Sensitivity analysis of two-temperature microscale heat transfer model with respect to the electron-phonon coupling factor

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Abstract

The microscale heat transfer model basing on the system of energy equations concerning the electron gas and phonon one is considered. The thermal interactions between electrons and lattice are determined by the parameter G called the coupling factor. To estimate the influence of this parameter perturbations on the course of thermal processes proceeding in the thin metal film subjected to an ultrashort laser pulse the direct variant of sensitivity analysis is applied. The problem of temporal and spatial evolution of the lattice and electrons temperatures calculations and the sensitivity one are solved using the finite difference method (a staggered geometrical grid is used). In the final part of the paper the examples of computations are shown.

Keywords: microscale heat transfer, laser heating, sensitivity analysis, two-temperature model, finite difference method

1. Introduction

The differences between the macroscopic heat conduction equation basing on the Fourier law and the models describing the microscale heat transfer appear because of extremely short duration, extreme temperature gradients and very small geometrical dimensions of an object considered. Ultrafast heating of thin metal film can be well described by the so-called two-temperature model [1, 2] (system of partial differential equations) which is supplemented by the adequate boundary and initial conditions. The thermal interactions between electrons temperature T_e and phonons temperature T_l are determined by the parameter G called a coupling factor (e.g. [6]). The assumption that the values of T_e and T_l are not big allows one to treat the parameter G as a constant value and a such situation is considered here. The changes of electrons and phonons temperatures due to the parameter G perturbations are estimated using the methods of sensitivity analysis [5]. At the stage of numerical computations both in a case of basic and sensitivity problems solution the finite difference method has been used.

2. Mathematical model

Let us consider a thin film of thickness L. A surface $x = 0$ is irradiated by a ultrashort laser pulse. Because the laser spot size is much larger than film thickness therefore it is possible to treat the problem as a 1D one [2].

The temporal and spatial evolution of the lattice and electrons temperatures in the irradiated metal is described by equations

$$C_e(T_e)\frac{\partial T_e(x,t)}{\partial t} = -\frac{\partial q_e(x,t)}{\partial x} + $$

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

and

$$C_l(T_l)\frac{\partial T_l(x,t)}{\partial t} = -\frac{\partial q_l(x,t)}{\partial x} + $$

$$+G(T_e)\left[T_e(x,t) - T_l(x,t)\right] \tag{2}$$

where $C_e(T_e)$, $C_l(T_l)$ are the volumetric specific heats of the electrons and lattice, respectively, $q_e(x,t)$, $q_l(x,t)$ are the heat fluxes for electron and lattice systems, G is the electron-phonon coupling factor related to the rate of the energy exchange between electrons and lattice. The internal heat source $Q(x,t)$ connected with the laser action is given as [2]

$$Q(x,t) = \sqrt{\frac{\beta}{\pi}}\frac{1-R}{t_p\,\delta}\,I_0\,\exp\left[-\frac{x}{\delta} - \beta\frac{(t-2t_p)^2}{t_p^2}\right] \tag{3}$$

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 $\beta = 4\ln 2$ [2].

Here, in a place of classical Fourier law the following formulas are introduced

$$q_e(x, t+\tau_e) = -\lambda_e(T_e, T_l)\frac{\partial T_e(x,t)}{\partial x} \tag{4}$$

and

$$q_l(x, t+\tau_l) = -\lambda_l(T_l)\frac{\partial T_l(x,t)}{\partial x} \tag{5}$$

where $\lambda_e(T_e, T_l)$, $\lambda_l(T_l)$ are the thermal conductivities, 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.

Taking into account the short period of laser heating, heat losses from front and back surfaces of thin film can be neglected [2], this means

$$q_e(0,t) = q_e(L,t) = q_l(0,t) = q_l(L,t) = 0 \tag{6}$$

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

$$t = 0:\quad T_e(x,0) = T_l(x,0) = T_p \tag{7}$$

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It should be pointed out that for constant coupling factor G the equations (1), (2) take a form

$$C_e(T_e)\frac{\partial T_e}{\partial t} = -\frac{\partial q_e}{\partial x} - G(T_e - T_l) + Q$$

$$C_l(T_l)\frac{\partial T_l}{\partial t} = -\frac{\partial q_l}{\partial x} + G(T_e - T_l) \tag{8}$$

Using the Taylor series expansions the following first-order approximation of equations (4), (5) can be taken into account

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

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

3. Sensitivity analysis

The differentiation of equations (8) with respect to the coupling factor G gives

$$\frac{\mathrm{d}C_e(T_e)}{\mathrm{d}T_e}\frac{\partial T_e}{\partial G}\frac{\partial T_e}{\partial t} + C_e(T_e)\frac{\partial}{\partial t}\left(\frac{\partial T_e}{\partial G}\right) =$$

$$= -\frac{\partial}{\partial x}\left(\frac{\partial q_e}{\partial G}\right) - (T_e - T_l) - G\left(\frac{\partial T_e}{\partial G} - \frac{\partial T_l}{\partial G}\right) \tag{10}$$

and

$$\frac{\mathrm{d}C_l(T_l)}{\mathrm{d}T_l}\frac{\partial T_l}{\partial G}\frac{\partial T_l}{\partial t} + C_l(T_l)\frac{\partial}{\partial t}\left(\frac{\partial T_l}{\partial G}\right) =$$

$$= -\frac{\partial}{\partial x}\left(\frac{\partial q_l}{\partial G}\right) + (T_e - T_l) + G\left(\frac{\partial T_e}{\partial G} - \frac{\partial T_l}{\partial G}\right) \tag{11}$$

The equations (9) are also differentiated with respect to the G and then

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

$$-\lambda_e(T_e,T_l)\frac{\partial}{\partial x}\left(\frac{\partial T_e}{\partial G}\right) \tag{12}$$

and

$$\frac{\partial q_l}{\partial G} + \tau_l\frac{\partial}{\partial t}\left(\frac{\partial q_l}{\partial G}\right) = -\frac{\mathrm{d}\lambda_l(T_l)}{\mathrm{d}T_l}\frac{\partial T_l}{\partial G}\frac{\partial T_l}{\partial x} - \lambda_l(T_l)\frac{\partial}{\partial x}\left(\frac{\partial T_l}{\partial G}\right) \tag{13}$$

