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APPLICATION OF THE TWO-TEMPERATURE MODEL FOR A NUMERICAL STUDY OF MULTIPLE LASER PULSES INTERACTIONS WITH THIN METAL FILMS

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Abstract. A thin metal film irradiated by multiple laser pulses is considered. The microscale heat transfer in the domain considered is described by hyperbolic two-temperature model. This model contains two energy equations determining the heat exchange in the electron gas and the metal lattice. The problem is solved by a explicit scheme of finite difference method. The influence of separation time between two laser pulses on the electrons and lattice temperatures is discussed.

Introduction

From the mathematical point of view, exist nowadays the different models describing the microscale heat transfer [1-5], namely Cattaneo-Vernotte equation, dual phase lag model, two-temperature models and Boltzmann equation. In this paper the heat conduction in thin metal film irradiated by multiple laser pulses is described using the microscopic hyperbolic two-temperature model supplemented by boundary and initial conditions. The problem formulated is solved by means of the finite difference method. The influence of separation time between two laser pulses on the electrons and lattice temperatures is analyzed and the conclusions are formulated.

1. Mathematical model

The two-temperature model describes the temporal and spatial evolution of the lattice and electrons temperatures (T_l and T_e) in the irradiated metal by two coupled nonlinear differential equations [1, 2] (1D problem)

$$C_e(T_e)\frac{\partial T_e(x,t)}{\partial t} = -\frac{\partial q_e(x,t)}{\partial x} - G(T_e)\left[T_e(x,t) - T_l(x,t)\right] + Q(x,t) \tag{1}$$

$$C_l(T_l)\frac{\partial T_l(x,\,t)}{\partial t}=-\frac{\partial q_l(x,\,t)}{\partial x}+G(T_e)\big[T_e(x,\,t)-T_l(x,\,t)\big] \tag{2}$$

where $T_e\,(x,\,t)$, $T_l\,(x,\,t)$ are the temperatures of electrons and lattice, respectively, $C_e(T_e)$, $C_l(T_l)$ are the volumetric specific heats, $G(T_e)$ is the electron-phonon coupling factor which characterizes the energy exchange between electrons and phonons [3], $Q(x,\,t)$ the source function associated with the irradiation.

In a place of classical Fourier law the following formulas are introduced

$$q_e(x,\,t+\tau_e)=-\lambda_e(T_e,T_l)\frac{\partial T_e(x,\,t)}{\partial x} \tag{3}$$

$$q_l(x,\,t+\tau_l)=-\lambda_l(T_l)\frac{\partial T_l(x,\,t)}{\partial x} \tag{4}$$

where $\lambda_e(T_e,\,T_l)$, $\lambda_l(T_l)$ are the thermal conductivities of electrons and lattice, respectively, τ_e is the relaxation time of free electrons in metals, τ_l is the relaxation time in phonon collisions.

Using the Taylor expansion the equations (3) and (4) can be written in the form

$$q_e(x,\,t)+\tau_e\frac{\partial q_e(x,\,t)}{\partial t}=-\lambda_e(T_e,T_l)\frac{\partial T_e(x,\,t)}{\partial x} \tag{5}$$

$$q_l(x,\,t)+\tau_l\frac{\partial q_l(x,\,t)}{\partial t}=-\lambda_l(T_l)\frac{\partial T_l(x,\,t)}{\partial x} \tag{6}$$

The laser irradiation is taken into account in the source term (c.f. equation (1))

$$Q(x,\,t)=\sqrt{\frac{\beta}{\pi}}\,\frac{1-R}{t_p\,\delta}\,I_0\,\exp\left[-\frac{x}{\delta}-\beta\frac{(t-2f\,t_p)^2}{t_p^2}\right] \tag{7}$$

where I_0 is the laser intensity, t_p is the characteristic time of laser pulse, δ is the optical penetration depth, R is the reflectivity of the irradiated surface and $\beta = 4\ln 2$ and f is the separation time between two laser pulses [6].

To define the thermal conductivity λ_e and heat capacity C_e of electrons the following formulas are widely used [1, 2, 7-10]

$$\lambda_e(T_e,\,T_l)=\lambda_0\frac{T_e}{T_l} \tag{8}$$

$$C_e(T_e)=\gamma T_e \tag{9}$$

where λ_0, γ are the material constants. It should be pointed out that the simple form of dependences (8), (9) is only suitable for low laser intensity. For such intensities, constant values of C_l and λ_l are also very commonly assumed.

