Journal of Applied Mathematics and Computational Mechanics 2015, 14(2), 31-39
www.amcm.pcz.pl p-ISSN 2299-9965
DOI: 10.17512/jamcm.2015.2.04 e-ISSN 2353-0588

ANALYSIS OF ULTRASHORT LASER PULSE INTERACTIONS WITH METAL FILMS USING A TWO-TEMPERATURE MODEL

Ewa Majchrzak, Jolanta Dziatkiewicz

Institute of Computational Mechanics and Engineering
Silesian University of Technology, Gliwice, Poland
ewa.majchrzak@polsl.pl, jolanta.dziatkiewicz@polsl.pl

Abstract. In the paper the problem of thin metal film subjected to the action of the high laser fluence and the ultrashort pulse width is considered. The mathematical model consists of the equations describing the electrons and phonons temperatures and the relationships between the heat fluxes and temperature gradients of electrons and phonons. The problem is solved using the explicit scheme of the finite difference method with staggered grid. In the final part the results of computations and conclusions are presented.

Keywords: *microscale heat transfer, two-temperature model, finite difference method*

1. Introduction

To describe the heat transfer process in thin metal film subjected to the ultrashort laser pulse action the two-temperature model is used. A key issue in the application of this model is the proper description of temperature dependent thermophysical properties of the material. Special attention should be given to the method for determining the thermal conductivity and volumetric heat capacity of electrons, as well as the coupling factor. This paper presents the dependencies describing the above-mentioned parameters which should be used in the case of high laser fluence and the ultrashort pulse. The problem discussed is solved using the explicit finite difference method. In the final part of the paper the results of the computations are shown.

2. Governing equations

Two-temperature model describing the temporal and spatial evolution of the lattice and electrons temperatures (T_l and T_e) in the irradiated metal is of the form [1, 2] (1D problem)

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

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 $T_e\,(x,\,t)$, $T_l\,(x,\,t)$ 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, $Q(x,\,t)$ is the source function associated with the irradiation.

Instead of classical Fourier law the following formulas are introduced:

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

and

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

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.

The laser irradiation is described by a source term introduced in equation (1)

$$Q(x,\,t)=\sqrt{\frac{\beta}{\pi}}\frac{1-R}{t_p\,\delta}\,I_0\,\exp\left[-\frac{x}{\delta}-\beta\frac{(t-t_p)^2}{t_p^2}\right] \tag{5}$$

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 $\beta = 4\ln 2$ [1].

The heat losses from front and back surface could be neglected, therefore the boundary conditions are as follows:

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

The initial condition was proposed as

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

3. Thermophysical parameters

A very important problem is the appropriate estimation of temperature-dependent thermophysical parameters appearing in the above presented model. Usually, the values of the volumetric specific heat $C_l(T_l)$ and thermal conductivity $\lambda_l(T_l)$

of the lattice are assumed as the constants. For low laser intensity the following relationships describing the electrons thermal capacity and volumetric specific heat are widely used [1-4]:

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

and

$$C_e(T_e) = A\,T_e \tag{9}$$

where λ_0 and A are the material constants, and [3, 5]

$$A = \frac{\pi^2 N\,k_B}{2T_F} \tag{10}$$

while N is the density of electrons, k_B is the Boltzmann constant and T_F is the Fermi temperature.

In this case also the remaining parameters, meaning coupling factor G and relaxation times τ_e, τ_l, usually are assumed to be the constant ones.

For high laser intensity, these formulas should not be used [3, 6-8]. For volumetric specific heat of electrons it is assumed that the dependence (9) is valid for the temperatures T_e below the Fermi temperature T_F divided by π^2, while for the temperatures T_e above the Fermi temperature the electrons volumetric specific heat is constant and equal to $3Nk_B/2$ [9]. For temperatures T_e in the range $[T_F/\pi^2,\ T_F]$ the linear temperature dependence can be accepted and then

$$C_e(T_e) = \begin{cases} AT_e, & T_e < T_F/\pi^2 \\ AT_F/\pi^2 + \dfrac{3Nk_B/2 - AT_F/\pi^2}{T_F - T_F/\pi^2}\left(T_e - T_F/\pi^2\right), & T_F/\pi^2 \le T_e < T_F \\ 3Nk_B/2, & T_e > T_F \end{cases} \tag{11}$$