Introducing

$$U_e = \frac{\partial T_e}{\partial G},\quad U_l = \frac{\partial T_l}{\partial G},\quad w_e = \frac{\partial q_e}{\partial G},\quad w_l = \frac{\partial q_l}{\partial G} \tag{14}$$

into equations (10), (11), (12) and (13) one has

$$\frac{\mathrm{d}C_e(T_e)}{\mathrm{d}T_e}U_e\frac{\partial T_e}{\partial t} + C_e(T_e)\frac{\partial U_e}{\partial t} =$$

$$= -\frac{\partial w_e}{\partial x} - (T_e - T_l) - G(U_e - U_l) \tag{15}$$

$$\frac{\mathrm{d}C_l(T_l)}{\mathrm{d}T_l}U_l\frac{\partial T_l}{\partial t} + C_l(T_l)\frac{\partial U_l}{\partial t} =$$

$$= -\frac{\partial w_l}{\partial x} + (T_e - T_l) + G(U_e - U_l) \tag{16}$$

and

$$w_e + \tau_e\frac{\partial w_e}{\partial t} = -\left[\frac{\partial \lambda_e(T_e,T_l)}{\partial T_e}U_e + \frac{\partial \lambda_e(T_e,T_l)}{\partial T_l}U_l\right]\frac{\partial T_e}{\partial x} +$$

$$-\lambda_e(T_e,T_l)\frac{\partial U_e}{\partial x} \tag{17}$$

$$w_l + \tau_l\frac{\partial w_l}{\partial t} = -\frac{\partial \lambda_l(T_l)}{\partial T_l}U_l\frac{\partial T_l}{\partial x} - \lambda_l(T_l)\frac{\partial U_l}{\partial x} \tag{18}$$

After some mathematical operations one obtains

$$C_e(T_e)\frac{\partial U_e}{\partial t} == -\frac{\partial w_e}{\partial x} - G(U_e - U_l) +$$

$$-(T_e - T_l) - \frac{\mathrm{d}C_e(T_e)}{\mathrm{d}T_e}U_e\frac{\partial T_e}{\partial t} \tag{19}$$

$$C_l(T_l)\frac{\partial U_l}{\partial t} == -\frac{\partial w_l}{\partial x} + G(U_e - U_l) +$$

$$+(T_e - T_l) - \frac{\mathrm{d}C_l(T_l)}{\mathrm{d}T_l}U_l\frac{\partial T_l}{\partial t} \tag{20}$$

and

$$w_e + \tau_e\frac{\partial w_e}{\partial t} = -\lambda_e(T_e,T_l)\frac{\partial U_e}{\partial x} +$$

$$-\left[\frac{\partial \lambda_e(T_e,T_l)}{\partial T_e}U_e + \frac{\partial \lambda_e(T_e,T_l)}{\partial T_l}U_l\right]\frac{\partial T_e}{\partial x} \tag{21}$$

$$w_l + \tau_l\frac{\partial w_l}{\partial t} = -\lambda_l(T_l)\frac{\partial U_l}{\partial x} - \frac{\partial \lambda_l(T_l)}{\partial T_l}U_l\frac{\partial T_l}{\partial x} \tag{22}$$

Finally

$$C_e(T_e)\frac{\partial U_e}{\partial t} == -\frac{\partial w_e}{\partial x} - G(U_e - U_l) +$$

$$-(T_e - T_l) - C_{e,e}U_e\frac{\partial T_e}{\partial t} \tag{23}$$

$$C_l(T_l)\frac{\partial U_l}{\partial t} == -\frac{\partial w_l}{\partial x} + G(U_e - U_l) +$$

$$+(T_e - T_l) - C_{l,l}U_l\frac{\partial T_l}{\partial t} \tag{24}$$

and

$$w_e + \tau_e\frac{\partial w_e}{\partial t} = -\lambda_e(T_e,T_l)\frac{\partial U_e}{\partial x} +$$

$$-\left[\lambda_{e,e}U_e + \lambda_{e,l}U_l\right]\frac{\partial T_e}{\partial x} \tag{25}$$

$$w_l + \tau_l\frac{\partial w_l}{\partial t} = -\lambda_l(T_l)\frac{\partial U_l}{\partial x} - \lambda_{l,l}U_l\frac{\partial T_l}{\partial x} \tag{26}$$

where

$$C_{e,e} = \frac{\mathrm{d}C_e(T_e)}{\mathrm{d}T_e},\quad C_{l,l} = \frac{\mathrm{d}C_l(T_l)}{\mathrm{d}T_l} \tag{27}$$

and

$$\lambda_{e,e}=\frac{\partial\lambda_e(T_e,T_l)}{\partial T_e}\,,\quad \lambda_{e,l}=\frac{\partial\lambda_l(T_e,T_l)}{\partial T_l}\,,\quad \lambda_{l,l}=\frac{\mathrm{d}\lambda_l(T_l)}{\mathrm{d}T_l} \tag{28}$$

Additionally, the differentiation of equations (6), (7) with respect to the coupling factor G gives

$$w_e(0,\,t)=w_e(L,\,t)=w_l(0,\,t)=w_l(L,\,t)=0 \tag{29}$$

$$t=0:\;\; U_e(x,\,0)=U_l(x,\,0)=T_p \tag{30}$$

Summing up, the equations (23), (24), (25), (26) supplemented by boundary conditions (29) and initial ones (30) create the additional problem connected with the sensitivity analysis of temperature fields T_e and T_l with respect to the coupling factor G.

4. Finite difference method

To solve the basic and additional problems formulated the finite difference method is adapted. A staggered grid [3, 7] is introduced as shown in Figure 1. Let us denote $T_i^f=T\,(ih,\,f\Delta t)$, $U_{ei}^f=U_e\,(ih,\,f\Delta t)$, $U_{li}^f=U_l\,(ih,\,f\Delta t)$, where h is a mesh size, Δt is a time step, $i=0,\,2,\,4,\,...,\,N$, $f=0,\,1,\,2,\,...,\,F$, and $q_j^f=q(jh,\;f\Delta t)$, $w_{ej}^f=w_e(jh,\;f\Delta t)$, $w_{lj}^f=w_l(jh,\;f\Delta t)$, where $j=1,\,3,\,....,\,N$-1.

The way of basic problem solution (equations (8), (9), (6), (7)) has been presented in details in [7]. Here, the method of additional problem solution (equations (23), (24), (25), (26), (29), (30)) is discussed.

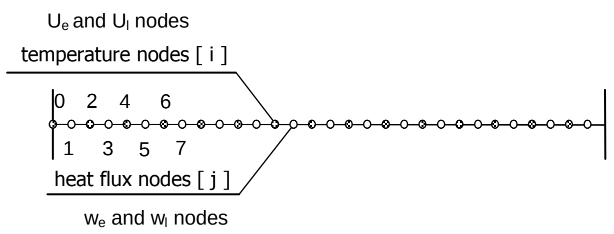

Figure 1: Discretization

The finite difference approximation the equations (25) and (26) using explicit scheme can be written in the form

$$w_{e\,j}^{f-1}+\tau_e\frac{w_{e\,j}^{f}-w_{e\,j}^{f-1}}{\Delta t}=-\lambda_{e\,j}^{f-1}\frac{U_{e\,j+1}^{f-1}-U_{e\,j-1}^{f-1}}{2h}+$$
$$-\left[\lambda_{e,e\,j}^{f-1}U_{e\,j}^{f-1}+\lambda_{e,l\,j}^{f-1}U_{l\,j}^{f-1}\right]\frac{T_{e\,j+1}^{f-1}-T_{e\,j-1}^{f-1}}{2h} \tag{31}$$

$$w_{l\,j}^{f-1}+\tau_l\frac{w_{l\,j}^{f}-w_{l\,j}^{f-1}}{\Delta t}=-\lambda_{l\,j}^{f-1}\frac{U_{l\,j+1}^{f-1}-U_{l\,j-1}^{f-1}}{2h}+$$
$$+\lambda_{l,l\,j}^{f-1}U_{l\,j}^{f-1}\frac{T_{l\,j+1}^{f-1}-T_{l\,j-1}^{f-1}}{2h} \tag{32}$$

where $j=1,\,3,\,....,\,N$-1.