2. Method of solutions

To solve the problem formulated the algorithm based on the finite difference method is proposed. A staggered grid is introduced [8, 11] (Fig. 1). Let us denote $T_i^f = T(ih, f\Delta t)$, where h is a mesh size, Δt is a time step, $i = 0, 2, 4, ..., N$, $f = 0, 1, 2, ..., F$, and $q_j^f = q(jh, f\Delta t)$, where $j = 1, 3, ..., N$-1.

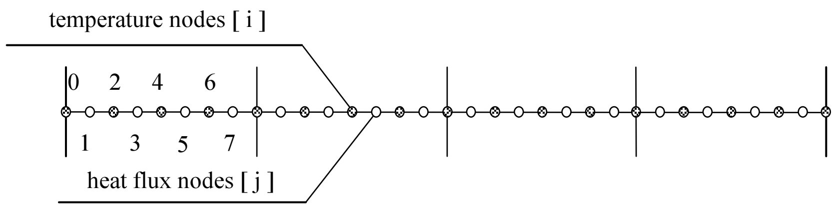

Fig. 1. Discretization

The finite difference approximation of equations (5) and (6) using the explicit scheme can be written in the form:

$$q_{e\,j}^{f-1} + \tau_e \frac{q_{e\,j}^{f} - q_{e\,j}^{f-1}}{\Delta t} = -\lambda_{e\,j}^{f-1} \frac{T_{e\,j+1}^{f-1} - T_{e\,j-1}^{f-1}}{2h} \tag{10}$$

$$q_{l\,j}^{f-1} + \tau_l \frac{q_{l\,j}^{f} - q_{l\,j}^{f-1}}{\Delta t} = -\lambda_{l\,j}^{f-1} \frac{T_{l\,j+1}^{f-1} - T_{l\,j-1}^{f-1}}{2h} \tag{11}$$

where index j corresponds to the 'heat flux nodes' (Fig. 1).

The dependencies (10), (11) allow one to construct the similar formulas for nodes i–1, i+1 and then one obtains

$$\begin{gathered} q_{e\,i-1}^{f} - q_{e\,i+1}^{f} = \frac{\tau_e - \Delta t}{\tau_e}\left(q_{e\,i-1}^{f-1} - q_{e\,i+1}^{f-1}\right) + \\ \frac{\Delta t}{2h\tau_e}\left[\lambda_{e\,i-1}^{f-1}(T_{e\,i-2}^{f-1} - T_{ei}^{f-1}) + \lambda_{e\,i+1}^{f-1}(T_{e\,i+2}^{f-1} - T_{ei}^{f-1})\right] \end{gathered} \tag{12}$$

$$\begin{gathered} q_{l\,i-1}^{f} - q_{l\,i+1}^{f} = \frac{\tau_l - \Delta t}{\tau_l}\left(q_{l\,i-1}^{f-1} - q_{l\,i+1}^{f-1}\right) + \\ \frac{\Delta t}{2h\tau_l}\left[\lambda_{l\,i-1}^{f-1}(T_{l\,i-2}^{f-1} - T_{li}^{f-1}) + \lambda_{l\,i+1}^{f-1}(T_{l\,i+2}^{f-1} - T_{li}^{f-1})\right] \end{gathered} \tag{13}$$

Now, the equations (1), (2) are discretized using the explicit scheme of the finite difference method

$$C_{ei}^{f-1}\frac{T_{ei}^{f}-T_{ei}^{f-1}}{\Delta t}=-\frac{q_{ei+1}^{f}-q_{ei-1}^{f}}{2h}-G\left[T_{ei}^{f-1}-T_{li}^{f-1}\right]+Q_{i}^{f-1} \tag{14}$$

$$C_{l}\frac{T_{li}^{f}-T_{li}^{f-1}}{\Delta t}=-\frac{q_{li+1}^{f}-q_{li-1}^{f}}{2h}+G\left[T_{ei}^{f-1}-T_{li}^{f-1}\right] \tag{15}$$

where index i corresponds to the 'temperature nodes' as shown in Figure 1.

