HEAT TRANSFER IN DOMAIN OF METAL SUPERFICIAL LAYER SUBJECTED TO A STRONG EXTERNAL HEAT FLUX

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Abstract. In the paper the thermal processes proceeding in a superficial layer of metal subjected to a strong external heat flux are analyzed. The different mathematical models of heat conduction in domain considered are taken into account. The first bases on the dual-phase-lag-equation describing a micro-scale heat transfer. DPLE contains the parameters corresponding to relaxation time τ_q and the normalization time τ_T. The second model considered here results from the assumption that $\tau_T = 0$ and then DPLE reduces to the Cattaneo equation. The last one ($\tau_q = \tau_T = 0$) corresponds to the well known Fourier equation. Using the implicit scheme of FDM algorithm the numerical simulations have been done and the conclusions resulting from the results obtained have been formulated.

Introduction

Thermal processes proceeding close to the surface of metal domain can be treated as the phenomena described by the energy equations corresponding to micro-scale heat conduction. This approach should be used in the case of small geometrical dimensions, strong thermal interactions between domain and external heat source, very big temperature gradients [1, 2]. The micro-scale heat transfer can be described in different ways [1-6]. In this paper the dual-phase-lag-model has been taken into account. The energy equation contains two positive constants corresponding to the relaxation time τ_q and the normalization time τ_T. The interpretation of τ_q and τ_T and the formulas determining above parameters will be presented in the next chapter. The characteristic feature of DPLE is a presence of second derivative of temperature with respect to time and the higher order derivative both in time and space.

The dual-phase-lag-equation can be reduced to the Cattaneo hyperbolic partial differential equation under the assumption that $\tau_T = 0$. Application of this type of heat transfer equation corresponds to the model in which the finite value of thermal wave velocity is taken into account.

If both relaxation time $\tau_q = 0$ and normalization time $\tau_T = 0$ then the DPLE is the same as the well known parabolic Fourier equation describing a heat conduction in a macro-scale.

In the paper we consider the superficial layer L which thermophysical parameters correspond to nickel (Ni). Taking into account the geometrical features of domain, the 1D solution is sufficiently exact. The thickness L of layer considered should secure the possibility of assumption of non-flux boundary condition for $x = L$ (it is the value of order 1 μm). The intensity of external heat flux and its duration have been assumed on the level assuring the values of local and temporary temperatures below a solidification point.

The numerical algorithm and computer program base on the implicit scheme of FDM [7]. The system of equations corresponding to transition from time t to time $t + \Delta t$ was solved using the Thomas algorithm [8].

1. Governing equations

The microscopic two-step model presented among others in [1, 2, 6] is discussed. The 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

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

and

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

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 which characterizes the energy exchange between phonon and electrons and is given as [6]

$$G = \frac{\pi^4 (n_e v_s k)^2}{\lambda_e} \tag{3}$$

where

$$v_s = \frac{k}{2\pi h}\left(6\pi^2 n_a\right)^{-1/3} \tag{4}$$

and n_e is the electron number density per unit volume, k [J/K] is the Boltzmann constant, v_s [m/s] is the speed of sound, h [J s] is the Planck constant, n_a is the

atomic density per unit volume. For the material considered (Ni) and the mean value of thermal conductivity for the temperature interval analyzed, the coupling factor G equals $3.6 \cdot 10^{17}$ W/m^{3}K [6].

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

$$c_e \frac{\partial T_e}{\partial t} = \nabla\left(\lambda_e \nabla T_e\right) - G\left(T_e - T_l\right) \tag{5}$$

and

$$c_l \frac{\partial T_l}{\partial t} = G\left(T_e - T_l\right) \tag{6}$$

This simplification, according to [1], results from the fact that the incident radiation and conductional heat flux are absorbed and diffused mainly by electrons. The equations (5), (6) 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 (6) results that

$$T_e = T_l + \frac{c_l}{G} \frac{\partial T_l}{\partial t} \tag{7}$$

Putting (7) into (5) one has

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

this means

$$\left(c_e + c_l\right)\frac{\partial T_l}{\partial t} + \frac{c_e c_l}{G} \frac{\partial^2 T_l}{\partial t^2} = \nabla\left(\lambda_e \nabla T_l\right) + \frac{c_l}{G} \frac{\partial}{\partial t}\left[\nabla\left(\lambda_e \nabla T_l\right)\right] \tag{9}$$

or

$$\left(c_e + c_l\right)\left[\frac{\partial T_l}{\partial t} + \frac{c_e c_l}{G\left(c_e + c_l\right)} \frac{\partial^2 T_l}{\partial t^2}\right] = \nabla\left(\lambda_e \nabla T_l\right) + \frac{c_l}{G} \frac{\partial}{\partial t}\left[\nabla \lambda_e \left(\nabla T_l\right)\right] \tag{10}$$