After some mathematical operations one has

$$w_{e\,j}^{f}=\frac{\tau_e-\Delta t}{\tau_e}w_{e\,j}^{f-1}-\frac{\left(\lambda_{e\,j-1}^{f-1}+\lambda_{e\,j+1}^{f-1}\right)\Delta t}{4h\tau_e}\left(U_{e\,j+1}^{f-1}-U_{e\,j-1}^{f-1}\right)+$$
$$-\frac{\Delta t}{8h\tau_e}\left[\left(\lambda_{e,e\,j-1}^{f-1}+\lambda_{e,e\,j+1}^{f-1}\right)\left(U_{e\,j-1}^{f-1}+U_{e\,j+1}^{f-1}\right)+\right.$$
$$\left.+\left(\lambda_{e,l\,j-1}^{f-1}+\lambda_{e,l\,j+1}^{f-1}\right)\left(U_{l\,j-1}^{f-1}+U_{l\,j+1}^{f-1}\right)\right]\left(T_{e\,j+1}^{f-1}-T_{e\,j-1}^{f-1}\right) \tag{33}$$

$$w_{l\,j}^{f}=\frac{\tau_l-\Delta t}{\tau_l}w_{l\,j}^{f-1}-\frac{\left(\lambda_{l\,j-1}^{f-1}+\lambda_{l\,j+1}^{f-1}\right)\Delta t}{4h\tau_l}\left(U_{l\,j+1}^{f-1}-U_{l\,j-1}^{f-1}\right)+$$
$$-\frac{\Delta t}{8h\tau_l}\left(\lambda_{l,l\,j-1}^{f-1}+\lambda_{l,l\,j+1}^{f-1}\right)\left(U_{l\,j-1}^{f-1}+U_{l\,j+1}^{f-1}\right)\left(T_{l\,j+1}^{f-1}-T_{l\,j-1}^{f-1}\right) \tag{34}$$

The stability criteria should be fulfilled

$$\frac{\tau_e-\Delta t}{2h\tau_e}\geq 0\;,\quad \frac{\tau_l-\Delta t}{2h\tau_l}\geq 0 \tag{35}$$

The dependences (33), (34) allow one to construct the similar formulas for nodes i-1, i+1 and then ($i=0,\,2,\,4,\,...,\,N$)

$$w_{ei-1}^{f}-w_{ei+1}^{f}=\frac{\tau_e-\Delta t}{\tau_e}\left(w_{ei-1}^{f-1}-w_{ei+1}^{f-1}\right)+\frac{\Delta t}{4h\tau_e}\left[\left(\lambda_{ei-2}^{f-1}+\lambda_{ei}^{f-1}\right)\left(U_{ei-2}^{f-1}-U_{ei}^{f-1}\right)+\right.$$
$$\left.+\left(\lambda_{ei}^{f-1}+\lambda_{ei+2}^{f-1}\right)\left(U_{ei+2}^{f-1}-U_{ei}^{f-1}\right)\right]+\frac{\Delta t}{8h\tau_e}\left[\left(\lambda_{e,ei-2}^{f-1}+\lambda_{e,ei}^{f-1}\right)\left(U_{ei-2}^{f-1}+U_{ei}^{f-1}\right)+\right.$$
$$\left.+\left(\lambda_{e,li}^{f-1}+\lambda_{e,li-2}^{f-1}\right)\left(U_{li-2}^{f-1}+U_{li}^{f-1}\right)\right]\left(T_{ei-2}^{f-1}-T_{ei}^{f-1}\right)+$$
$$+\frac{\Delta t}{8h\tau_e}\left[\left(\lambda_{e,ei+2}^{f-1}+\lambda_{e,ei}^{f-1}\right)\left(U_{ei}^{f-1}+U_{ei+2}^{f-1}\right)+\right.$$
$$\left.+\left(\lambda_{e,li+2}^{f-1}+\lambda_{e,li}^{f-1}\right)\left(U_{li}^{f-1}+U_{li+2}^{f-1}\right)\right]\left(T_{ei+2}^{f-1}-T_{ei}^{f-1}\right) \tag{36}$$

$$w_{li-1}^{f}-w_{li+1}^{f}=\frac{\tau_l-\Delta t}{\tau_l}\left(w_{li-1}^{f-1}-w_{li+1}^{f-1}\right)+\frac{\Delta t}{4h\tau_e}\left[\left(\lambda_{li-2}^{f-1}+\lambda_{li}^{f-1}\right)\left(U_{li-2}^{f-1}-U_{li}^{f-1}\right)+\right.$$
$$\left.+\left(\lambda_{li}^{f-1}+\lambda_{l\,i+2}^{f-1}\right)\left(U_{l\,i+2}^{f-1}-U_{li}^{f-1}\right)\right]+$$
$$+\frac{\Delta t}{8h\tau_e}\left(\lambda_{l,l\,i-2}^{f-1}+\lambda_{l,li}^{f-1}\right)\left(U_{li-2}^{f-1}+U_{li}^{f-1}\right)\left(T_{li-2}^{f-1}-T_{li}^{f-1}\right)+$$
$$+\frac{\Delta t}{8h\tau_e}\left(\lambda_{l,l\,i+2}^{f-1}+\lambda_{l,li}^{f-1}\right)\left(U_{li}^{f-1}+U_{l\,i+2}^{f-1}\right)\left(T_{l\,i+2}^{f-1}-T_{li}^{f-1}\right) \tag{37}$$

Now, equations (23) and (24) are discretized

$$C_{ei}^{f-1}\frac{U_{ei}^{f}-U_{ei}^{f-1}}{\Delta t}==-\frac{w_{ei+1}^{f-1}-w_{ei-1}^{f-1}}{2h}-G(U_{ei}^{f-1}-U_{li}^{f-1})+$$
$$-(T_{ei}^{f-1}-T_{li}^{f-1})-C_{e,ei}U_{ei}^{f-1}\frac{T_{ei}^{f}-T_{ei}^{f-1}}{\Delta t} \tag{38}$$

$$C_{li}^{f-1}\frac{U_{li}^{f}-U_{li}^{f-1}}{\Delta t}==-\frac{w_{li+1}^{f-1}-w_{li-1}^{f-1}}{2h}+G(U_{ei}^{f-1}-U_{li}^{f-1})+$$
$$+(T_{ei}^{f-1}-T_{li}^{f-1})-C_{l,li}U_{li}^{f-1}\frac{T_{li}^{f}-T_{li}^{f-1}}{\Delta t} \tag{39}$$

