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TWO-TEMPERATURE MODEL OF MICROSCOPIC HEAT TRANSFER

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Abstract

Thin metal film subjected to a short-pulse laser heating is considered. The hyperbolic two-temperature model describing the temporal and spatial evolution of the lattice and electrons temperatures is discussed. At a stage of numerical computations the finite difference method is used under the assumption that a part of thermophysical parameters in mathematical model of the process considered is temperature-dependent. In the final part of the paper the examples of computations are shown.

Key words: microscale heat transfer, laser heating, thin metal film, two temperature model, finite difference method

1. INTRODUCTION

The usage of femtosecond lasers in practical applications requires (at a stage of mathematical modelling) the description of very complex physical phenomena appearing in the fast heating solids. The differences between the macroscopic heat conduction equation basing on the Fourier law and the models describing the ultrafast heating or cooling processes appear because of extremely short duration, extreme temperature gradients and geometrical features of domain considered (Ozisik & Tzou, 1994; Tamma & Zhou, 1998; Smith & Norris, 2003; Zhang, 2007).

Fast and highly nonequilibrium processes induced in the material, for example by the laser excitation, are a very active research area. From the mathematical point of view exist the different models describing the mechanism of process analyzed (Chen et al., 2004; Zhang, 2007; Escobar, et al., 2006; Majchrzak et al, 2009), in particular the two temperature models (Lin & Zhigilei, 2008; Chen & Beraun, 2001) are also considered.

The microscopic two-temperature models involve two energy equations determining the thermal processes in the electron gas and the metal lattice. Usually, the parabolic two-temperature model is considered (Lin & Zhigilei, 2008). In the case of hyperbolic two-temperature model application the heat conduction in a lattice is not taken into account (Chen & Beraun, 2001).

In this paper the microscopic hyperbolic two-temperature model involving the heat conduction in the lattice is discussed, at the same time a part of parameters appearing in governing equations is assumed to be temperature-dependent (e.g. thermal conductivity and thermal capacity of free electron gas) (Lin & Zhigilei, 2008; Chen & Beraun, 2001). The same model has been used by Majchrzak and Poteralska (2010), but here the different method of the problem solution is proposed. The interactions between external heat source generated by the laser and the domain considered are taken into account by introduction of internal heat source in the equation describing the electron gas temperature (Lin & Zhigilei, 2008). The numerical model bases on a certain variant of finite difference method. At the stage of computations the different thin metal films have been analyzed - the results of simulations are presented in the final part of the paper.

2. MATHEMATICAL MODEL

Let us consider a thin film of thickness L as shown in figure 1. A front surface $x = 0$ is irradiated by a laser pulse. Usually, the laser spot size is much larger than film thickness and then it is possible to treat the interactions as a one-dimensional (1D) heat transfer process (Chen & Beraun, 2001). The mathematical form of the laser heat source constituting the component of energy equation concerning the distribution of electrons temperature is given as

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

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 $\beta = 4 \ln 2$ (Chen & 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.

Taking into account the short period of laser heating, heat losses from front and back surfaces of thin film can be neglected, this means

$$q_e(0, t) = q_e(L, t) = q_l(0, t) = q_l(L, t) = 0 \tag{2}$$

where $q_e(x, t)$, $q_l(x, t)$ are the heat fluxes for electron and lattice systems, respectively.

The initial conditions are assumed to be constant

$$t = 0: \quad T_e(x, 0) = T_l(x, 0) = T_p \tag{3}$$

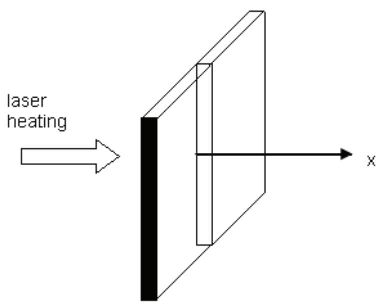

Fig. 1. Thin film.

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 (Lin & Zhigilei, 2008; Chen & Beraun, 2001; Majchrzak & Poteralska, 2010) (1D problem)

$$C_e(T_e)\frac{\partial T_e(x, t)}{\partial t} = -\frac{\partial q_e(x, t)}{\partial x} - G\left[T_e(x, t) - T_l(x, t)\right] + Q(x, t) \tag{4}$$

and

$$C_l(T_l)\frac{\partial T_l(x, t)}{\partial t} = -\frac{\partial q_l(x, t)}{\partial x} + G\left[T_e(x, t) - T_l(x, t)\right] \tag{5}$$

where $C_e(T_e)$, $C_l(T_l)$ are the volumetric specific heats of the electrons and lattice, respectively, G is the electron-phonon coupling factor related to the rate of the energy exchange between electrons and lattice.

