\partial T / \partial t)$ one obtains

$$c\left[\frac{\partial T(x,t)}{\partial t} + \tau_q \frac{\partial^2 T(x,t)}{\partial t^2} \right] = \nabla \left[\lambda \nabla T(x,t) \right] + \tau_T \nabla \left[\lambda \frac{\partial \nabla T(x,t)}{\partial t} \right] \tag{16}$$

this means the same equation as equation (10).

In this paper the problem of heat diffusion in the presence of volumetric internal heat sources $Q(x, t)$ is considered. It can be shown that in this case the equation (16) must be supplemented by additional components, in particular

$$c\left[\frac{\partial T(x,t)}{\partial t} + \tau_q \frac{\partial^2 T(x,t)}{\partial t^2} \right] = \nabla \left[\lambda \nabla T(x,t) \right] + \tau_T \nabla \left[\lambda \frac{\partial \nabla T(x,t)}{\partial t} \right] + Q(x,t) + \tau_q \frac{\partial Q(x,t)}{\partial t} \tag{17}$$

3 Multi-layered domain

Let us consider a multi-layered thin film of thickness $L = L_1 + L_2 + ... + L_M$ (as in Figure 1) with an initial temperature distribution $T(x, 0) = T_0$, constant thermal properties of successive layers and ideal thermal contact between the layers.

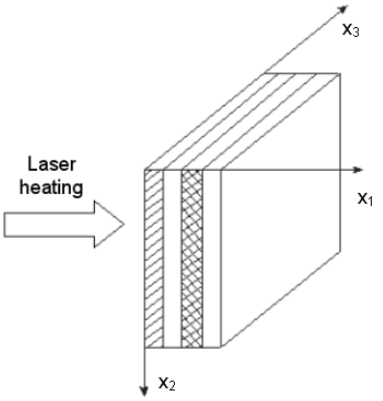

Figure 1: Multi-layered domain

The 1D problem is analyzed (heat transfer in direction perpendicular to the layers is taken into account). A front surface x= 0 is irradiated by a laser pulse and according to ref. [Tang and Araki (1999)], the conductional heat transfer can be modeled by the equation (17) with internal volumetric heat sources $Q(x, t)$, at the same time for x= 0 and x= L the non-flux conditions can be assumed. In this paper the following formula [Kaba and Dai (2005); Tang and Araki (1999)] determining the capacity of internal heat sources has been applied

$$Q(x,t) = \sqrt{\frac{\beta}{\pi}} \frac{1-R}{t_p \delta} I_0 \exp\left[-\frac{x}{\delta} - \beta \frac{(t-2t_p)^2}{t_p^2} \right] \tag{18}$$

where I_0 is the laser intensity which is defined as total energy carried by a laser pulse per unit cross-section of the laser beam, t_p is the characteristic time of laser pulse, δ is the characteristic transparent length of irradiated photons called the absorption depth, R is the reflectivity of the irradiated surface and β= 4ln2 [Chen and Beraun (2001)]. The local and temporary value of $Q(x, t)$ results from the distance x between surface subjected to laser action and the point considered.

So, the following system of equations is taken into account

$$x \in \Omega_m : \quad c_m \left[\frac{\partial T_m(x,t)}{\partial t} + \tau_{qm} \frac{\partial^2 T_m(x,t)}{\partial t^2} \right] = \frac{\partial}{\partial x} \left[\lambda_m \frac{\partial T_m(x,t)}{\partial x} \right] + \tau_{Tm} \frac{\partial}{\partial t} \left[\frac{\partial}{\partial x} \left(\lambda_m \frac{\partial T_m(x,t)}{\partial x} \right) \right] + Q_m(x,t) + \tau_{qm} \frac{\partial Q_m(x,t)}{\partial t} \tag{19}$$

where m= 1, 2, ..., M identifies the layers of domain considered.