Putting (36) and (37) into (38) and (39), respectively, one has

$$C_{ei}^{f-1}\frac{U_{ei}^{f}-U_{ei}^{f-1}}{\Delta t}==-\frac{\tau_e-\Delta t}{2h\tau_e}\left(w_{ei-1}^{f-1}-w_{ei+1}^{f-1}\right)+$$
$$\frac{\Delta t}{8h^2\tau_e}\left[\left(\lambda_{ei-2}^{f-1}+\lambda_{ei}^{f-1}\right)\left(U_{ei-2}^{f-1}-U_{ei}^{f-1}\right)+\right.$$
$$\left.+\left(\lambda_{ei}^{f-1}+\lambda_{ei+2}^{f-1}\right)\left(U_{ei+2}^{f-1}-U_{ei}^{f-1}\right)\right]+$$
$$\frac{\Delta t}{16h^2\tau_e}\left[\left(\lambda_{e,ei-2}^{f-1}+\lambda_{e,ei}^{f-1}\right)\left(U_{ei-2}^{f-1}+U_{ei}^{f-1}\right)+\right.$$

$$+\left(\lambda_{e,li}^{f-1}+\lambda_{e,li-2}^{f-1}\right)\left(U_{li-2}^{f-1}+U_{li}^{f-1}\right)\Big]\left(T_{ei-2}^{f-1}-T_{ei}^{f-1}\right)+$$

$$+\frac{\Delta t}{16h^2\tau_e}\Big[\left(\lambda_{e,ei+2}^{f-1}+\lambda_{e,ei}^{f-1}\right)\left(U_{ei}^{f-1}+U_{ei+2}^{f-1}\right)+$$

$$+\left(\lambda_{e,li+2}^{f-1}+\lambda_{e,li}^{f-1}\right)\left(U_{li}^{f-1}+U_{li+2}^{f-1}\right)\Big]\left(T_{ei+2}^{f-1}-T_{ei}^{f-1}\right)+$$

$$-G(U_{ei}^{f-1}-U_{li}^{f-1})-(T_{ei}^{f-1}-T_{li}^{f-1})-C_{e,ei}U_{ei}^{f-1}\frac{T_{ei}^{f}-T_{ei}^{f-1}}{\Delta t} \tag{40}$$

and

$$C_{li}^{f-1}\frac{U_{li}^{f}-U_{li}^{f-1}}{\Delta t}==-\frac{\tau_l-\Delta t}{2h\tau_l}\left(w_{li-1}^{f-1}-w_{li+1}^{f-1}\right)+$$

$$\frac{\Delta t}{8h^2\tau_l}\Big[\left(\lambda_{li-2}^{f-1}+\lambda_{li}^{f-1}\right)\left(U_{li-2}^{f-1}-U_{li}^{f-1}\right)+$$

$$+\left(\lambda_{li}^{f-1}+\lambda_{li+2}^{f-1}\right)\left(U_{li+2}^{f-1}-U_{li}^{f-1}\right)\Big]+$$

$$\frac{\Delta t}{16h^2\tau_l}\left(\lambda_{l,li-2}^{f-1}+\lambda_{l,li}^{f-1}\right)\left(U_{li-2}^{f-1}+U_{li}^{f-1}\right)\left(T_{li-2}^{f-1}-T_{li}^{f-1}\right)+$$

$$+\frac{\Delta t}{16h^2\tau_l}\left(\lambda_{l,li+2}^{f-1}+\lambda_{l,li}^{f-1}\right)\left(U_{li}^{f-1}+U_{li+2}^{f-1}\right)\left(T_{li+2}^{f-1}-T_{li}^{f-1}\right)+$$

$$+G(U_{ei}^{f-1}-U_{li}^{f-1})+(T_{ei}^{f-1}-T_{li}^{f-1})-C_{l,li}U_{li}^{f-1}\frac{T_{li}^{f}-T_{li}^{f-1}}{\Delta t} \tag{41}$$

From equation (40) one has

$$U_{ei}^{f}=\left(1-A_{ei}^{f-1}-B_{ei}^{f-1}+D_{ei}^{f-1}+E_{ei}^{f-1}-\frac{G\,\Delta t}{C_{ei}^{f-1}}-\frac{C_{e,ei}^{f-1}}{C_{ei}^{f-1}}\left(T_{ei}^{f}-T_{ei}^{f-1}\right)\right)U_{ei}^{f-1}+$$

$$+\left(A_{ei}^{f-1}+D_{ei}^{f-1}\right)U_{ei-2}^{f-1}+\left(B_{ei}^{f-1}+E_{ei}^{f-1}\right)U_{ei+2}^{f-1}+P_{ei}^{f-1}\left(U_{li-2}^{f-1}-U_{li}^{f-1}\right)+$$

$$+R_{ei}^{f+1}\left(U_{li*2}^{f-1}-U_{li}^{f-1}\right)+\frac{G\,\Delta t}{C_{ei}^{f-1}}U_{li}^{f-1}-\frac{\Delta t}{C_{ei}^{f-1}}\left(T_{ei}^{f-1}-T_{li}^{f-1}\right)+$$

$$+\frac{(\tau_e-\Delta t)\Delta t}{2h\tau_e C_{ei}^{f-1}}\left(w_{ei-1}^{f-1}-w_{ei+1}^{f-1}\right) \tag{42}$$

where

$$A_{ei}^{f-1}=\frac{(\Delta t)^2\left(\lambda_{ei-2}^{f-1}+\lambda_{ei}^{f-1}\right)}{8h^2\tau_e C_{ei}^{f-1}}$$

$$B_{ei}^{f-1}=\frac{(\Delta t)^2\left(\lambda_{ei}^{f-1}+\lambda_{ei+2}^{f-1}\right)}{8h^2\tau_e C_{ei}^{f-1}}$$

$$D_{ei}^{f-1}=\frac{(\Delta t)^2\left(\lambda_{e,ei-2}^{f-1}+\lambda_{e,ei}^{f-1}\right)}{16h^2\tau_e C_{ei}^{f-1}}\left(T_{ei-2}^{f-1}-T_{ei}^{f-1}\right)$$

$$E_{ei}^{f-1}=\frac{(\Delta t)^2\left(\lambda_{e,ei+2}^{f-1}+\lambda_{e,ei}^{f-1}\right)}{16h^2\tau_e C_{ei}^{f-1}}\left(T_{ei+2}^{f-1}-T_{ei}^{f-1}\right) \tag{43}$$

and

$$R_{ei}^{f-1}=\frac{(\Delta t)^2\left(\lambda_{e,li+2}^{f-1}+\lambda_{e,li}^{f-1}\right)}{16h^2\tau_e C_{ei}^{f-1}}\left(T_{ei+2}^{f-1}-T_{ei}^{f-1}\right) \tag{44}$$

Stability criterion is as follows

$$\left(1-A_{ei}^{f-1}-B_{ei}^{f-1}+D_{ei}^{f-1}+E_{ei}^{f-1}-\frac{G\,\Delta t}{C_{ei}^{f-1}}-\frac{C_{e,ei}^{f-1}}{C_{ei}^{f-1}}\left(T_{ei}^{f}-T_{ei}^{f-1}\right)\right)\geq 0 \tag{45}$$