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

$$q_e(x, t + \tau_e) = -\lambda_e(T_e, T_l)\frac{\partial T_e(x, t)}{\partial x} \tag{6}$$

and

$$q_l(x, t + \tau_l) = -\lambda_l(T_l)\frac{\partial T_l(x, t)}{\partial x} \tag{7}$$

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

Using the Taylor series expansions the following first-order approximations of equations (6), (7) can be taken into account

$$q_e(x, t) + \tau_e \frac{\partial q_e(x, t)}{\partial t} = -\lambda_e(T_e, T_l)\frac{\partial T_e(x, t)}{\partial x} \tag{8}$$

and

$$q_l(x, t) + \tau_l \frac{\partial q_l(x, t)}{\partial t} = -\lambda_l(T_l)\frac{\partial T_l(x, t)}{\partial x} \tag{9}$$

Introducing (8) into (4) and (9) into (5), respectively, one has

$$C_e(T_e)\frac{\partial T_e(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[\tau_e \frac{\partial q_e(x,t)}{\partial t} + \lambda_e(T_e,T_l)\frac{\partial T_e(x,t)}{\partial x}\right] - G\left[T_e(x,t)-T_l(x,t)\right]+Q(x,t) \tag{10}$$

and

$$C_l(T_l)\frac{\partial T_l(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[\tau_l \frac{\partial q_l(x,t)}{\partial t} + \lambda_l(T_l)\frac{\partial T_l(x,t)}{\partial x}\right] + G\left[T_e(x,t)-T_l(x,t)\right] \tag{11}$$

Assuming that τ_e and τ_l are the constant values, the equations (10), (11) can be written in the form

$$C_e(T_e)\frac{\partial T_e(x,t)}{\partial t} = \tau_e\frac{\partial}{\partial t}\left(\frac{\partial q_e(x,t)}{\partial x}\right) + \frac{\partial}{\partial x}\left(\lambda_e(T_e,T_l)\frac{\partial T_e(x,t)}{\partial x}\right) - G\left[T_e(x,t)-T_l(x,t)\right]+Q(x,t) \tag{12}$$

and

$$C_l(T_l)\frac{\partial T_l(x,t)}{\partial t} = \tau_l\frac{\partial}{\partial t}\left(\frac{\partial q_l(x,t)}{\partial x}\right) + \frac{\partial}{\partial x}\left(\lambda_l(T_l)\frac{\partial T_l(x,t)}{\partial x}\right) + G\left[T_e(x,t)-T_l(x,t)\right] \tag{13}$$

From equations equations (4), (5) results that

$$-\frac{\partial q_e(x,t)}{\partial x} = C_e(T_e)\frac{\partial T_e(x,t)}{\partial t} + G\left[T_e(x,t)-T_l(x,t)\right]-Q(x,t) \tag{14}$$

and

$$-\frac{\partial q_l(x,t)}{\partial x} = C_l(T_l)\frac{\partial T_l(x,t)}{\partial t} - G\left[T_e(x,t)-T_l(x,t)\right] \tag{15}$$

Introducing (14) into (12) and (15) into (13), respectively, under the assumption that the coupling factor G is a constant value, the equations (12), (13) have a form

$$C_e(T_e)\frac{\partial T_e(x,t)}{\partial t} + \tau_e\frac{\partial}{\partial t}\left[C_e(T_e)\frac{\partial T_e(x,t)}{\partial t}\right] + \tau_e G\left[\frac{\partial T_e(x,t)}{\partial t} - \frac{\partial T_l(x,t)}{\partial t}\right] = \frac{\partial}{\partial x}\left(\lambda_e(T_e,T_l)\frac{\partial T_e(x,t)}{\partial x}\right) - G\left[T_e(x,t)-T_l(x,t)\right] + Q(x,t)+\tau_e\frac{\partial Q(x,t)}{\partial t} \tag{16}$$

and

$$C_l(T_l)\frac{\partial T_l(x,t)}{\partial t} + \tau_l\frac{\partial}{\partial t}\left[C_l(T_l)\frac{\partial T_l(x,t)}{\partial t}\right] - \tau_l G\left[\frac{\partial T_e(x,t)}{\partial t} - \frac{\partial T_l(x,t)}{\partial t}\right] = \frac{\partial}{\partial x}\left(\lambda_l(T_l)\frac{\partial T_l(x,t)}{\partial x}\right) + G\left[T_e(x,t)-T_l(x,t)\right] \tag{17}$$