Putting (12) into (14) and (13) into (15) one has:

$$\begin{gathered}C_{ei}^{f-1}\frac{T_{ei}^{f}-T_{ei}^{f-1}}{\Delta t}=\frac{(\tau_e-\Delta t)}{2h\tau_e}(q_{ei-1}^{f-1}-q_{ei+1}^{f-1})+\frac{\Delta t}{4h^2\,\tau_e}\Big[\lambda_{ei-1}^{f-1}(T_{ei-2}^{f-1}-T_{ei}^{f-1})+\\ \lambda_{ei+1}^{f-1}(T_{ei+2}^{f-1}-T_{ei}^{f-1})\Big]-G\left[T_{ei}^{f-1}-T_{li}^{f-1}\right]+Q_{i}^{f-1}\end{gathered} \tag{16}$$

$$\begin{gathered}C_{li}^{f-1}\frac{T_{li}^{f}-T_{li}^{f-1}}{\Delta t}=\frac{(\tau_l-\Delta t)}{2h\tau_l}(q_{li-1}^{f-1}-q_{li+1}^{f-1})+\frac{\Delta t}{4h^2\,\tau_l}\Big[\lambda_{li-1}^{f-1}(T_{li-2}^{f-1}-T_{li}^{f-1})+\\ \lambda_{li+1}^{f-1}(T_{li+2}^{f-1}-T_{li}^{f-1})\Big]+G\left[T_{ei}^{f-1}-T_{li}^{f-1}\right]\end{gathered} \tag{17}$$

From equation (16) results that

$$\begin{gathered}T_{ei}^{f}=\left(1-\frac{(\Delta t)^2\,\lambda_{ei-1}^{f-1}}{4h^2\,\tau_e\,C_{ei}^{f-1}}-\frac{(\Delta t)^2\,\lambda_{ei+1}^{f-1}}{4h^2\,\tau_e\,C_{ei}^{f-1}}-\frac{G\Delta t}{C_{ei}^{f-1}}\right)T_{ei}^{f-1}+\frac{(\Delta t)^2\,\lambda_{ei-1}^{f-1}}{4h^2\,\tau_e\,C_{ei}^{f-1}}T_{ei-2}^{f-1}+\\ \frac{(\Delta t)^2\,\lambda_{ei+1}^{f-1}}{4h^2\,\tau_e\,C_{ei}^{f-1}}T_{ei+2}^{f-1}+\frac{G\Delta t}{C_{ei}^{f-1}}T_{li}^{f-1}+\frac{\Delta t(\tau_e-\Delta t)}{2h\tau_e\,C_{ei}^{f-1}}\left(q_{ei-1}^{f-1}-q_{ei+1}^{f-1}\right)+\frac{Q_i^{f-1}\Delta t}{C_{ei}^{f-1}}\end{gathered} \tag{18}$$

From equation (17) results that

$$\begin{gathered}T_{li}^{f}=\left(1-\frac{(\Delta t)^2\,\lambda_{li-1}^{f-1}}{4h^2\,\tau_l\,C_l}-\frac{(\Delta t)^2\,\lambda_{li+1}^{f-1}}{4h^2\,\tau_l\,C_l}-\frac{G\Delta t}{C_l}\right)T_{li}^{f-1}+\frac{(\Delta t)^2\,\lambda_{li-1}^{f-1}}{4h^2\,\tau_l\,C_l}T_{li-2}^{f-1}+\\ \frac{(\Delta t)^2\,\lambda_{li+1}^{f-1}}{4h^2\,\tau_l\,C_l}T_{li+2}^{f-1}+\frac{G\Delta t}{C_l}T_{ei}^{f-1}+\frac{\Delta t(\tau_l-\Delta t)}{2h\tau_l\,C_l}\left(q_{li-1}^{f-1}-q_{li+1}^{f-1}\right)\end{gathered} \tag{19}$$