From equation (41) one has

$$U_{li}^{f}=\left(1-A_{li}^{f-1}-B_{li}^{f-1}+D_{li}^{f-1}+E_{li}^{f-1}-\frac{G\,\Delta t}{C_{li}^{f-1}}-\frac{C_{l,li}^{f-1}}{C_{li}^{f-1}}\left(T_{li}^{f}-T_{li}^{f-1}\right)\right)U_{li}^{f-1}+$$

$$+\left(A_{li}^{f-1}+D_{li}^{f-1}\right)U_{li-2}^{f-1}+\left(B_{li}^{f-1}+E_{li}^{f-1}\right)U_{li+2}^{f-1}+$$

$$+\frac{G\,\Delta t}{C_{li}^{f-1}}U_{ei}^{f-1}-\frac{\Delta t}{C_{li}^{f-1}}\left(T_{ei}^{f-1}-T_{li}^{f-1}\right)+\frac{(\tau_l-\Delta t)\Delta t}{2h\tau_l C_{li}^{f-1}}\left(w_{li-1}^{f-1}-w_{li+1}^{f-1}\right) \tag{46}$$

where

$$A_{li}^{f-1}=\frac{(\Delta t)^2\left(\lambda_{li-2}^{f-1}+\lambda_{li}^{f-1}\right)}{8h^2\tau_l C_{li}^{f-1}}$$

$$B_{li}^{f-1}=\frac{(\Delta t)^2\left(\lambda_{li}^{f-1}+\lambda_{li+2}^{f-1}\right)}{8h^2\tau_l C_{li}^{f-1}}$$

$$D_{li}^{f-1}=\frac{(\Delta t)^2\left(\lambda_{l,li-2}^{f-1}+\lambda_{l,li}^{f-1}\right)}{16h^2\tau_l C_{li}^{f-1}}\left(T_{li-2}^{f-1}-T_{li}^{f-1}\right)$$

$$E_{li}^{f-1}=\frac{(\Delta t)^2\left(\lambda_{l,li+2}^{f-1}+\lambda_{l,li}^{f-1}\right)}{16h^2\tau_l C_{li}^{f-1}}\left(T_{li+2}^{f-1}-T_{li}^{f-1}\right) \tag{47}$$

And stability criterion is as follows

$$\left(1-A_{li}^{f-1}-B_{li}^{f-1}+D_{li}^{f-1}+E_{li}^{f-1}-\frac{G\,\Delta t}{C_{li}^{f-1}}-\frac{C_{l,li}^{f-1}}{C_{li}^{f-1}}\left(T_{li}^{f}-T_{li}^{f-1}\right)\right)\geq 0 \tag{48}$$

Summing up, for transition $t^{f-1}\rightarrow t^{f}$,at first the equations (8), (9), (6), (7) should be solved [7] and next using the equations (33), (34), (42), (46) the sensitivity functions U$_e$ and U_l are determined.

5. Results of computations

At first, the gold films of thicknesses L = 100 nm (1nm =10^{-9} m) and L = 20 nm, respectively, are considered. The layer is subjected to a short-pulse laser irradiation (R = 0.93, I_0 = 13.4 J/m^2, t_p = 0.1 ps, δ =15.3 nm). 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 = 70 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]. Initial temperature equals T_p = 300 K.

The problem is solved using finite difference method under the assumption that Δt =0.001 ps and h =1 nm.

In Figures 2 and 3 the comparison of numerical results for thin gold film (x = 0) with experimental data presented in [2] is shown. The line and the symbols represent calculated temperature of electrons and experimental data, respectively. One can see that the agreement of the results obtained and measured temperatures is very good.

In Figures 4, 5, 6 and 7 the calculated sensitivity functions $U_e=\partial T_e/\partial G$ and $U_l=\partial T_l/\partial G$ at the front surface x =0 are presented.

Similar calculations have been done for others materials, this means Cu, W and Ti – c.f. Table 1. In Figures 8-19 the results of computations are shown.

Knowledge of sensitivity functions U_e, U_l allows one, among others, to estimate the temperature changes due to the parameter G perturbations, this means

$$\Delta T_e=T_e(x,t,G+\Delta G)-T_e(x,t,G-\Delta G)=2U_e\Delta G \tag{49}$$

$$\Delta T_l=T_l(x,t,G+\Delta G)-T_l(x,t,G-\Delta G)=2U_l\Delta G \tag{50}$$

where ΔG is the change of parameter..

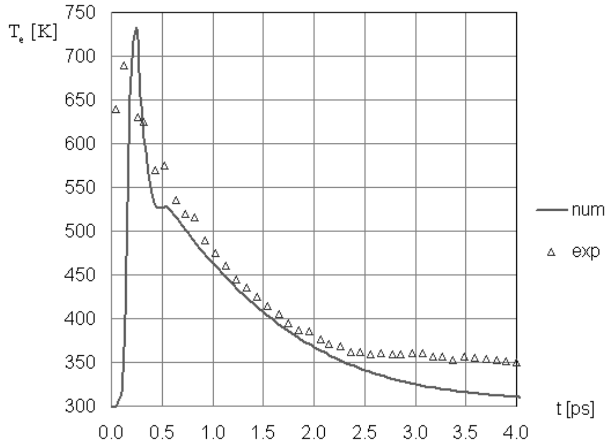

Figure 2: Comparison of calculated electron temperature with experimental data for 100 nm gold film [2]

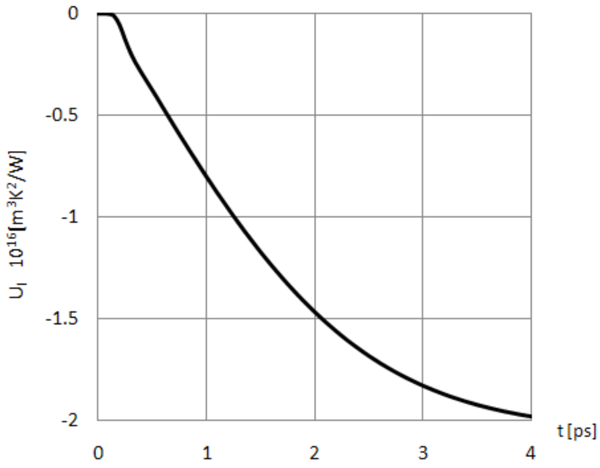

Figure 5: Sensitivity function $U_l(0, t)$ – gold film (100 nm)