Because

$$\frac{\partial C_e(T_e)}{\partial t} = \frac{\mathrm{d}C_e(T_e)}{\mathrm{d}T_e}\frac{\partial T_e}{\partial t}, \quad \frac{\partial C_l(T_l)}{\partial t} = \frac{\mathrm{d}C_l(T_l)}{\mathrm{d}T_l}\frac{\partial T_l}{\partial t} \tag{18}$$

therefore

$$C_e(T_e)\frac{\partial T_e(x,t)}{\partial t} + \tau_e\frac{\mathrm{d}C_e(T_e)}{\mathrm{d}T_e}\left[\frac{\partial T_e(x,t)}{\partial t}\right]^2 + \tau_e C_e(T_e)\frac{\partial^2 T_e(x,t)}{\partial t^2} + \tau_e G\left[\frac{\partial T_e(x,t)}{\partial t} - \frac{\partial T_l(x,t)}{\partial t}\right] = \frac{\partial}{\partial x}\left(\lambda_e(T_e,T_l)\frac{\partial T_e(x,t)}{\partial x}\right) - G\left[T_e(x,t)-T_l(x,t)\right] + Q(x,t)+\tau_e\frac{\partial Q(x,t)}{\partial t} \tag{19}$$

and

$$C_l(T_l)\frac{\partial T_l(x,t)}{\partial t} + \tau_l\frac{\mathrm{d}C_l(T_l)}{\mathrm{d}T_l}\left[\frac{\partial T_l(x,t)}{\partial t}\right]^2 + \tau_l C_l(T_l)\frac{\partial^2 T_l(x,t)}{\partial t^2} + \tau_l G\left[\frac{\partial T_l(x,t)}{\partial t} - \frac{\partial T_e(x,t)}{\partial t}\right] =$$

$$\frac{\mathrm{d}C_l(T_l)}{\mathrm{d}T_l}\left[\frac{\partial T_l(x,t)}{\partial t}\right]^2 + \tau_l\, C_l(T_l)\frac{\partial^2 T_l(x,t)}{\partial t^2}+$$

$$\frac{(x,t)}{\partial t}\Bigg] = \frac{\partial}{\partial x}\left(\lambda_l(T_l)\,\frac{\partial T_l(x,t)}{\partial x}\right) - G\left[T_l(x,t)-T_e(x,t)\right] \tag{20}$$

The following thermophysical properties appear in the two-temperature model (19), (20): C_e, C_l, λ_e, λ_l, G, τ_e, τ_l. To define the thermal conductivity λ_e and heat capacity C_e of electrons the following relationships are widely used (Lin & Zhigilei, 2008; Chen & Beraun, 2001)

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

$$C_e(T_e) = A_e T_e \tag{21}$$

where λ_0, A_e are the constants. The remaining parameters, this means λ_l, C_l, G, τ_e, τ_l usually are assumed to be the constant ones. It should be pointed out that the simple form of formulas (21) is only suitable for temperatures T_e much smaller than Fermi temperature $T_F = E_F / k_B$, where E_F, k_B are the Fermi energy and Boltzmann constant, respectively (Lin & Zhigilei, 2008).

3. EXAMPLES OF COMPUTATIONS

To solve the problem formulated, this means the equations (19), (20) supplemented by boundary and initial conditions (2), (3), the finite difference method is used and the numerical algorithm bases on the extended version of FDM presented by Majchrzak at al. (2009).

The film of thickness L = 100 nm and initial temperature T_p = 300 K is considered. 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 (1)). The computations have been done for different metals – table 1.

Table 1. *Thermophysical parameters for selected metals (Z.Lin, L.V. Zhigilei, 2008)*

	Au	Cu	Ti	W
λ_0 [W/(mK)]	315	409	21.9	173
A_e [J/(m^{3}K^2)]	62.9	71.0	328.9	137.3
C_l [J/(m^{3}K)]	$2.5\cdot10^6$	$3.39\cdot10^6$	$2.34\cdot10^6$	$3\cdot10^6$
G [W/(m^{3}K)]	$2.6\cdot10^{16}$	10^{17}	$1.3\cdot10^{18}$	$5\cdot10^{17}$
τ_e [ps]	0.04	0.03	0.01	0.01
τ_l [ps]	0.8	0.6	0.5	0.2

In figures 2-9 the calculated electrons and lattice temperature profiles in Au, Cu, Ti and W thin films are shown. Figure 10 illustrates the heating (cooling) curves T_e, T_l at the front surface (x = 0) for these materials.

