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Dual-phase lag model of thermal processes in a multi-layered microdomain subjected to a strong laser pulse using the implicit scheme of FDM

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ABSTRACT

In the paper, the thermal processes occurring in the axially-symmetrical domain of multi-layered thin metal film subjected to a strong laser pulse are considered. The problem is described by the system of dual-phase lag equations (DPLE) supplemented by the appropriate boundary and initial conditions (in the form corresponding to the model considered). The possibility of domain melting is also taken into account. At the stage of numerical computations, the implicit scheme of the finite difference method is used. The problems connected with the modeling of the thermal contact conditions between sub-domains and finally the simulations of the melting and resolidification processes are discussed in detail.The continuity condition given on the contact surface is considered in the form in which the lag times are taken into account. The results confirm the differences between often presented solutions, using the dual-phase lag model supplemented by the 'macroscopic' type of these conditions. The model of melting and resolidification results from the modified form of the DPLE for which the derivative of temperature with respect to time is equal to zero. It results from the fact that the melting of pure metals proceeds at the constant temperature.

1. Introduction

The considerations presented in this paper are based on the application of the dual-phase lag equation (e.g. [1–4]) for numerical modeling of the microscale heat transfer problems. As one knows, the mathematical form of this equation results from the generalization of the Fourier law, namely

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

where $\mathbf{q}$ is a heat flux vector, ∇T is a temperature gradient, λ is a thermal conductivity, X, t denote the geometrical co-ordinates and time. The positive constants τ_q, τ_T correspond to relaxation time and thermalization time, respectively. 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 [5].

Using the Taylor series expansions, the following first-order approximation of equation (1) can be taken into account

$$\mathbf{q}(X,\ t) + \tau_q \frac{\partial \mathbf{q}(X,\ t)}{\partial t} = -\lambda \left[\nabla T(X,\ t) + \tau_T \frac{\partial \nabla T(X,\ t)}{\partial t}\right] \tag{2}$$

The well-known energy balance equation is of the form

$$c\frac{\partial T(X,\ t)}{\partial t} = -\nabla \cdot \mathbf{q}(X,\ t) + Q(X, t) \tag{3}$$

where c is the volumetric specific heat and $Q(X, t)$ is the capacity of internal heat sources. In the paper presented the function $Q(X, t)$ results from the laser heating.

From equation (2) it results that

$$-\mathbf{q}(X,\ t) = \tau_q \frac{\partial \mathbf{q}(X,\ t)}{\partial t} + \lambda \left[\nabla T(X,\ t) + \tau_T \frac{\partial \nabla T(X,\ t)}{\partial t}\right] \tag{4}$$

Introducing this formula to equation (3) one has

$$c\frac{\partial T(X,\ t)}{\partial t} = \tau_q \frac{\partial}{\partial t}[\nabla \cdot \mathbf{q}(X,\ t)] + \nabla[\lambda \nabla T(X,\ t)] + \tau_T \nabla\left[\lambda \frac{\partial \nabla T(X,\ t)}{\partial t}\right] \tag{5}$$

Because (c.f. equation (3))

$$\nabla \cdot \mathbf{q}(X,\ t) = -c\frac{\partial T(X,\ t)}{\partial t} + Q(X, t) \tag{6}$$

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Nomenclature

c	volumetric specific heat [W/(m^{3}K)]
f	level of time
I_0	laser intensity [J/m^2]
L	volumetric heat of fusion [J/m^3]
$\mathbf{q}$	heat flux vector [W/m^2]
Q	capacity of internal heat sources [W/m^3]
Q_m	source function related to melting [W/m^3]
q_b	boundary heat flux [W/m^2]
R	reflectivity of the irradiated surface
R_0	domain radius [m]
r_D	laser beam radius [m]
S	volumetric molten state fraction
T	temperature [K]
T_m	melting temperature [K]
T_0	initial temperature [K]
t	time [s]
t_p	characteristic time of laser pulse [s]
$X=\{r,\ z\}$	geometrical co-ordinates
w	initial heating rate [K/s]
Z	domain depth [m]

Greek letters

δ	optical penetration depth [m]
λ	thermal conductivity [W/(mK)]
Φ	shape functions of FDM mesh
τ_T	thermalization time [s]
τ_q	relaxation time [s]
Ω_e	subdomains

consequently

$$c\left[\frac{\partial T(X,\ t)}{\partial t}+\tau_q\frac{\partial^2 T(X,\ t)}{\partial t^2}\right]=\nabla\left[\lambda\nabla T(X,\ \ t)\right]+\tau_T\frac{\partial}{\partial t}\{\nabla\left[\lambda\nabla T(X,\ \ t)\right]\}+Q\,(X,t)+\tau_q\frac{\partial Q\,(X,\ t)}{\partial t} \tag{7}$$

In literature the other forms of DPLE are also presented. In particular, the second order Taylor expression of thermal flux and the first order Taylor expression of temperature gradient are applied to describe the phase lagging behavior [6]. In the papers [7,8], both the heat flux $\mathbf{q}$ and the temperature gradient ∇T are expanded using the second order Taylor formula.