In numerical computations the following approximation of thermal conductivities has been used (c.f. equations (18), (19)) and (c.f. equations (10), (11))

$$\lambda_{e\,i-1}^{f-1}=\frac{\lambda_{e\,i}^{f-1}+\lambda_{e\,i-2}^{f-1}}{2},\quad \lambda_{e\,i+1}^{f-1}=\frac{\lambda_{e\,i}^{f-1}+\lambda_{e\,i+2}^{f-1}}{2}$$
$$\lambda_{l\,i-1}^{f-1}=\frac{\lambda_{l\,i}^{f-1}+\lambda_{l\,i-2}^{f-1}}{2},\quad \lambda_{l\,i+1}^{f-1}=\frac{\lambda_{l\,i}^{f-1}+\lambda_{l\,i+2}^{f-1}}{2} \tag{20}$$

$$\lambda_{e\,j}^{f-1}=\frac{\lambda_{e\,j-1}^{f-1}+\lambda_{e\,j+1}^{f-1}}{2},\quad \lambda_{l\,j}^{f-1}=\frac{\lambda_{l\,j-1}^{f-1}+\lambda_{l\,j+1}^{f-1}}{2} \tag{21}$$

It should be pointed out that adequate stability criteria for explicit scheme must be fulfilled, this means (equations (10), (11))

$$\frac{\tau_e-\Delta t}{2h\tau_e}\ge 0,\quad \frac{\tau_l-\Delta t}{2h\tau_l}\ge 0 \tag{22}$$

and (c.f. equations (18), (19)):

$$\left(1-\frac{(\Delta t)^2\lambda_{e\,i-1}^{f-1}}{4h^2\tau_e C_{e\,i}^{f-1}}-\frac{(\Delta t)^2\lambda_{e\,i+1}^{f-1}}{4h^2\tau_e C_{e\,i}^{f-1}}-\frac{G\Delta t}{C_{e\,i}^{f-1}}\right)\ge 0$$
$$\left(1-\frac{(\Delta t)^2\lambda_{l\,i-1}^{f-1}}{4h^2\tau_l C_l}-\frac{(\Delta t)^2\lambda_{l\,i+1}^{f-1}}{4h^2\tau_l C_l}-\frac{G\Delta t}{C_{l\,i}^{f-1}}\right)\ge 0 \tag{23}$$

3. Results of computations

The gold film of thickness L = 100 nm (1 nm = 10^{-9} m) is considered. Initial temperature is equal to T_p = 300 K. The layer is subjected to a short-pulse laser irradiation (R = 0.93, I_0 = 10 J/m^2, t_p = 0.1 ps, δ = 15.3 nm - c.f. equation (7)). Thermophysical parameters are following: $\lambda_l = \lambda_0$, $\lambda_e = \lambda_0 T_e / T_l$, where λ_0 = = 315 W/(mK), C_l = 2.5 MJ/(m^3 K), $C_e = \gamma T_e$, where γ = 62.9 J/(m^3 K^2), τ_e = 0.04 ps (1 ps = 10^{-12}s), τ_l = 0.8 ps, $G = 2.6\cdot 10^{16}$ W/(m^{3}K) [2]. The problem is solved using the finite difference method under the assumption that Δt = 0.001 ps and h = 1 nm.

Figure 2 shows the comparison of numerical results for thin gold film (x = 0 and I_0 = 13.4 J/m^2) with experimental data presented in [2]. The line and the symbols represent calculated temperature of electrons and experimental data, respectively. The agreement of the results obtained and measured temperatures is very good.

In Figure 3 the heat source profiles for different separation times between laser pulses, namely $f = 4t_p$, $f = 6t_p$ and $f = 8t_p$, respectively are presented.

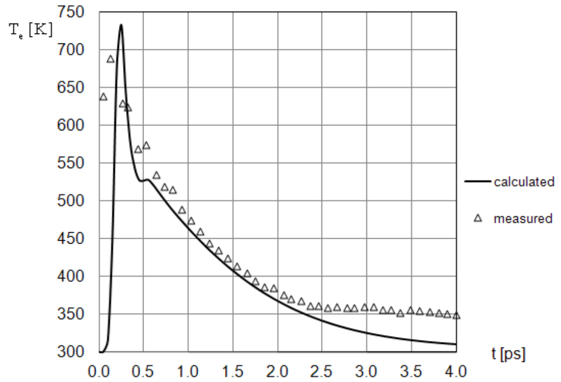

Fig. 2. Comparison of calculated electron temperature with experimental data for 100 nm gold film