The boundary conditions on the contact surfaces between sub-domains have the form of continuity ones, this means

$$x \in \Gamma_m : \quad \begin{cases} T_m(x,t) = T_{m+1}(x,t) \\ q_m(x,t) = q_{m+1}(x,t) \end{cases} , \quad m = 1,2,...,M-1 \tag{20}$$

On the outer surfaces of the system the no-flux conditions are introduced

$$x \in \Gamma_0 : \quad q_1(x,t) = 0, \quad x \in \Gamma_M : \quad q_M(x,t) = 0 \tag{21}$$

The initial conditions are assumed in the following way

$$t = 0 : \quad T_m(x,0) = T_{m0}, \quad \left. \frac{\partial T_m(x,t)}{\partial t} \right|_{t=0} = 0 \tag{22}$$

4 Numerical model

At the stage of numerical computations the finite difference method has been used. A geometrical mesh is shown in Figure 2. One can see that the internal nodes close to the external or internal boundaries are located at the distance of $0.5h$ from Γ_m. Additionally a time grid

$$t^0 < t^1 < ... < t^{f-2} < t^{f-1} < t^f < ... < t^F < \infty \tag{23}$$

with constant time step Δt is introduced.

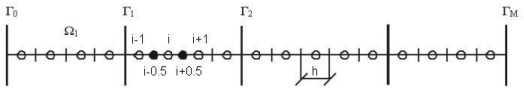

Figure 2: The mesh

We shall seek the differential analogue of 1D operator $\nabla(\lambda\nabla T)$ for a 3-point star – as in Figure 2. At the distances of $0.5h$ on the arms of the star, auxiliary points were distinguished. We shall make use of the approximation of a derivative by mean quotient. Thus

$$\begin{aligned}\left(\lambda\frac{\partial T}{\partial x}\right)^f_{i+0.5} &= \lambda^{f-1}_{i+0.5}\frac{T^f_{i+1}-T^f_i}{h}\\ \left(\lambda\frac{\partial T}{\partial x}\right)^f_{i-0.5} &= \lambda^{f-1}_{i-0.5}\frac{T^f_i-T^f_{i-1}}{h}\end{aligned} \tag{24}$$

An index f shows that the implicit differential scheme will be used here, at the same time the thermal conductivities are taken for time t^{f-1} to obtain the linear form of final FDM equations.

The conductivities λ in directions i+1 and $i-1$ will be approximated by the mean harmonics of the conductivities in the star nodes, namely

$$\lambda^{f-1}_{i+0.5}=\frac{2\lambda^{f-1}_i\lambda^{f-1}_{i+1}}{\lambda^{f-1}_i+\lambda^{f-1}_{i+1}},\quad \lambda^{f-1}_{i-0.5}=\frac{2\lambda^{f-1}_i\lambda^{f-1}_{i-1}}{\lambda^{f-1}_i+\lambda^{f-1}_{i-1}} \tag{25}$$

Then

$$\begin{aligned}\left(\lambda\frac{\partial T}{\partial x}\right)^f_{i+0.5} &= \frac{T^f_{i+1}-T^f_i}{R^{f-1}_{i+1}},\\ \left(\lambda\frac{\partial T}{\partial x}\right)^f_{i-0.5} &= \frac{T^f_i-T^f_{i-1}}{R^{f-1}_{i-1}}\end{aligned} \tag{26}$$

where

$$R^{f-1}_{i+1}=\frac{0.5h}{\lambda^{f-1}_i}+\frac{0.5h}{\lambda^{f-1}_{i+1}},\quad R^{f-1}_{i-1}=\frac{0.5h}{\lambda^{f-1}_i}+\frac{0.5h}{\lambda^{f-1}_{i-1}} \tag{27}$$

are the thermal resistances from the node i to the nodes i+ 1 and $i-1$.

Still making use of the mean quotient definition, we can write

$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)^f_i=\frac{1}{h}\left[\left(\lambda\frac{\partial T}{\partial x}\right)^f_{i+0.5}-\left(\lambda\frac{\partial T}{\partial x}\right)^f_{i-0.5}\right] \tag{28}$$

or

$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)^f_i=\frac{T^f_{i+1}-T^f_i}{R^{f-1}_{i+1}}\Psi_{i+1}+\frac{T^f_{i-1}-T^f_i}{R^{f-1}_{i-1}}\Psi_{i-1} \tag{29}$$

where $\Psi_{i+1} = \Psi_{i-1} = 1/h$.