It should be pointed out that in paper [6] the interval $[T_F/\pi^2,\ T_F]$ is divided into two sub-intervals $[T_F/\pi^2,\ 3T_F/\pi^2]$, $[3T_F/\pi^2,\ T_F]$ and for $T_e = 3T_F/\pi^2$ it is assumed that $C_e(T_e) = Nk_B$. Next, the linear temperature dependences in the sub-intervals are proposed, namely

$$C_e(T_e) = \begin{cases} AT_e, & T_e < T_F/\pi^2 \\ AT_F/\pi^2 + \dfrac{N\,k_B - AT_F/\pi^2}{2T_F/\pi^2}\left(T_e - T_F/\pi^2\right), & T_F/\pi^2 \le T_e < 3T_F/\pi^2 \\ N\,k_B + \dfrac{N\,k_B/2}{T_F - 3T_F/\pi^2}\left(T_e - 3T_F/\pi^2\right), & 3T_F/\pi^2 \le T_e < T_F \\ 3N\,k_B/2, & T_e > T_F \end{cases} \tag{12}$$

In Figure 1 the courses of functions (11) and (12) for gold are shown.

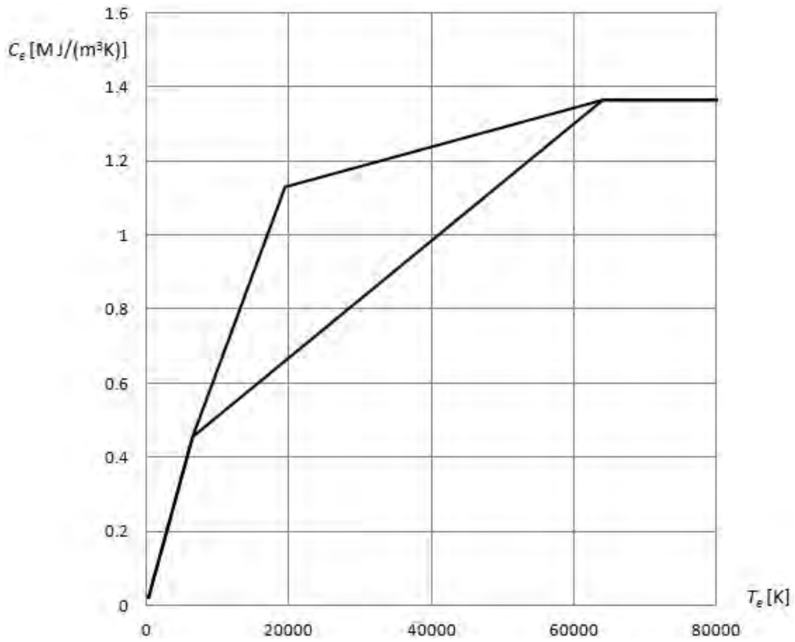

Fig. 1. Function $C_e(T_e)$

In the case of electrons thermal conductivity the following dependence is used [10]

$$\lambda_e(T_e,T_l)=\chi\frac{\left[(T_e/T_F)^2+0.16\right]^{5/4}\left[(T_e/T_F)^2+0.44\right](T_e/T_F)}{\left[(T_e/T_F)^2+0.092\right]^{1/2}\left[(T_e/T_F)^2+\eta(T_l/T_F)\right]} \tag{13}$$

while for the coupling factor

$$G(T_e,T_l)=G_{rt}\left[\frac{A_e}{B_l}(T_e+T_l)+1\right] \tag{14}$$

where χ, η, A_e, B_l are the constants and G_{rt} is the coupling factor at room temperature [10].

In Figure 2 the course of electrons thermal conductivity for $300 \le T_e \le 24\,000$ K (gold) under the assumption that $T_l = 300$ K is shown.