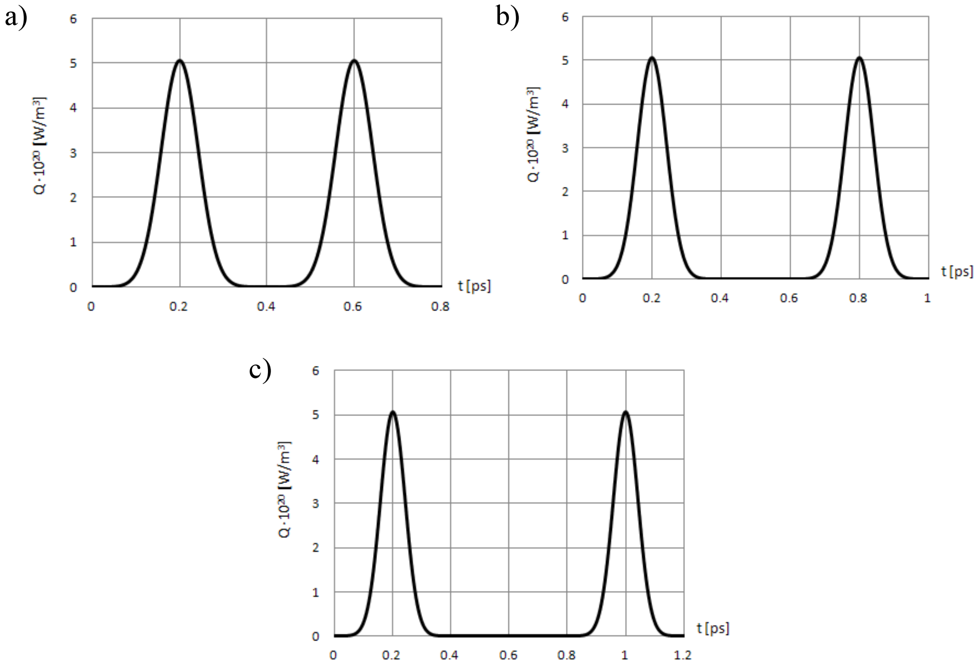

Fig. 3. Heat source profiles for different values of separation time: a) $f = 4t_p$, b) $f = 6t_p$, c) $f = 8t_p$

In Figures 4 and 5 the calculated electrons and lattice temperature profiles at the irradiated surface ($x = 0$) in Au thin film for different values of separation time f are presented. This is visible that the separation time has a greater effect on electron temperature than the temperature of lattice. The longer separation time between laser pulses the later equilibrium of electrons and lattice temperatures is observed.

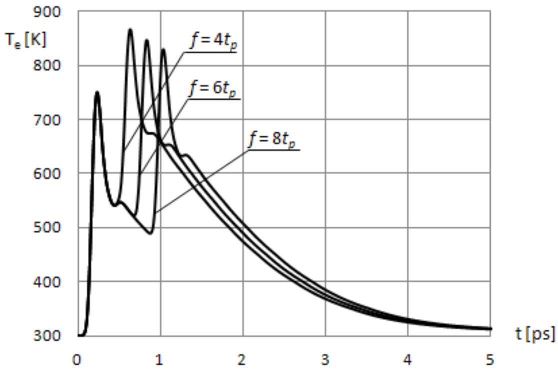

Fig. 4. Profiles of electrons temperatures for different values of f

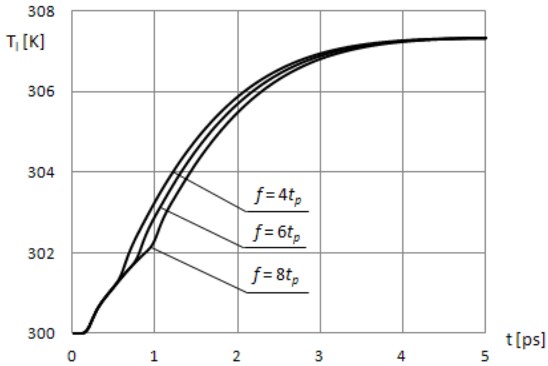

Fig. 5. Profiles of lattice temperatures for different values of f

Conclusions

The hyperbolic two-temperature model assures a good agreement between calculated and measured electron temperatures. It should be emphasized that the use of multiple laser pulses and different separation times allows the lattice to achieve the assumed temperature without increasing the laser power.

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