ARCHIVES of FOUNDRY ENGINEERING

ISSN (1897-3310)
Volume 11
Special Issue
3/2011

277 – 281

48/3

Published quarterly as the organ of the Foundry Commission of the Polish Academy of Sciences

Estimation of dual phase lag model parameters using the evolutionary algorithms

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Received 21.06.2011; accepted in revised form 27.07.2011

Abstract

Generalization of Fourier law, in particular the introduction of two 'delay times' (relaxation time τ_q and thermalization time τ_T) leads to the new form of energy equation called the dual-phase-lag model (DPLM). This equation should be applied in a case of microscale heat transfer modeling. In particular, DPLM constitutes a good approximation of thermal processes which are characterized by extremely short duration (e.g. ultrafast laser pulse), extreme temperature gradients and geometrical features of domain considered (e.g. thin metal film). The aim of considerations presented in this paper is the identification of two above mentioned positive constants τ_q, τ_T. 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. In this paper the DPLM equation is applied for analysis of thermal processes proceeding in a thin metal film subjected to a laser beam. At the stage of computations connected with the identification problem solution the evolutionary algorithms are used. To solve the problem the additional information concerning the transient temperature distribution on a metal film surface is assumed to be known.

Keywords: Microscale heat transfer, Dual phase lag model, Inverse problem, Numerical modeling

1. Governing equations

The following form of generalized Fourier law is considered

$$\mathbf{q}\left(x, t+\tau_q\right) = -\lambda \nabla T\left(x, t+\tau_T\right) \tag{1}$$

where $\mathbf{q}$ is the unitary heat flux, λ is the thermal conductivity, ∇T is the temperature gradient. One can see that for $\tau_T = 0$ one obtains the formula leading to the Cattaneo-Vernotte equation, while when $\tau_q=0$ and $\tau_T=0$ the equation (1) corresponds to the typical Fourier law.

The DPLM equation can be, among others, educed from the considerations concerning the parabolic two-temperature model [1, 2, 3]. This model involves two energy equations determining the heat exchange in the electron gas and the metal lattice. The equations creating the model discussed (in a case of metals) are of the form

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

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

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 [1], which characterizes the energy exchange between phonon and electrons [4]. The equations (1), (2) under the assumption that volumetric specific heats c_e and c_l are the constant values, 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 (2) results that

$$T_e = T_l + \frac{c_l}{G}\frac{\partial T_l}{\partial t} \tag{4}$$

Putting (3) into (1) one has

$$c_e\left(\frac{\partial T_l}{\partial t} + \frac{c_l}{G}\frac{\partial^2 T_l}{\partial t^2}\right) = \nabla\left(\lambda_e \nabla T_l\right) + \frac{c_l}{G}\nabla\left[\lambda_e \frac{\partial}{\partial t}\left(\nabla T_l\right)\right] - c_l\frac{\partial T_l}{\partial t} \tag{5}$$

this means

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

Denoting

$$\tau_T = \frac{c_l}{G}, \qquad \tau_q = \frac{1}{G}\left(\frac{1}{c_e} + \frac{1}{c_l}\right)^{-1} \tag{7}$$

finally one obtains

$$\begin{aligned}&c\left[\frac{\partial T(x,t)}{\partial t} + \tau_q\frac{\partial^2 T(x,t)}{\partial t^2}\right] = \\ &\nabla\left[\lambda\nabla T(x,t)\right] + \tau_T\nabla\left[\lambda\frac{\partial\nabla T(x,t)}{\partial t}\right]\end{aligned} \tag{8}$$

where $T(x, t) = T_l(x, t)$ is the macroscopic lattice temperature [5], $c = c_l + c_e$ is the effective volumetric specific heat resulting from the serial assembly of electrons and phonons and $\lambda = \lambda_e$ [6].

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. In Figure 1 the numerical solution obtained on a basis of two temperature parabolic model is shown (equations (2) and (3)). In particular the heating/cooling curves refer to the surface of domain (Ti) subjected to a laser pulse. The time for which the electrons and lattice temperatures are equalized correspond to the thermalization one τ_T. So it seems that the physical interpretation of this parameter is self-evident. Figure 1 was taken from [11].