The FDM approximation of equations (19) for transition $t^{f-1} \to t^f$ takes a form

$$c_i \frac{T_i^f - T_i^{f-1}}{\Delta t} + c_i \tau_{qi} \frac{T_i^f - 2T_i^{f-1} + T_i^{f-2}}{(\Delta t)^2} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right)_i^f + \frac{\tau_{Ti}}{\Delta t}\left[\frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right)_i^f - \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right)_i^{f-1}\right] + Q_i^f + \tau_{qi}\left(\frac{\partial Q}{\partial t}\right)_i^f \quad (30)$$

and next

$$c_i \frac{T_i^f - T_i^{f-1}}{\Delta t} + c_i \tau_{qi} \frac{T_i^f - 2T_i^{f-1} + T_i^{f-2}}{(\Delta t)^2} = \frac{T_{i+1}^f - T_i^f}{R_{i+1}^{f-1}}\Psi_{i+1} + \frac{T_{i-1}^f - T_i^f}{R_{i-1}^{f-1}}\Psi_{i-1} + \frac{\tau_{Ti}}{\Delta t}\left(\frac{T_{i+1}^f - T_i^f}{R_{i+1}^{f-1}}\Psi_{i+1} + \frac{T_{i-1}^f - T_i^f}{R_{i-1}^{f-1}}\Psi_{i-1}\right) - \frac{\tau_{Ti}}{\Delta t}\left(\frac{T_{i+1}^{f-1} - T_i^{f-1}}{R_{i+1}^{f-1}}\Psi_{i+1} + \frac{T_{i-1}^{f-1} - T_i^{f-1}}{R_{i-1}^{f-1}}\Psi_{i-1}\right) + Q_i^f + \tau_{qi}\left(\frac{\partial Q}{\partial t}\right)_i^f \quad (31)$$

The last equation can be written in the form

$$A_i T_{i-1}^f + B_i T_i^f + C_i T_{i+1}^f = D_i T_{i-1}^{f-1} + E_i T_i^{f-1} + F_i T_{i+1}^{f-1} + \frac{\tau_{qi}}{(\Delta t)^2} T_i^{f-2} - \frac{Q_i^f}{c_i} - \frac{\tau_{qi}}{c_i}\left(\frac{\partial Q}{\partial t}\right)_i^f \quad (32)$$

where

$$A_i = \frac{\Psi_{i-1}}{c_i R_{i-1}^{f-1}}\left(1 + \frac{\tau_{Ti}}{\Delta t}\right) \quad (33)$$

$$C_i = \frac{\Psi_{i+1}}{c_i R_{i+1}^{f-1}}\left(1 + \frac{\tau_{Ti}}{\Delta t}\right) \quad (34)$$

$$B_i = -\frac{1}{\Delta t}\left(1 + \frac{\tau_{qi}}{\Delta t}\right) - A_i - C_i \quad (35)$$

$$D_i = \frac{\Psi_{i-1}}{c_i R_{i-1}^{f-1}} \frac{\tau_{Ti}}{\Delta t} \quad (36)$$

$$F_i = \frac{\Psi_{i+1}}{c_i R_{i+1}^{f-1}} \frac{\tau_{Ti}}{\Delta t} \quad (37)$$

$$E_i = -\frac{1}{\Delta t}\left(1+\frac{2\tau_{qi}}{\Delta t}\right) - D_i - F_i \tag{38}$$

Finally

$$A_i T_{i-1}^f + B_i T_i^f + C_i T_{i+1}^f = G_i^f \tag{39}$$

where

$$G_i^f = D_i T_{i-1}^{f-1} + E_i T_i^{f-1} + F_i T_{i+1}^{f-1} + \frac{\tau_{qi}}{(\Delta t)^2} T_i^{f-2} - \frac{Q_i^f}{c_i} - \frac{\tau_{qi}}{c_i}\left(\frac{\partial Q}{\partial t}\right)_i^f \tag{40}$$

The same equations are accepted for the nodes close to external and internal boundaries. If a central node is located near an internal boundary Γ_m for which an ideal contact is assumed, then one should remember that in formulas determining the thermal resistances, the values of thermal conductivities corresponding to different sub-domains must be introduced. No-flux condition given for Γ_0 and Γ_M is modelled by substitution of very big number (e.g. 10^{10}) in place of thermal resistance in direction to an external boundary, at the same time the 'missing' left or right hand sides temperatures can be assumed in an optional way (e.g. ambient temperatures). A start point of numerical simulation process results from the initial conditions, in particular $T_i^0 = T_i^1 = T_0$, $i = 1,2,...,N$. The system of FDM equations (39) has been solved using the Thomas algorithm [Majchrzak and Mochnacki (2004)] for three-diagonal linear system.