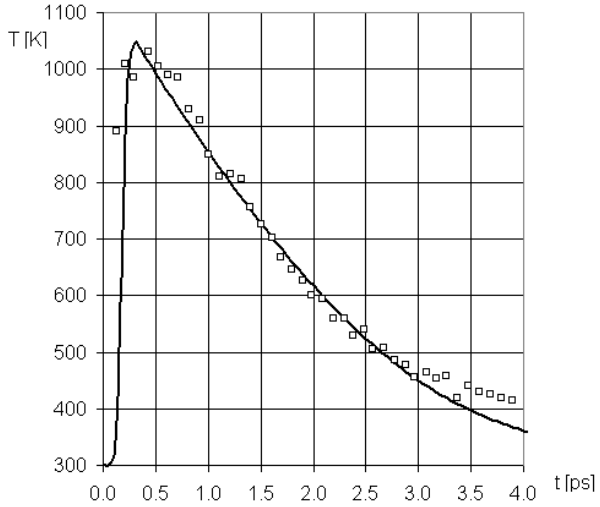

Figure 3: Comparison of calculated electron temperature with experimental data for 20nm gold film [2]

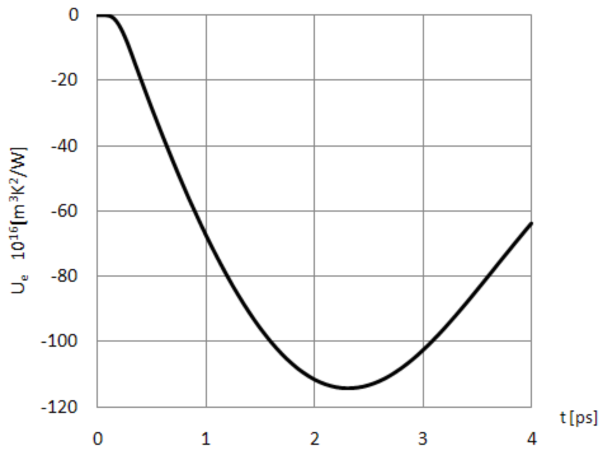

Figure 6: Sensitivity function $U_e(0, t)$ – gold film (20 nm)

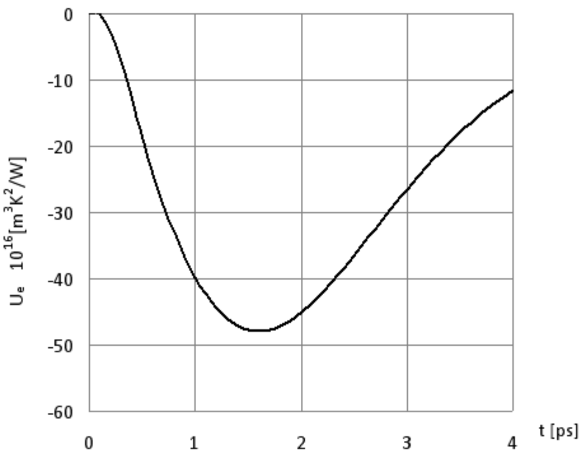

Figure 4: Sensitivity function $U_e(0, t)$ – gold film (100 nm)

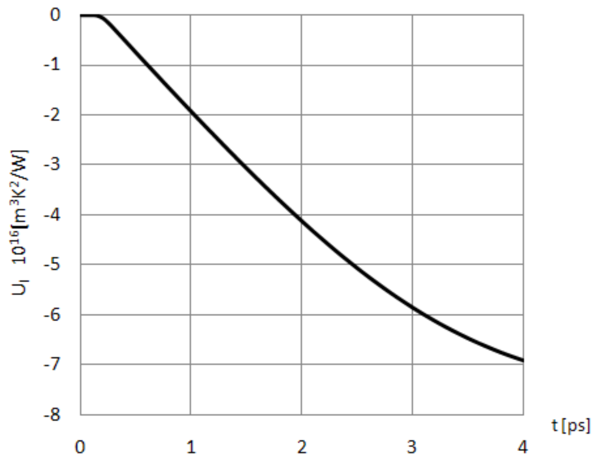

Figure 7: Sensitivity function $U_l(0, t)$ – gold film (20 nm)

Table 1: Thermophysical parameters for selected metals [4]

	Cu	Au	W	Ti
λ_0 [W/(mK)]	409	315	173	21.9
A_e [J/(m^{3}K^2)]	71.0	62.9	137.3	328.9
C_l [J/(m^{3}K)]	$3.39\cdot 10^6$	$2.5\cdot 10^6$	$3\cdot 10^6$	$2.34\cdot 10^6$
G [W/(m^{3}K)]	10^{17}	$2.6\cdot 10^{16}$	$5\cdot 10^{17}$	$1.3\cdot 10^{18}$
τ_e [ps]	0.03	0.04	0.01	0.01
τ_l [ps]	0.6	0.8	0.2	0.5
T_m [K]	1358	1337	3695	1941

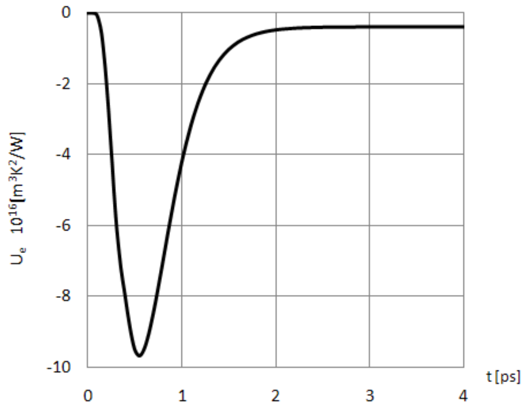

Figure 8: Sensitivity function $U_e(0, t)$ - Cu film (100 nm)

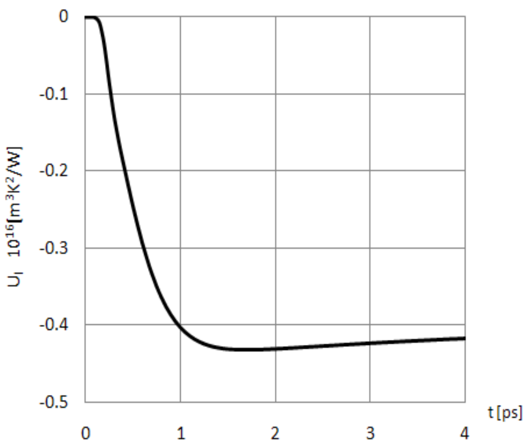

Figure 9: Sensitivity function $U_l(0, t)$ - Cu film (100 nm)

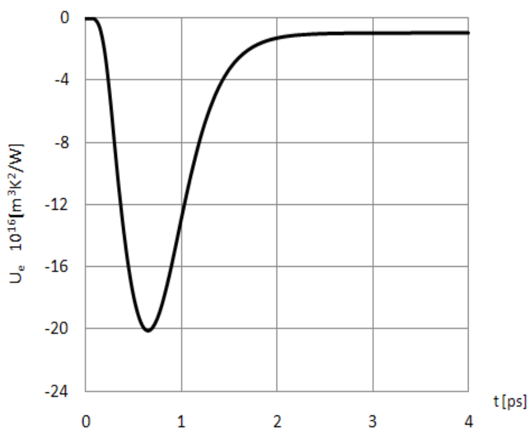

Figure 10: Sensitivity function $U_e(0, t)$ – Cu film (20nm)