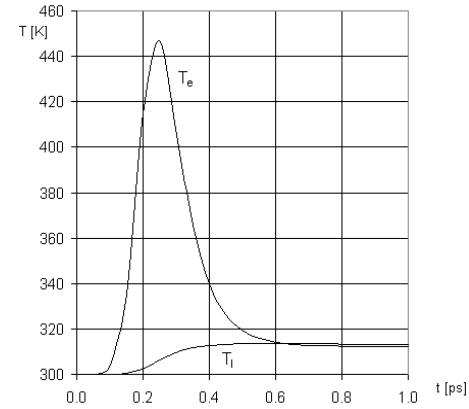

Fig. 1. Surface temperatures

The other approach leading to the DPLM equation results from the following considerations. The well known macroscopic energy equation

$$c\frac{\partial T(x,t)}{\partial t} = -\nabla\cdot\mathbf{q}(x,t) \tag{9}$$

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 formula (1). Next using the Taylor series expansions the following first-order approximation of equation (1) can be taken into account

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

or

$$-\mathbf{q}(x,t) = \tau_q\frac{\partial\mathbf{q}(x,t)}{\partial t} + \lambda\nabla T(x,t) + \tau_T\,\lambda\frac{\partial\nabla T(x,t)}{\partial t} \tag{11}$$

This formula should be introduced to equation (9) and then

$$\begin{aligned}&c\frac{\partial T(x,t)}{\partial t} = \tau_q\frac{\partial}{\partial t}\left[\nabla\mathbf{q}(x,t)\right] + \\ &\nabla\left[\lambda\nabla T(x,t)\right] + \tau_T\nabla\left[\lambda\frac{\partial\nabla T(x,t)}{\partial t}\right]\end{aligned} \tag{12}$$

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

$$\begin{aligned}&c\left[\frac{\partial T(x,t)}{\partial t} + \tau_q\frac{\partial^2 T(x,t)}{\partial t^2}\right] = \\ &\nabla\left[\lambda\nabla T(x,t)\right] + \tau_T\nabla\left[\lambda\frac{\partial\nabla T(x,t)}{\partial t}\right]\end{aligned} \tag{13}$$

this means the same equation as equation (8).

In this paper the problem of heat diffusion in the presence of volumetric internal heat sources $Q(x, t)$ is considered. The introduction of source function results from the thermal interactions between the metal film and external heat source (laser pulse) [2] – Figure 2. It can be shown that in this case the equation (13) must be supplemented by additional components, in particular

$$c\left[\frac{\partial T(x,t)}{\partial t}+\tau_q\frac{\partial^2 T(x,t)}{\partial t^2}\right]=\nabla\left[\lambda\nabla T(x,t)\right]+$$
$$\tau_T\nabla\left[\lambda\frac{\partial\nabla T(x,t)}{\partial t}\right]+Q(x,t)+\tau_q\frac{\partial Q(x,t)}{\partial t} \tag{14}$$

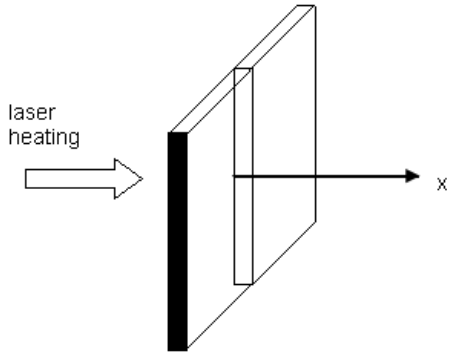

Fig. 2. Domain considered

As was mentioned, the laser-film interaction is taken into account by use of internal volumetric heat source appearing in the microscopic heat transfer equation. In this paper the following formula [7, 8] determining the capacity of internal heat sources is applied (1D problem)

$$Q(x,t)=\sqrt{\frac{\beta}{\pi}}\frac{1-R}{t_p\delta}I_0\exp\left[-\frac{x}{\delta}-\beta\frac{(t-2t_p)^2}{t_p^2}\right] \tag{15}$$

where I_0 is the laser intensity which is defined as the 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 $\beta = 4\ln 2$ [8]. The local and temporary value of Q results from the distance x between surface subjected to laser action and the point considered.