5 Examples of computations

To test the accuracy and effectiveness of the method proposed, at first the following task has been solved. The single layer of thickness $L = 10^{-4}$ which thermophysical parameters equal λ = 1, c= 1, $\tau_q = 1/\pi^2 + 100$, $\tau_T = 1/\pi^2 + 10^{-6}$, $Q(x, t)$ = 0 is considered. So, the following equation is taken into account

$$\frac{\partial T(x,t)}{\partial t} + \left(\frac{1}{\pi^2}+100\right)\frac{\partial^2 T(x,t)}{\partial t^2} = \frac{\partial^2 T(x,t)}{\partial x^2} + \left(\frac{1}{\pi^2}+10^{-6}\right)\frac{\partial^3 T(x,t)}{\partial t \partial x^2} \tag{41}$$

Additionally

$$T(0,t) = 0, \quad T(L,t) = 0 \tag{42}$$

and

$$\begin{aligned} &T(x,0) = \sin(10^4 \pi x), \\ &\left.\frac{\partial T(x,t)}{\partial t}\right|_{t=0} = -\pi^2 \sin(10^4 \pi x) \end{aligned} \tag{43}$$

Analytical solution of the problem formulated above is [Dai and Nassar (2001)]:

$$T(x,t) = \exp(-\pi^2 t)\sin(10^4 \pi x) \tag{44}$$

Using the algorithm presented in the previous chapter under the assumption that N= 200 (h= 5·10^{-7}) and Δt= 0.001 the transient temperature field has been found. In Figure 3 the comparison of numerical and analytical solutions for times t= 0.02, 0.04, 0.06, 0.08 and 0.1 is shown. A good agreement between both solutions is visible.

To show convergence, the error of numerical solution is calculated [Dai and Nassar (2001)]

$$B^f = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(T_i^f - T_{di}^f\right)^2} \tag{45}$$

where T_{di}^f is the analytical solution at the node i for time t^f. Figure 4 illustrates the courses of curves at the central point (x= 0.5·10^{-4}) for time steps Δt= 0.001, 0.005 and 0.01, respectively, while in Figure 5 the errors of numerical solutions are shown. Figure 6 shows the influence of mesh step on the results of computations. Summing up, the exactness of numerical solution is connected with the proper choice of time and mesh steps but very essential feature of numerical algorithm consisting in the error decrease with time is visible in every case of discretization.

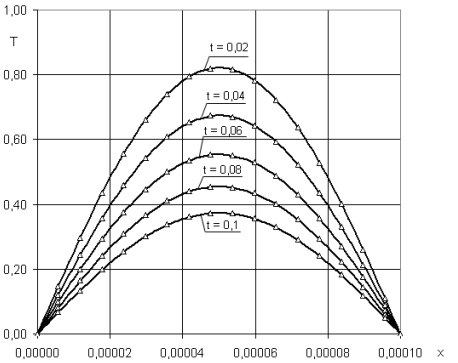

Figure 3: Analytical (lines) and numerical (symbols) solutions (N = 200, Δt= 0.001)

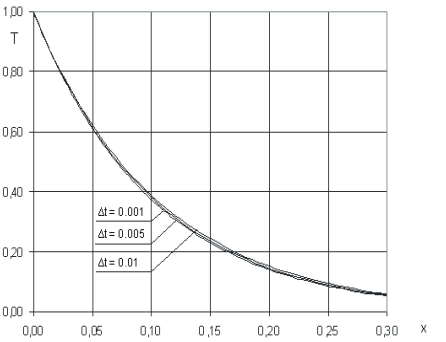

Figure 4: Course of curve at the central point

The second example concerns the gold layer with thickness L= 0.2 μm. The layer is subjected to a short-pulse laser irradiation (R= 0.93, I_0= 13.7 J/m^2, t_p= 96 fs, δ =