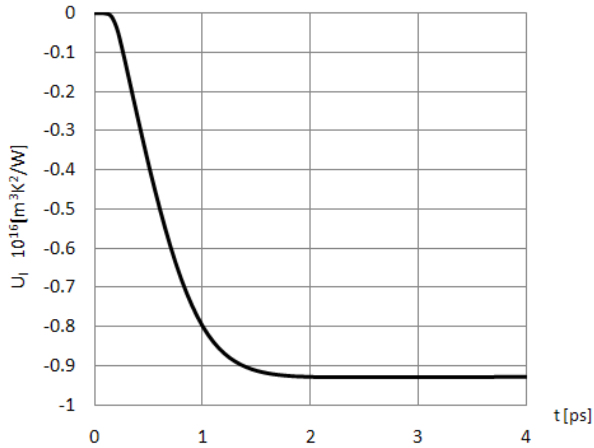

Figure 11: Sensitivity function $U_l(0, t)$ - Cu film (20nm)

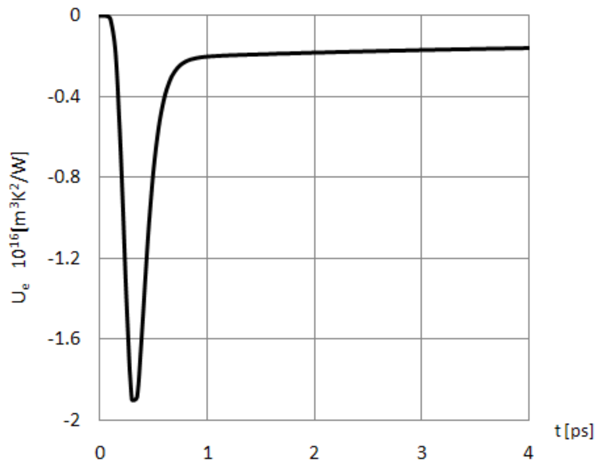

Figure 12: Sensitivity function $U_e(0, t)$ - W film (100 nm)

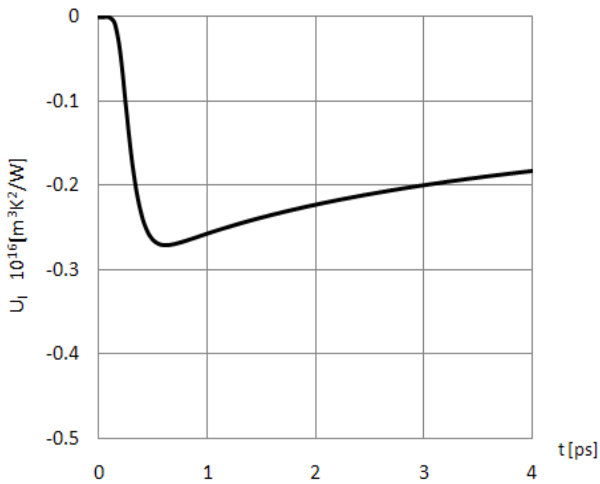

Figure 13: Sensitivity function $U_l(0, t)$ - W film (100 nm)

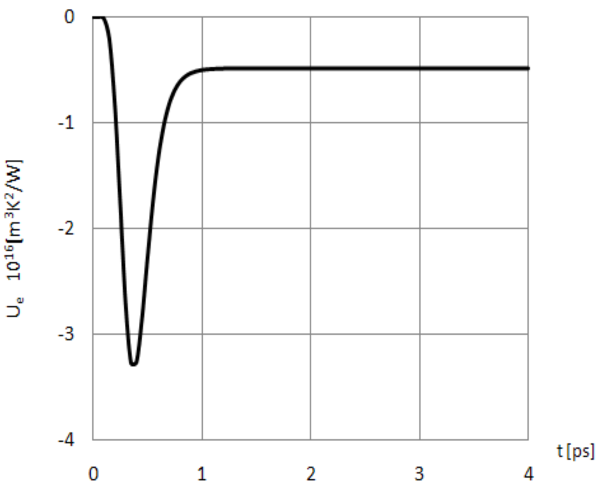

Figure 14: Sensitivity function $U_e(0, t)$ - W film (20nm)

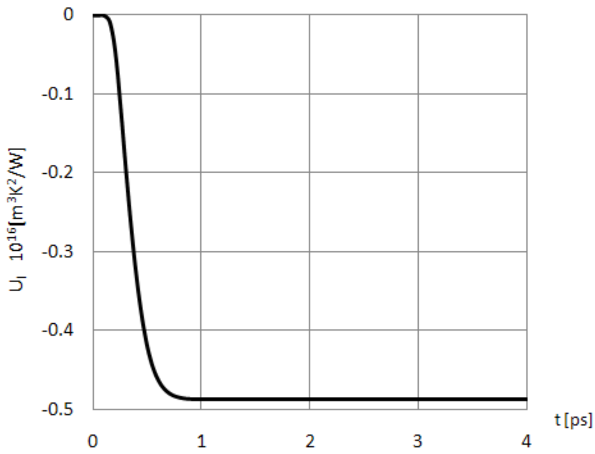

Figure 15: Sensitivity function $U_l(0, t)$ - W film (20nm)

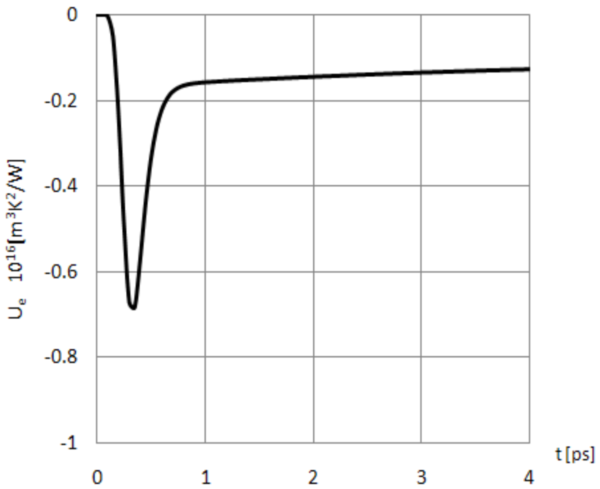

Figure 16: Sensitivity function $U_e(0, t)$ for Ti (100 nm)

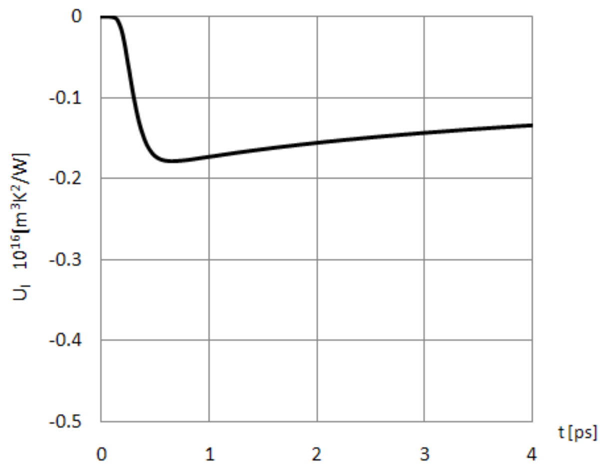

Figure 17: Sensitivity function $U_l(0, t)$ - Ti film (100 nm)