2. Numerical solution of direct problem

On the stage of numerical computations the finite difference method has been used. The differential mesh is a Cartesian product of spatial Δ_h and time Δ_t meshes. Time grid is defined as follows

$$\Delta_t:\ t^0<t^1<...<t^{f-2}<t^{f-1}<t^f<...<t^F<\infty \tag{16}$$

while the spatial mesh is shown in Figure 1.

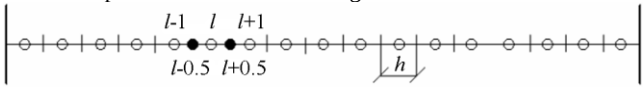

Fig. 3. The mesh

It is visible that the 'boundary' nodes are located at the distance $0.5h$ from real boundaries (this type of discretization assures a very simple and exact approximation of boundary conditions [9]).

It can be shown that FDM approximation of spatial differential operator can be taken in the form [9]

$$\frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right)_i^f=\frac{T_{i+1}^f-T_i^f}{R_{i+1}^{f-1}}\Psi_{i+1}+\frac{T_{i-1}^f-T_i^f}{R_{i-1}^{f-1}}\Psi_{i-1} \tag{17}$$

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

$$R_{i+1}^{f-1}=\frac{0.5h}{\lambda_i^{f-1}}+\frac{0.5h}{\lambda_{i+1}^{f-1}},\quad R_{i-1}^{f-1}=\frac{0.5h}{\lambda_i^{f-1}}+\frac{0.5h}{\lambda_{i-1}^{f-1}} \tag{18}$$

are the thermal resistances between node i and adjoining nodes $i+1$, $i-1$. An index f in formula (17) 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 FDM approximation of equation (14) for transition $t^{f-1}\to t^f$ is of the form

$$c\frac{T_i^f-T_i^{f-1}}{\Delta t}+c\tau_q\frac{T_i^f-2T_i^{f-1}+T_i^{f-2}}{(\Delta t)^2}=$$
$$\frac{T_{i+1}^f-T_i^f}{R_{i+1}^{f-1}}\Psi_{i+1}+\frac{T_{i-1}^f-T_i^f}{R_{i-1}^{f-1}}\Psi_{i-1}+$$
$$\frac{\tau_T}{\Delta t}\left(\frac{T_{i+1}^f-T_i^f}{R_{i+1}^{f-1}}\Psi_{i+1}+\frac{T_{i-1}^f-T_i^f}{R_{i-1}^{f-1}}\Psi_{i-1}\right)- \tag{19}$$
$$\frac{\tau_T}{\Delta t}\left(\frac{T_{i+1}^{f-1}-T_i^{f-1}}{R_{i+1}^{f-1}}\Psi_{i+1}+\frac{T_{i-1}^{f-1}-T_i^{f-1}}{R_{i-1}^{f-1}}\Psi_{i-1}\right)+Q_i^f+\tau_q\left(\frac{\partial Q}{\partial t}\right)_i^f$$

and the last formula can be written as follows

$$A_iT_{i-1}^f+B_iT_i^f+C_iT_{i+1}^f=$$
$$D_iT_{i-1}^{f-1}+E_iT_i^{f-1}+F_iT_{i+1}^{f-1}+\frac{\tau_q}{(\Delta t)^2}T_i^{f-2}- \tag{20}$$
$$\frac{Q_i^f}{c}-\frac{\tau_q}{c}\left(\frac{\partial Q}{\partial t}\right)_i^f,\quad i=1,2,...,N$$

where

$$A_i=\frac{\Psi_{i-1}}{cR_{i-1}^{f-1}}\left(1+\frac{\tau_T}{\Delta t}\right),\qquad C_i=\frac{\Psi_{i+1}}{cR_{i+1}^{f-1}}\left(1+\frac{\tau_T}{\Delta t}\right) \tag{21}$$