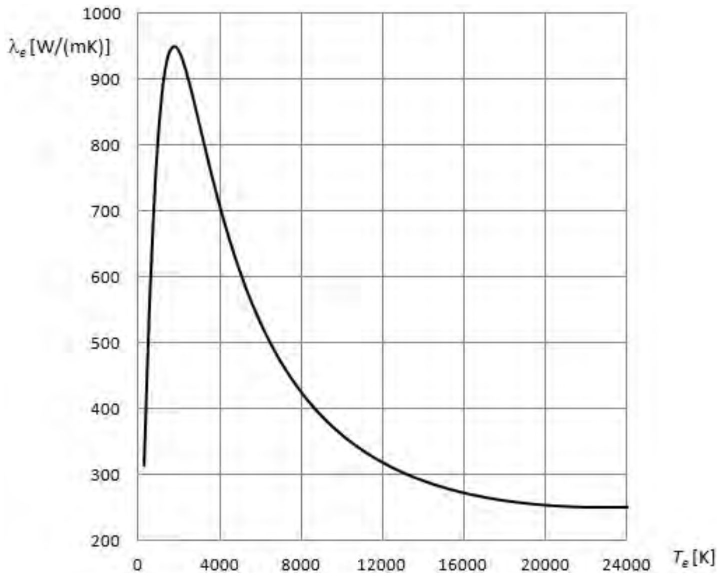

Fig. 2. Electrons thermal conductivity (T_l = 300 K)

4. Method of solution

To solve the problem formulated the algorithm based on the finite difference method is used [2]. A staggered grid is introduced in which the temperature nodes $i = 0,2,4,..., N$ and the heat fluxes nodes $j = 1,3,....,N - 1$ are distinguished. Let us denote $T_i^f = T(ih, f\Delta t)$ and $q_j^{\,f} = q(jh, f\Delta t)$, where h is the mesh size, Δt is the time step, $f = 0,1,2,...,F$.

The finite difference approximation of equations (1)-(4) using the explicit scheme is as follows

$$C_{ei}^{f-1}\frac{T_{ei}^{f}-T_{ei}^{f-1}}{\Delta t}=-\frac{q_{ei+1}^{f}-q_{ei-1}^{f}}{2h}-G_i^{f-1}\left(T_{ei}^{f-1}-T_{li}^{f-1}\right)+Q_i^{f-1} \tag{15}$$

$$C_{li}^{f-1}\frac{T_{li}^{f}-T_{li}^{f-1}}{\Delta t}=-\frac{q_{li+1}^{f}-q_{li-1}^{f}}{2h}+G_i^{f-1}\left(T_{ei}^{f-1}-T_{li}^{f-1}\right) \tag{16}$$

and

$$q_{ej}^{f-1}+\tau_e\frac{q_{ej}^{f}-q_{ej}^{f-1}}{\Delta t}=-\lambda_{ej}^{f-1}\frac{T_{ej+1}^{f-1}-T_{ej-1}^{f-1}}{2h} \tag{17}$$

$$q_{lj}^{f-1}+\tau_l\frac{q_{lj}^{f}-q_{lj}^{f-1}}{\Delta t}=-\lambda_{lj}^{f-1}\frac{T_{lj+1}^{f-1}-T_{lj-1}^{f-1}}{2h} \tag{18}$$

After the mathematical manipulations one obtains [2]

$$T_{ei}^{f}=\left(1-\frac{(\Delta t)^2\lambda_{ei-1}^{f-1}}{4h^2\tau_e C_{ei}^{f-1}}-\frac{(\Delta t)^2\lambda_{ei+1}^{f-1}}{4h^2\tau_e C_{ei}^{f-1}}-\frac{G_i^{f-1}\Delta t}{C_{ei}^{f-1}}\right)T_{ei}^{f-1}+\frac{(\Delta t)^2\lambda_{ei-1}^{f-1}}{4h^2\tau_e C_{ei}^{f-1}}T_{ei-2}^{f-1}+$$
$$\frac{(\Delta t)^2\lambda_{ei+1}^{f-1}}{4h^2\tau_e C_{ei}^{f-1}}T_{ei+2}^{f-1}+\frac{G_i^{f-1}\Delta t}{C_{ei}^{f-1}}T_{li}^{f-1}+\frac{\Delta t(\tau_e-\Delta t)}{2h\tau_e C_{ei}^{f-1}}\left(q_{ei-1}^{f-1}-q_{ei+1}^{f-1}\right)+\frac{Q_i^{f-1}\Delta t}{C_{ei}^{f-1}} \tag{19}$$