Denoting

$$\tau_T = \frac{c_l}{G}, \quad \tau_q = \frac{1}{G}\left(\frac{1}{c_e} + \frac{1}{c_l}\right)^{-1} \tag{11}$$

finally one obtains

$$c\left[\frac{\partial T(x,t)}{\partial t}+\tau_q\frac{\partial^2 T(x,t)}{\partial t^2}\right]=\nabla\left[\lambda\,\nabla T(x,t)\right]+\tau_T\nabla\left[\lambda\,\frac{\partial \nabla T(x,t)}{\partial t}\right] \quad (12)$$

where $T(x, t) = T_l(x, t)$ is the macroscopic lattice temperature [1], $c = c_l + c_e$ 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.

This general form of energy equation can be simplified and then one obtains well known heat conduction model basing on the Cattaneo equation and the Fourier one. In particular, assuming $\tau_T = 0$ one obtains the Cattaneo model

$$c\left[\frac{\partial T(x,t)}{\partial t}+\tau_q\frac{\partial^2 T(x,t)}{\partial t^2}\right]=\nabla\left[\lambda\,\nabla T(x,t)\right] \quad (13)$$

while for $\tau_T = \tau_q = 0$ one obtains the Fourier model

$$c\,\frac{\partial T(x,t)}{\partial t}=\nabla\left[\lambda\,\nabla T(x,t)\right] \quad (14)$$

The solution of problem describing by Equations (12) or (13) requires the formulation of two initial conditions, namely

$$t=0:\quad T(x,0)=T_0(x) \quad (15)$$

and

$$t=0:\quad \left.\frac{\partial T(x,0)}{\partial t}\right|_{t=0}=U_0(x) \quad (16)$$

while in a case of equation (14) only knowledge of initial temperature distribution (15) is required.

In a general case the dependence between heat flux $\mathbf{q}$ [W/m^2] and the temperature gradient ∇T [K/m] results from the formula

$$\mathbf{q}(x,t+\tau_q)=-\lambda\nabla T(x,t+\tau_T) \quad (17)$$

Using the Taylor series expansions the following first-order approximation of Equation (17) can be taken into account

$$\mathbf{q}(x, t) + \tau_q \frac{\partial \mathbf{q}(x, t)}{\partial t} = -\lambda \left[\nabla T(x, t) + \tau_T \frac{\partial \nabla T(x, t)}{\partial t} \right] \tag{18}$$

In special cases for $\tau_T = 0$ one has

$$\mathbf{q}(x, t) + \tau_q \frac{\partial \mathbf{q}(x, t)}{\partial t} = -\lambda \nabla T(x, t) \tag{19}$$

and for $\tau_T = \tau_q = 0$

$$\mathbf{q}(x, t) = -\lambda \nabla T(x, t) \tag{20}$$

Taking into account the geometrical features of metal superficial layer, the heat transfer processes proceeding in the domain considered can be described by 1D task (Fig. 1) and then the following boundary-initial problem can be formulated

$$x \in \Omega: \quad c \left[\frac{\partial T(x, t)}{\partial t} + \tau_q \frac{\partial^2 T(x, t)}{\partial t^2} \right] = \lambda \frac{\partial^2 T(x, t)}{\partial x^2} + \lambda \tau_T \frac{\partial^3 T(x, t)}{\partial t \partial x^2} \tag{21}$$

Let us assume that the surface Γ_0 is subjected to the external heat flux q_b (x, t) and then

$$x \in \Gamma_0: \quad q_b(x, t) + \tau_q \frac{\partial q_b(x, t)}{\partial t} = -\lambda \frac{\partial T(x, t)}{\partial x} - \lambda \tau_T \frac{\partial}{\partial t} \left[\frac{\partial T(x, t)}{\partial x} \right] \tag{22}$$

On the conventionally assumed boundary Γ_∞ limiting the superficial layer the no-flux condition can be taken into account

$$x \in \Gamma_\infty: \quad 0 = -\lambda \frac{\partial T(x, t)}{\partial x} - \lambda \tau_T \frac{\partial}{\partial t} \left[\frac{\partial T(x, t)}{\partial x} \right] \tag{23}$$

Additionally

$$t = 0: \quad T(x, 0) = T_0, \quad \left. \frac{\partial T(x, 0)}{\partial t} \right|_{t=0} = 0 \tag{24}$$

where T_0 is the constant initial temperature of layer.

The assumption of constant values λ, c, τ_T, τ_q results from the input data quoted and approachable in literature.

On a stage of numerical modelling both the dual-phase-lag model and the others above discussed models have been taken into account and the aim of our research is to compare the results obtained by means of these models.