$$B_i=-\frac{1}{\Delta t}\left(1+\frac{\tau_q}{\Delta t}\right)-A_i-C_i \tag{22}$$

$$D_i=\frac{\Psi_{i-1}}{cR_{i-1}^{f-1}}\frac{\tau_T}{\Delta t},\qquad F_i=\frac{\Psi_{i+1}}{cR_{i+1}^{f-1}}\frac{\tau_T}{\Delta t} \tag{23}$$

$$E_i=-\frac{1}{\Delta t}\left(1+\frac{2\tau_q}{\Delta t}\right)-D_i-F_i \tag{24}$$

Finally

$$A_iT_{i-1}^f+B_iT_i^f+C_iT_{i+1}^f=G_i^f \tag{25}$$

where

$$G_i^f = D_i T_{i-1}^{f-1} + E_i T_i^{f-1} + F_i T_{i+1}^{f-1} + \frac{\tau_q}{(\Delta t)^2} T_i^{f-2} - \frac{Q_i^f}{c} - \frac{\tau_q}{c}\left(\frac{\partial Q}{\partial t}\right)_i^f \quad (26)$$

The same equations are accepted for the nodes close to boundaries. It is enough to assume that the thermal resistances in directions 'to boundary' are sufficiently big (e.g. 10^{10}) and then the non-flux condition is taken into account. The 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. As was mentioned, the system of FDM equations (26) has been solved using the Thomas algorithm [9] for three-diagonal linear system.

3. Formulation of inverse problem

To solve the inverse problem the least squares criterion is applied

$$S(\tau_q, \tau_T) = \frac{1}{MF}\sum_{i=1}^{M}\sum_{f=1}^{F}\left(T_i^f - T_{di}^f\right)^2 \quad (27)$$

where T_{di}^f and $T_i^f = T(x_i, t^f)$ are the measured and estimated temperatures, respectively, M is the number of sensors. The optimum of functional (27) has been found using the evolutionary algorithms. So the direct problems have been solved and the results allow ones to determine the time dependent surface temperature (x = 0). Because the temperature history resulting from numerical solution for the basic input data is very close to experimental ones quoted in [10] – Figure 4 therefore this undisturbed numerical solution is assumed to be a base of identification problem solution ('measured surface temperature'). So, the laser parameters determining capacity of internal source function $Q(x, t)$ and also the thermal conductivity and volumetric specific heat of gold are known, the parameters τ_q, τ_T should be determined (from the practical standpoint the experimental estimation of τ_q, τ_T is not easy).

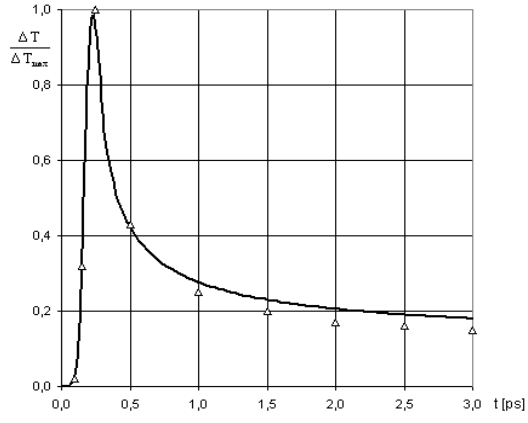

Fig. 4. Comparison with experimental data [10]

In Figures 5 and 6 the example of direct problem solution is shown. The layer is subjected to a short-pulse laser irradiation which parameters are equal to: R = 0.93 (reflectivity), I_0 = 13.7 [J/m^2] (intensity), t_p = 0.1 ps = 10^{-13} s (time of laser pulse), δ = 15.3 nm (absorption depth). The following parameters of gold thin film are assumed: thermal conductivity λ = 317 [W/(mK)], volumetric specific heat c = 2.4897 [MJ/(m^{3}K)], relaxation time τ_q = 8.5 ps, thermalization time τ_T = 90 ps. Initial temperature equals T_0 = 20°C. Using the algorithm presented in the previous chapter under the assumption that N = 200 and Δt = 0.005 ps the transient temperature field has been found. In Figure 5 the temperature profiles are shown, while Figure 6 illustrates the courses of heating (cooling) curves at the points selected from the domain considered. Figure 7 illustrates the differences between solutions basing on the DPLM equation and the Fourier one.