5 nm). Thermophysical parameters of material are the following: λ = 317 W/(mK), c= 2.4897 MJ/(m^{3}K), τ_q= 8.5ps (1ps = 10^{-12}s), τ_T= 90ps. The mesh step: h= 1nm, time step: Δt= 0.005 ps. The results of simulation have been compared with the experimental data quoted in [Tang and Araki (1999)]. In Figure 7 the heating (cooling) curves at the point corresponding to x= 0 are shown (on the vertical axis the dimensionless temperature $[T(0, t)- T_0] / (T_{max} - T_0)$ is marked). The good agreement of numerical simulation and experiment is clearly visible.

Figure 8 illustrates the differences between the solution obtained using the model discussed here and the solution resulting from Fourier one.

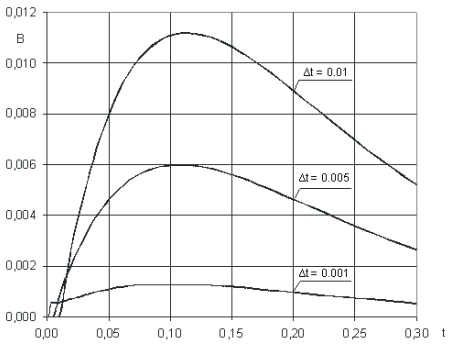

Figure 5: Errors of the numerical solutions with different time steps (N = 200)

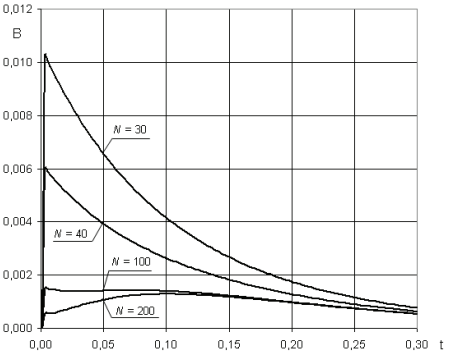

Figure 6: Errors of the numerical solutions with different meshes (Δ t= 0.001)

In the paper [Dai and Nassar (2000)] the problem of heat transport in a double-layered thin film (gold and chromium) subjected to a laser pulse has been discussed. For the same input data (the necessary differences have been introduced in the definition of $Q(x, t)$), a similar example has been solved using the approach presented here, and the results proved to be close to the results shown in the quoted paper. The layer of thickness L= 100nm being a composition of gold layer L_1= 50nm and chromium layer L_2= 50nm is subjected to a short-pulse laser heating (R= 0.93, I_0= 13.7 J/m^2, t_p= 96 fs, δ = 15.3 nm). Thermophysical parameters of sub-domains are the following: λ = 17 W/(mK), c= 2.4897 MJ/(m^{3}K), τ_q= 8.5ps, τ_T= 90ps (gold), λ = 93 W/(mK), c= 3.2148 MJ/(m^{3}K), τ_q= 0.136ps, τ_T= 7.86ps (chromium). The mesh step: h= 0.5nm, time step: Δt= 0.005 ps.

In Figure 9 the normalized heating (cooling) curves at the points close to external surface (1), interface (3) and in the middle of gold (2) layer are shown.

The last example concerns the multi-layer domain (gold-chromium-gold-chromium).