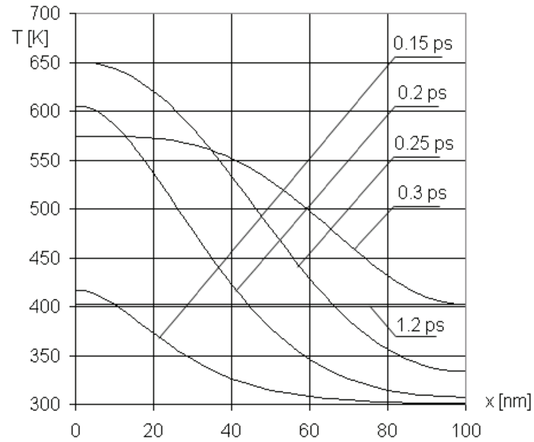

Fig. 2. *Electron temperature profiles (Au).*

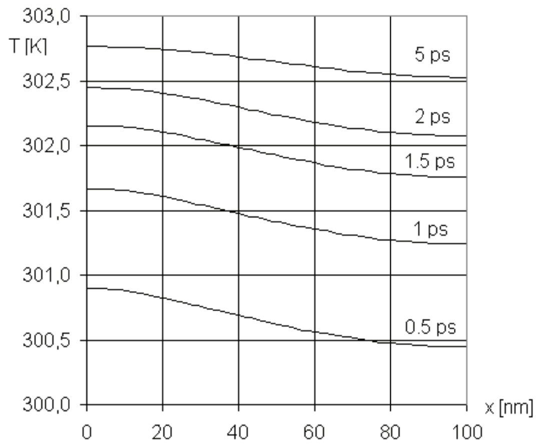

Fig. 3. *Lattice temperature profiles (Au).*

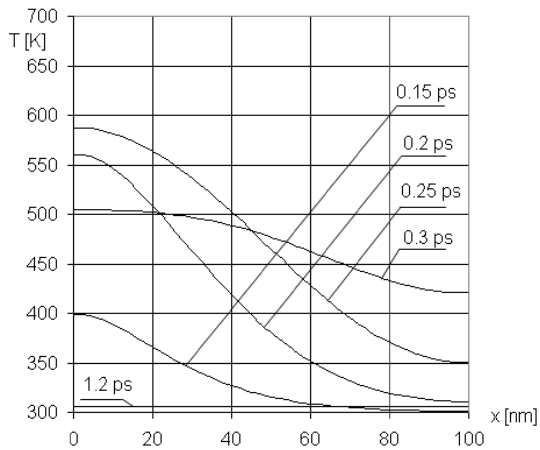

Fig. 4. *Electron temperature profiles (Cu).*

It is visible, that the results of computations for successive materials are different. For example, although the thermal conductivity of copper λ_0 is greater than the thermal conductivity of gold, both the electrons and the lattice temperatures in Cu film are lower in comparison with Au film (figures 2-5). This results from the differences in values of coupling factor between these materials - the coupling factor for Cu is essentially greater than coupling factor for Au.

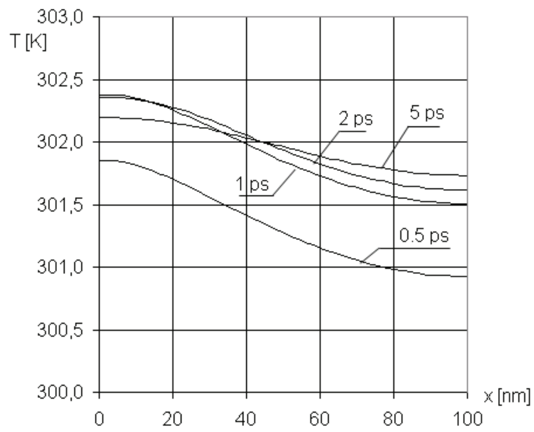

Fig. 5. Lattice temperature profiles (Cu).