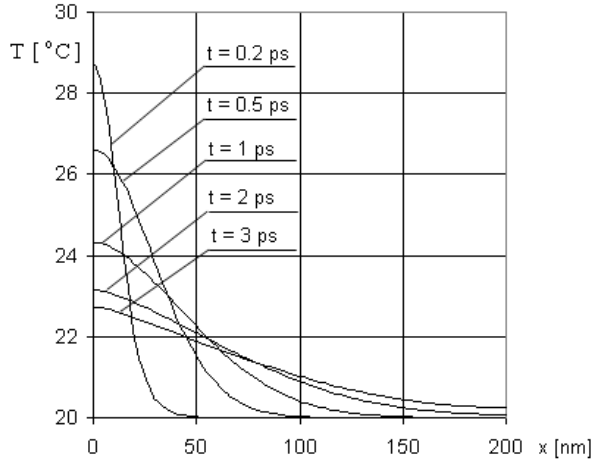

Fig. 5. Temperature profiles for different times

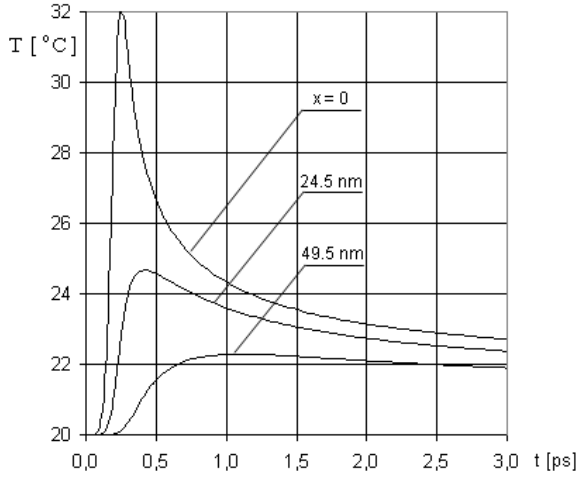

Fig. 6. Cooling (heating) curves

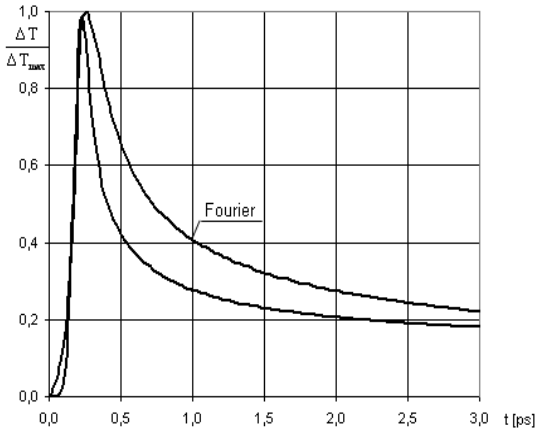

Fig. 7. Comparison of dual-phase-lag model (DPLM) and Fourier model

The identification of 'delay' times has been done using the evolutionary algorithms. In Table 1 the algorithm parameters are collected. The results obtained are presented in Table 2 and they are quite satisfactory.

Table 1.
Evolutionary algorithm parameters

Number of generations	50
Number of chromosomes	20
Prob. of uniform mutation	20%
Prob. of non-uniform mutation	30%
Prob. of arithmetic crossover	50%
Prob. of cloning	10%

Table 2.
Result of computations using the EA

design variable	exact value	found value	error %
τ_q	$8.5 \cdot 10^{-12}$	$8.499999 \cdot 10^{-12}$	0
τ_T	$90 \cdot 10^{-12}$	$89.99999 \cdot 10^{-12}$	0

Acknowledgement

This work was supported by Grant No N N501 2176 37 from the Polish Ministry of Science and Higher Education.

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