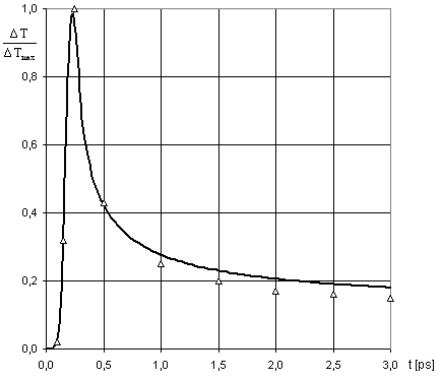

Figure 7: Comparison with experimental data ([Tang and Araki (1999)]

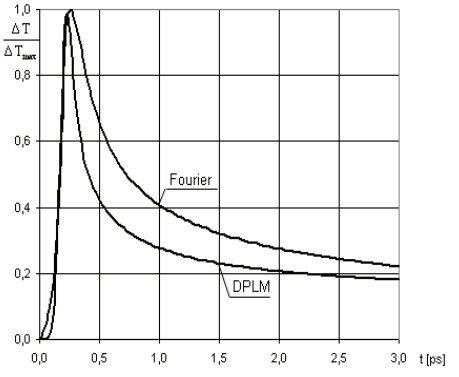

Figure 8: Comparison of dual-phase-lag model (DPLM) and Fourier model

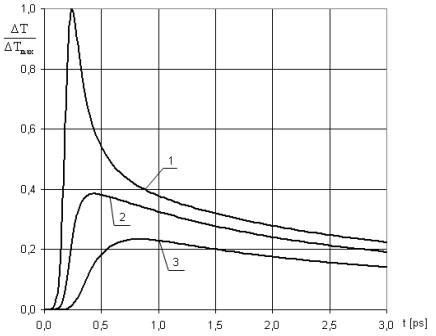

Figure 9: Heating (cooling) curves 1 – x = 0.25 nm, 2 – x = 24.75 nm, 3 – x = 49.75 nm

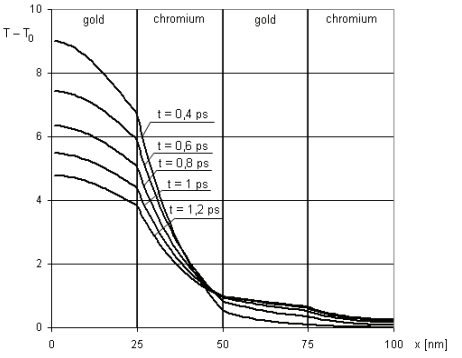

Figure 10: Temperature profiles

The thicknesses of successive layers are the same L_1= L_2= L_3= L_4= 25nm. Thermophysical parameters of sub-domains are assumed as in previous example. In Figure 10 the temperature profiles for times 0.4, 0.6, 0.8 and 1ps are shown, while the next Figure shows the heating (cooling) curves, more exactly the temperature rise over T_0, at the points corresponding to the external boundary x= 0 (1) and interfaces Γ_1(2), Γ_2(3), Γ_3(4). One can see that because of short duration of laser pulse and a low value of absorption depth, the changes of temperature for domains 'of secondary importance' are small.

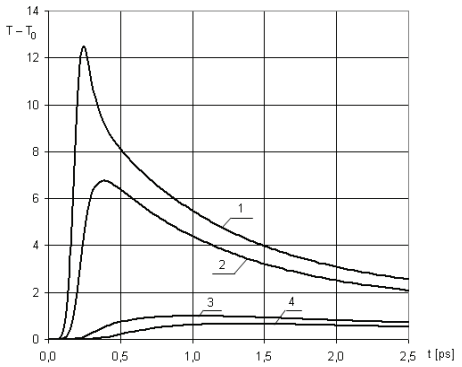

Figure 11: Heating (cooling) curves for multi-layered domain

6 Final remarks

The model presented basing on the dual-phase-lag approach contains both the relaxation time τ_q and additionally the thermalization time τ_T. In literature concerning the micro-scale heat transfer [Escobar at al. (2006); Smith and Norris (2003)] one can find also the models for which only the relaxation time is taken into account. In this place the well known Cataneo equation can be mentioned. According to present opinions resulting mainly from experiments [Özişik and Tzou (1994); Tang and Araki (1999); Chen et al. (2004)] it seems that the assumption concerning a non-zero value of τ_T gives the results closer to real physical conditions of microscale heat transfer.

The algorithm presented can be simply generalized on the cases of 2D or 3D tasks, but at the stage of computations the problems connected with a very large number of nodes and a short time interval can appear.

The model 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 to treat such a domain as a conventionally homogeneous one. The application of Thomas algorithm for implicit FDM schemes causes that the algorithm proposed is very quick and effective.

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