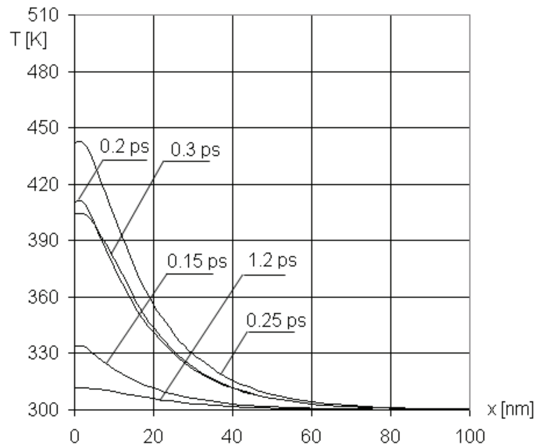

Fig. 6. Electron temperature profiles (Ti).

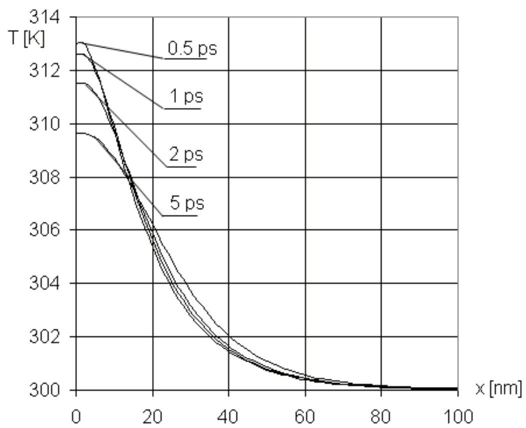

Fig. 7. Lattice temperature profiles (Ti)

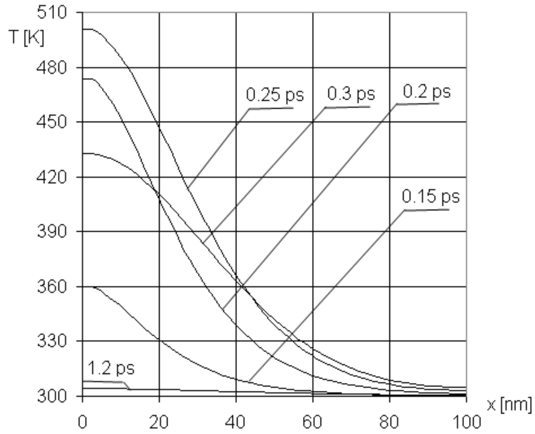

Fig. 8. Electron temperature profiles (W).

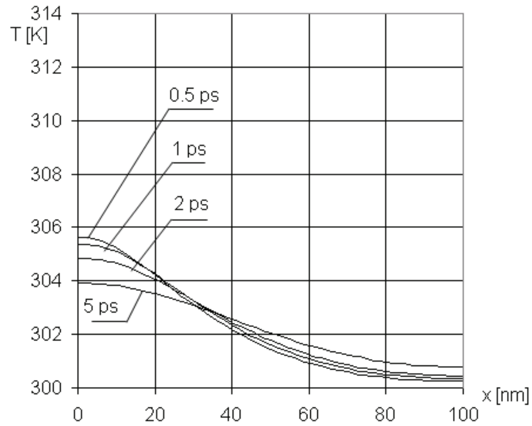

Fig. 9. Lattice temperature profiles (W).

It should be pointed out that for Au thin film the temperatures obtained quite good agree with experimental results presented by Chen & Beraun (2001) and Qiu et al. (1994) as shown in figure 11 (the results presented in the quoted papers correspond to $I_0 = 13.4$ J/m^2, $t_p = 0.1$ ps). The normalized temperature used in the last figure is defined as $(T_e - T_p)/(T_e - T_{max})$, where T_{max} denotes the maximum electrons temperature.

The numerical experiments concerning the same material but different laser intensities show that the results from the qualitative point of view are similar and the main differences are connected with the changes of maximum electrons temperature.