$$T_{li}^{f}=\left(1-\frac{(\Delta t)^2\lambda_{li-1}^{f-1}}{4h^2\tau_l C_l}-\frac{(\Delta t)^2\lambda_{li+1}^{f-1}}{4h^2\tau_l C_l}-\frac{G_i^{f-1}\Delta t}{C_l}\right)T_{li}^{f-1}+\frac{(\Delta t)^2\lambda_{li-1}^{f-1}}{4h^2\tau_l C_l}T_{li-2}^{f-1}+$$
$$\frac{(\Delta t)^2\lambda_{li+1}^{f-1}}{4h^2\tau_l C_l}T_{li+2}^{f-1}+\frac{G_i^{f-1}\Delta t}{C_l}T_{ei}^{f-1}+\frac{\Delta t(\tau_l-\Delta t)}{2h\tau_l C_l}\left(q_{li-1}^{f-1}-q_{li+1}^{f-1}\right) \tag{20}$$

and

$$q_{ej}^{f}=\frac{\tau_e-\Delta t}{\tau_e}q_{ej}^{f-1}-\frac{\lambda_{ej}^{f-1}\Delta t}{2h\tau_e}\left(T_{ej+1}^{f-1}-T_{ej-1}^{f-1}\right) \tag{21}$$

$$q_{lj}^{f}=\frac{\tau_l-\Delta t}{\tau_l}q_{lj}^{f-1}-\frac{\lambda_{lj}^{f-1}\Delta t}{2h\tau_l}\left(T_{lj+1}^{f-1}-T_{lj-1}^{f-1}\right) \tag{22}$$

where

$$\lambda_{ei-1}^{f-1}=\frac{\lambda_{ei}^{f-1}+\lambda_{ei-2}^{f-1}}{2},\quad \lambda_{ei+1}^{f-1}=\frac{\lambda_{ei}^{f-1}+\lambda_{ei+2}^{f-1}}{2} \tag{23}$$

$$\lambda_{li-1}^{f-1}=\frac{\lambda_{li}^{f-1}+\lambda_{li-2}^{f-1}}{2},\quad \lambda_{li+1}^{f-1}=\frac{\lambda_{li}^{f-1}+\lambda_{li+2}^{f-1}}{2} \tag{24}$$

$$\lambda_{ej}^{f-1}=\frac{\lambda_{ej-1}^{f-1}+\lambda_{ej+1}^{f-1}}{2},\quad \lambda_{lj}^{f-1}=\frac{\lambda_{lj-1}^{f-1}+\lambda_{lj+1}^{f-1}}{2} \tag{25}$$

It should be pointed out that adequate stability criteria for the explicit scheme must be fulfilled [2].

5. Results of computations

The gold film of thickness $L = 100$ nm (1 nm = 10^{-9} m) is considered. The initial temperature is equal to $T_p = 300$ K. The constants in equations (13), (14) are the following: $\chi = 353$ W/(mK), $\eta = 0.16$, $A_e = 1.2\cdot10^7$ 1/(K^{2}s), $B_l = 1.23\cdot10^{11}$ 1/(Ks) and $G_{rt} = 2.2\cdot10^{16}$ W/(m^{3}K) [9]. The Fermi temperature is equal to $T_F = 64\,200$ K and the density of electrons is equal to $N = 5.9\cdot10^{28}$ 1/m (cf. equation (11)) [9]. The other parameters are as follows: thermal conductivity of lattice $\lambda_l = 315$ W/(mK), volumetric specific heat of lattice $C_l = 2.5$ MJ/(m^{3}K), electrons relaxation time $\tau_e = 0.04$ ps, phonons relaxation time $\tau_l = 0.8$ ps [1], reflectivity $R = 0.93$, optical penetration depth $\delta = 15.3$ nm. The problem is solved using the finite difference method under the assumption that $\Delta t = 0.002$ ps and $h = 1$ nm.