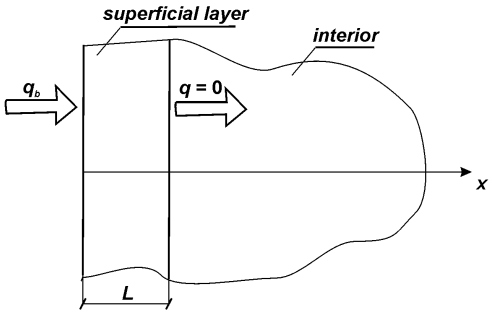

Fig. 1. Domain considered

3. Results of computations

The superficial layer of thickness L = 1 μm is considered. Thermophysical parameter of material (nickel) are the following: $\lambda = \lambda_e = 90.8$ W/(mK), $c = c_l + c_e = 0.32 \cdot 10^6 + 3.68 \cdot 10^6 = 4 \cdot 10^6$ J/(m^3 K). Because $G = 3.6 \cdot 10^{17}$ W/(m^3 K) therefore (c.f. equations (11)) $\tau_q = 0.82$ ps (1ps = 10^{-12} s), $\tau_T = 10$ ps. For $x = 0$ and $t \geq 100$ ps (exposure time) $q_b = 10^{12}$ W/m^2, while for $t > 100$ ps: $q_b = 0$. Initial temperature $T_0 = 20$°C. The computations have been realized by means of the finite difference method under the assumption that $h = 0.002$ μm and $\Delta t = 0.05$ ps.

In Figure 2 the temperature profiles for time $t = 0.5$ ps at the region close to the external boundary obtained using the different models are shown. The differences between temperature profiles are visible but only for the first stages of the process and points close to the boundary Γ_0.

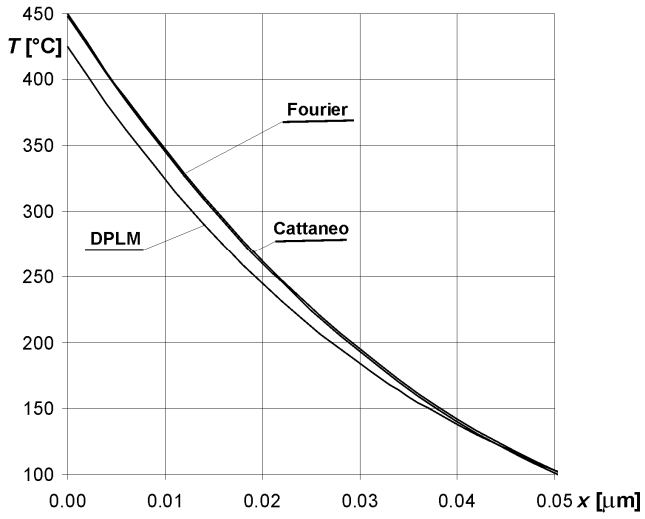

Fig. 2. Comparison of temperature profiles for time $t = 0.5$ ps

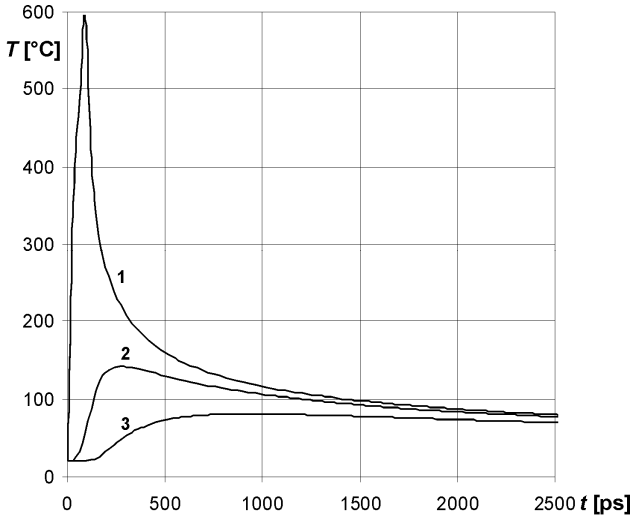

Fig. 3. Heating-cooling curves (1 - $x = 0$, 2 - $x = 1/5\,L$, 3 - $x = 2/5\,L$)

The next Figure shows the heating (cooling) curves at the points $x = 0$, $x = 1/5L$ and $x = 2/5L$. For the assumed axes intervals the differences between successive solutions are not visible.

3. Final remarks

From the theoretical point of view the process analyzed should be described by the micro-scale heat conduction equation. In practice, it turned out, that the numerical solution obtained using the Cattaneo model and even the Fourier one are sufficiently exact. It results from the small values of τ_q and τ_T for material considered and the boundary condition assumed on Γ_0. According to our experience, the more visible differences appear in the case of thermal interaction between ultrashort laser pulse and the metal surface.

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