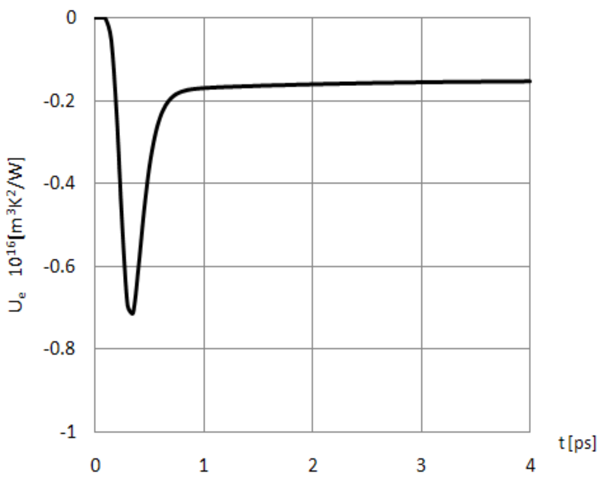

Figure 18: Sensitivity function $U_e(0, t)$ - Ti (20nm)

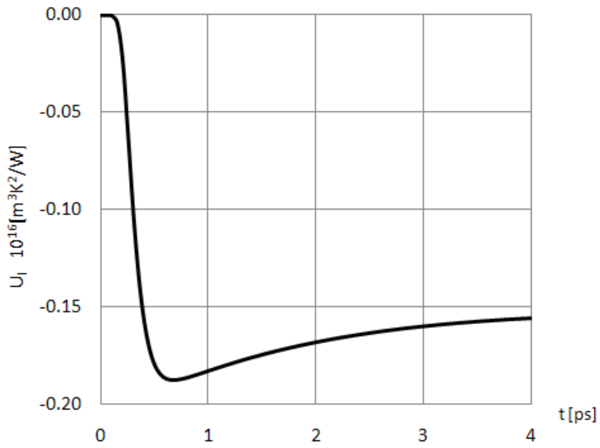

Figure 19: Sensitivity function $U_l(0, t)$ - Ti (20nm)

In Figures 20-23 the changes of temperatures T_e, T_l due to the change of parameter G ($\Delta G = 0.1G$) for different materials and different layers thicknesses are shown.

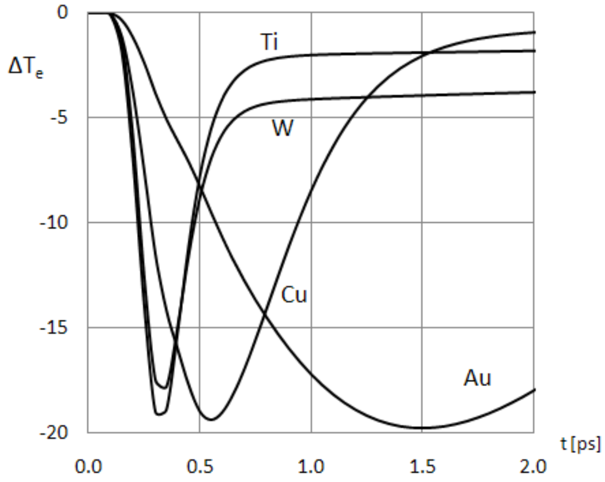

Figure 20: Time history of ΔT_e for Au, Cu, W and Ti (100 nm)

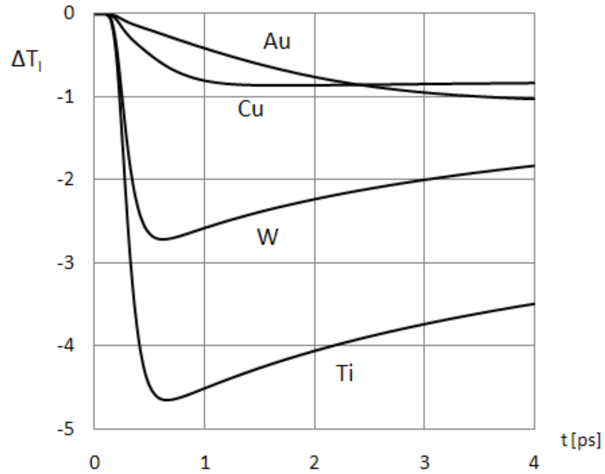

Figure 21: Time history of ΔT_l for Au, Cu, W and Ti (100 nm)

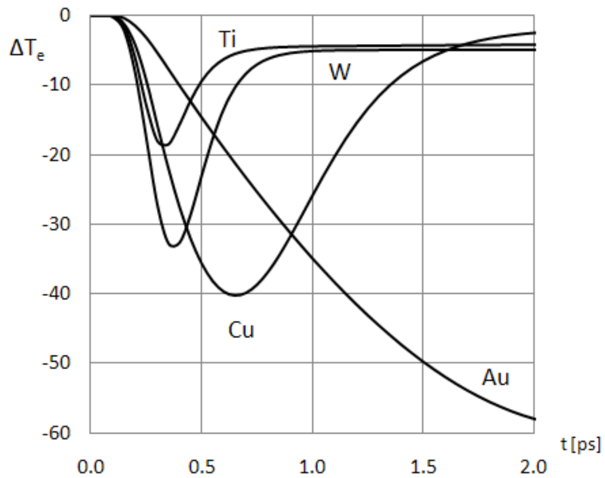

Figure 22: Time history of ΔT_e for Au, Cu, W and Ti (20 nm)

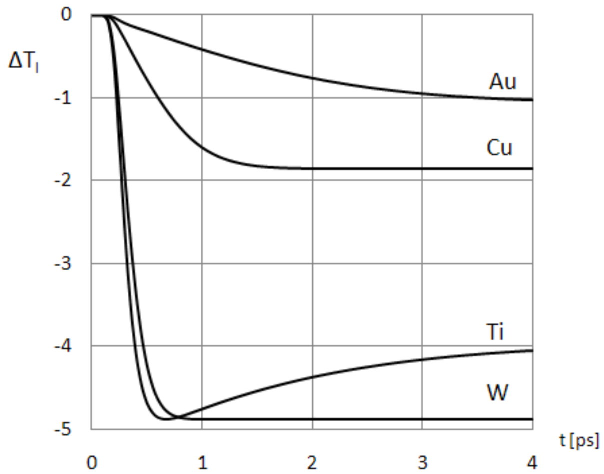

Figure 23: Time history of ΔT_l for Au, Cu, W and Ti (20 nm)

6. Conclusions

Different materials and different geometrical properties of metal films subjected to a laser pulse have been considered. Thermal processes proceeding in the domains have been described using the two-temperature model. Equations determining the transient temperature field in the electron gas and lattice are coupled by the parameter called a coupling factor.

Sensitivity analysis of electrons and phonons temperatures with respect to this parameter in a case of thin metal film has been presented. It turned out, that the perturbations of coupling factor have an essential influence on the electron temperatures especially when the thickness of film is small.

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