In Figure 3 the electrons and lattice temperature at the irradiated surface $x = 0$ for the laser intensity $I_0 = 4182$ W/m^2 and the characteristic time of laser pulse $t_p = 100$ ps is shown.

It should be pointed out that the results are compared with those obtained using the dependences (8), (9) and the constant value of coupling factor $G = G_{rt}$. The differences between the temperatures for this variant of parameters and those previously assumed are shown in Figures 4 and 5.

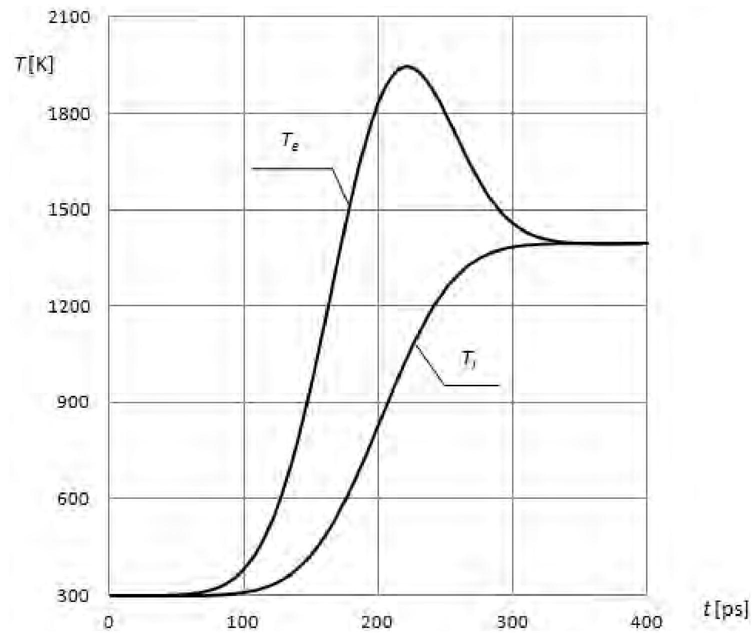

Fig. 3. Electrons and lattice temperature at the irradiated surface

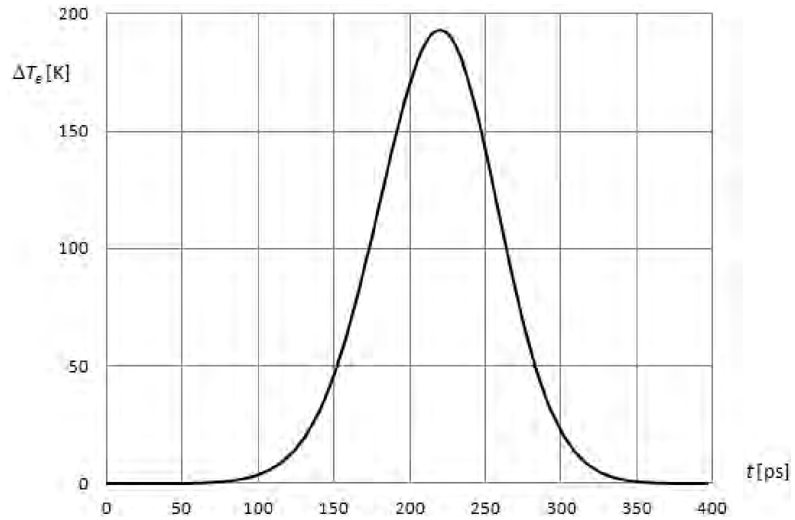

Fig. 4. Electrons temperature differences

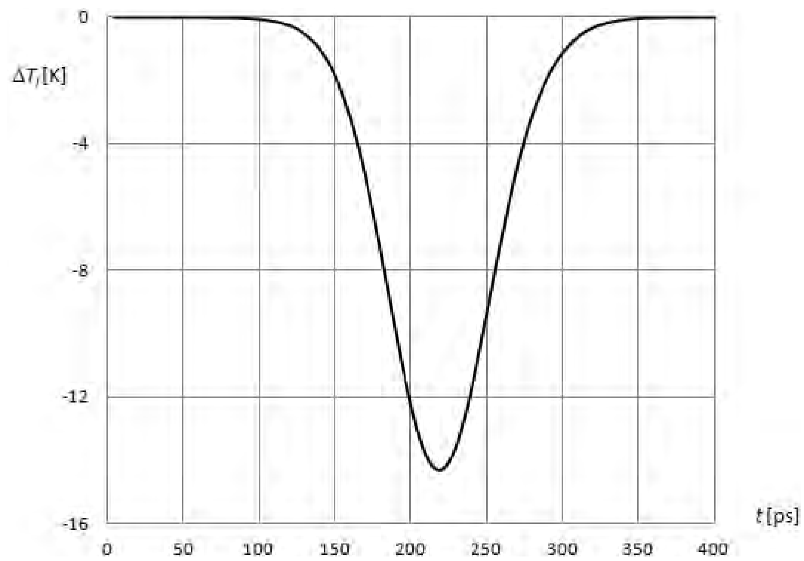

Fig. 5. Lattice temperature differences

6. Conclusions

The problem of the heat exchange proceeding in the domain of thin metal film subjected to the ultrashort laser pulse described by the two-temperature model is considered. Two sets of parameters occurring in the model have been taken into account and the differences in the electrons and lattice temperatures between them are presented. Temperature-dependent parameters and the way they are estimated have more influence on the electrons temperature distribution than on the lattice temperature distribution, but in the case considered the differences are not big.

Acknowledgement

This work is supported by the project No. 2012/05/B/ST8/01477 and sponsored by the Polish National Science Centre.

References

[1] Chen J.K., Beraun J.E., Numerical study of ultrashort laser pulse interactions with metal films, Numerical Heat Transfer, Part A 2001, 40, 1-20.