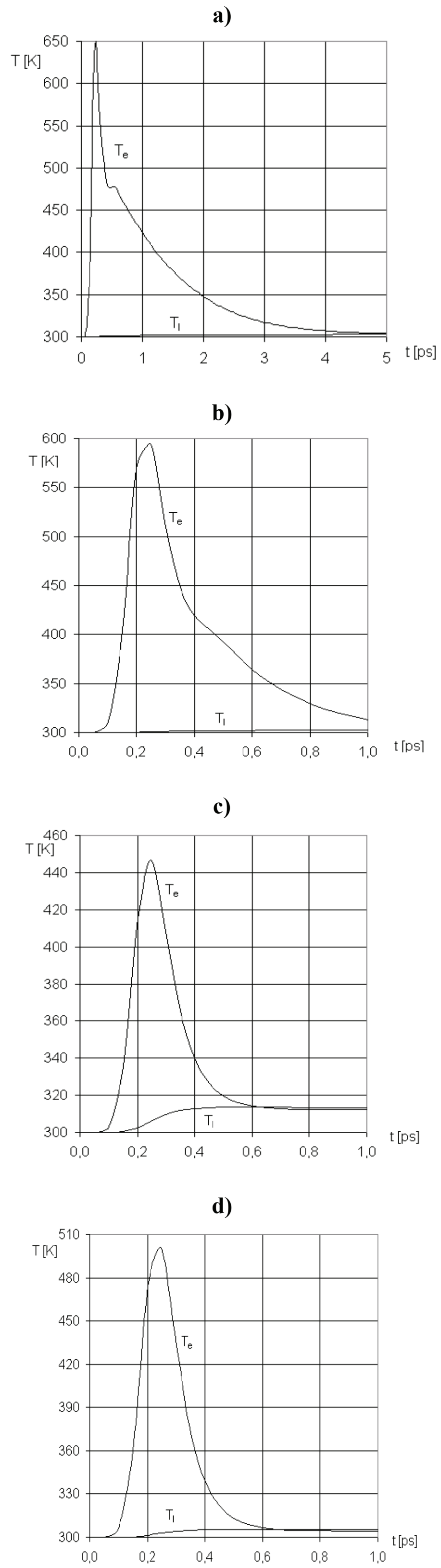

Fig. 10. Time history of the electron and lattice temperatures at the front surface (x = 0): a) Au, b) Cu, c) Ti, d) W

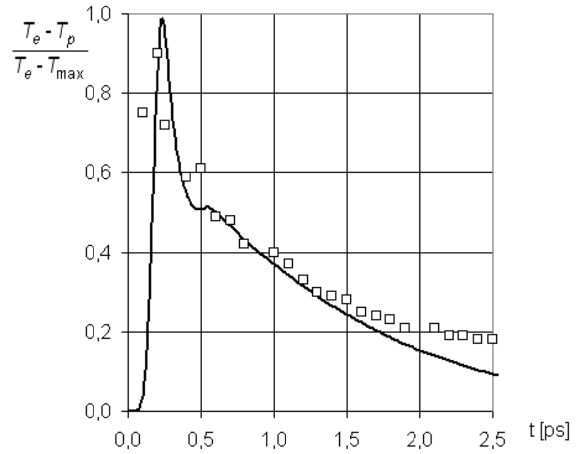

***Fig. 11.** Comparison of the normalized electron temperature at the front surface of gold film (full line) with the experimental data presented by Chen & Beraun (2001) and Qiu et al. (1994).*

4. CONCLUSIONS

The two-temperature hyperbolic model of thermal processes in thin metal films subjected to ultrafast laser pulse is considered. The same problem can be also described using the different approaches but it seems that the non-equilibrium model presented gives the very interesting information about the course of the process which cannot be obtained using the others models. Among others, this model allows one to determine the thermalization time appearing in the equation called the dual phase lag model (time for which the equalization of electrons and lattice temperatures takes place – c.f. figure 10).

The thermal interactions between external heat source and the film domain can be taken into account in a 'natural' way (the real boundary condition on external surface is introduced) or this condition is substituted by introduction of internal heat source (equation concerning the free electron gas) and this approach has been here used. The further investigations will be connected with the generalization of model considered on a case of 2D or 3D tasks.

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DWU-TEMPERATUROWY MODEL PRZEPŁYWU CIEPŁA W SKALI MIKRO

Streszczenie

Rozpatrywano cienką warstwę metalową poddaną działaniu lasera. Procesy cieplne w analizowanym obszarze opisano dwu-temperaturowym hiperbolicznym modelem, który uwzględnia zmiany temperatury elektronów i sieci krystalicznej. Zadanie rozwiązano za pomocą metody różnic skończonych, przy czym uwzględniono zmienne z temperaturą wartości niektórych parametrów termofizycznych W końcowej części artykułu przedstawiono wyniki obliczeń.

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