The 'classical' form of the DPLE (with some assumptions corresponding to the heat conduction proceeding in the domains of pure metals) can be obtained on the basis of the microscopic two-step parabolic model (e.g. [9,10]). 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, using a certain elimination technique, can be substituted by a single equation containing a second derivative of temperature with respect to time and a higher-order mixed derivative in both time and space. A detailed discussion of the transition discussed is presented in [11].

The other group of heat transfer problems using the model resulting from the generalized Fourier law is connected with the heat exchange in domain of biological tissue. Recently here is a view that taking into account the specific inner tissue structure the DPL model (or the Cattaneo-Vernotte one) better than the well known Pennes equation describes the bioheat transfer problems.

Some quite simple initial-boundary problems described by DPLE can be solved using the analytical and semi-analytical methods. For example, in the paper [12], the solution concerning the heating of the semi-infinite plate in which the thermal processes are described by the higher order DPLE supplemented by the simple boundary-initial conditions is presented.The interesting analytical solution is discussed in [13]. The author solved the 1D classical DPLE taking into account the presence of internal heat sources caused by the laser interaction.The solution has been obtained using the separation of the variables technique and Green's function method. The analytical solution of the dual phase lag bioheat transfer equation using the finite integral transform has been presented in [14]. A problem of the analysis of thermal damage to laser irradiated tissue has been solved analytically in the paper [15]. In turn, the Adomian decomposition method (ADM) and the Adomian double decomposition method (ADDM) for solving the 3D DPLE is proposed in the paper [16]. In the paper [17], the Laplace transformation method has been used to solve the 1D dual-phase lag model for a non-homogeneous (multilayered) cylindrical or spherical domain. The boundary conditions have been assumed in the macroscale convention, wherein between the subdomains the thermal resistance has been taken into account.

The discussed works are not, of course, a complete review of the analytical solutions of the problems in question.

To solve the heat transfer problems described by the dual-phase lag equation, the different numerical methods are, definitely more often, used. In most of the work in this area, the different variants of the FDM are applied. The solutions based on the boundary element method [18], the finite element method [19–21], the control volume method [22–24] or the lattice Boltzmann method can be also found, for example [25,26].

As mentioned, the most commonly used, however, are the different variants of the FDM (see: e.g. [27–30]). In the paper [27], the numerical model of heating of the double-layered thin film has been applied for the analysis of the thermal deformation process. In the paper [28] the 3D FDM numerical model of the thin metal film heating has been presented. In [29] the explicit scheme of the FDM has been used. The stability problem of the algorithm of this type is discussed in [30]. The FDM numerical solutions of the inverse problems are also discussed (e.g. [24,31]). In turn, the numerical solution of 2D DPLE using the alternating directions approach can be found in [32]. It should be emphasized that the number of papers devoted to the FDM applications for the numerical solution of the problems described by DPLE is, of course, much bigger.

As previously mentioned, recently there is the view of the DPLE usefulness to describe the heat transfer in the biological tissue domain [14,15,18–23,25,29], but these problems will not be discussed in more detail here. So, without going into particularities in the papers [19–21] the problems of hyperthermia treatment are analyzed. In [22,23] the DPL model has been coupled with the radiative transfer equation (the analysis of laser-irradiated tissue), additionally in [23] the nanoparticles have been introduced to the tissue region. The similar problem has been discussed in [25] in which the thermal processes proceeding in domain of the tissue during the laser-based photo-thermal therapy are considered. In turn, in the paper [29] the cryosurgical treatment is analyzed.

In the paper presented the multi-layered domain is considered. Modeling of thermal processes in such objects, apart from the scientific aspects, is of major practical importance (micro-technologies design). The mathematical model of heat transfer processes is in this case created by the system of the dual-phase lag equations, typical boundary conditions on the external surface of the system and the continuity conditions given on the contact surfaces (the ideal contact is, as a rule, assumed). The initial conditions are also known, of course. The FDM solution discussed in literature differ, among other things, in the choice of the differential grid. Besides the typical meshes (the boundary nodes are located directly on the boundary) one can find the solutions in which the nodes are located not on the contact surface but at a certain