[2] Dziatkiewicz J., Kuś W., Majchrzak E., Burczyński T., Turchan Ł., Bioinspired identification of parameters in microscale heat transfer, International Journal for Multiscale Computational Engineering 2014, 12(1), 79-89.

[3] Dziatkiewicz J., Analiza przepływu ciepła w mikroobszarach z wykorzystaniem modeli dwu-temperaturowych, Politechnika Śląska, Gliwice 2012.

[4] Majchrzak E., Dziatkiewicz J., Identification of electron-phonon coupling factor in a thin metal film subjected to an ultrashort laser pulse, Computer Assisted Methods in Engineering and Science 2012, 19, 383-392.

[5] Smith A.N., Norris P.M., Microscale heat transfer, Chapter 18 [in:] Heat Transfer Handbook, John Wiley & Sons, 2003.

[6] Lin Z., Zhigilei L.V., Electron-phonon coupling and electron heat capacity of metals under conditions of strong electron-phonon nonequilibrium, Physical Review B 2008, 77, 075133-1-075133-17.

[7] Majchrzak E., Poteralska J., Two-temperature microscale heat transfer model, Part I: Determination of electron parameters, Scientific Research of the Institute of Mathematics and Computer Science 2010, 1(9), 99-108.

[8] Majchrzak E., Poteralska J., Two-temperature microscale heat transfer model. Part II: Determination of lattice parameters, Scientific Research of the Institute of Mathematics and Computer Science 2010, 1(9), 109-120.

[9] Chen J.K., Tzou D.Y., Beraun J.E., A semiclassical two-temperature model for ultrafast laser heating, International Journal of Heat and Mass Transfer 2006, 49, 307-316.

[10] Huang J., Baheti K., Chen J.K., Zhang Y., An axisymmetric model for solid-liquid-vapor phase change in thin metal films induced by an ultrashort laser pulse, Frontiers in Heat and Mass Transfer 2011, 2, 013005.