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MODELING OF IRRADIATION BY SHORT LASER PULSE – COMPARISON OF BOLTZMANN TRANSPORT EQUATION AND A TWO-TEMPERATURE MODEL WITH EXPERIMENTAL DATA

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Abstract: *The presented paper investigates two methods of heat transfer problem in nanoscale. Simulations are takeover thin metal film irradiated by the ultrashort laser pulse. The first simulation is based on the Boltzmann transport equation and solved using the lattice Boltzmann method. The second applied method was the finite difference method with a two-temperature model. Results of both simulations were compared with experimental data what is presented in Calculations.*

Keywords: Boltzmann transport equation, Two-temperature model, Heat transfer, Lattice Boltzmann method, Finite difference method.

1. Introduction

In the presented research, comparison of two methods of heat transfer modeling was carried out. Next the error between numerical and experimental results was investigated. In the modeled example a laser beam influences thin metal film, what was modeled numerically and considered as the one-dimensional case. The base of result evaluation is the outcome of the experiment described in (Chen, 2001) where experimental data are shown for electron temperatures in chosen node in a function of time.

We can use various models and numerical methods to deal with heat flow in solids, sometimes even in use of artificial intelligence (Mucha, 2020). But when analyzing objects of nano scale dimensions and with fast heating processes, comparable to relaxation times, then there are only a few methods. The most popular are molecular dynamics, the Boltzmann transport equation and a two-temperature model. The presented further two methods have the advantage over molecular dynamics that they have a less complicated mathematical apparatus and calculations proceed faster. Both models consist of coupled system of equations that consider relaxation times of energy carriers (phonons-lattice vibrations and electrons).

In the mathematical model the internal heat source is applied in a shape of the temporal variation of the laser pulse approximated by a form of exponential function (Lin, 2008)

$$Q(t,x)=\sqrt{\frac{\beta}{\pi}}\frac{1-R}{t_p\delta_s}I_0\cdot e^{\frac{-x}{\delta_s}-\beta\left(\frac{t-2t_p}{t_p}\right)^2} \tag{1}$$

where I_0 is the laser intensity, R the reflectivity, t_p the laser pulse duration defined as full width at half maximum of the laser pulse, δ_s the optical penetration depth, x the depth measured from the front surface, $\beta = 4\ln(2)$.

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2. The Boltzmann transport equation

In this chapter is presented the Boltzmann transport equation (BTE) as the governing equation. To take into account both types of energy carriers it must be analyzed as a coupled problem (Hopkins, 2009).

The coupled system of equations is written using the partial differential equations (where denote: e-electrons and ph-phonons) (Escobar, 2006)

$$\frac{\partial e_e}{\partial t} + \mathbf{c}_e \cdot \frac{\partial e_e}{\partial x} = -\frac{e_e - e_e^0}{\tau_e} + Q_e \tag{2}$$

$$\frac{\partial e_l(x,t)}{\partial t} + \mathbf{v}_l \cdot \nabla e_l(x,t) = -\frac{e_l(x,t) - e_l^0(x,t)}{\tau_l} + Q_l(x,t) \tag{3}$$

The energy densities of electrons and phonons are combined with their equivalent nonequilibrium temperatures using following formulas (Escobar, 2006)

$$e_e(T_e) = \left(n_e \frac{\pi^2}{2} \frac{k_b^2}{\varepsilon_F} \right) T_e^2 \tag{4}$$

$$e_l(T_l) = \left(\frac{9\eta_{ph} k_b}{\Theta_D^3} \int_0^{\Theta_D/T_l} \frac{z^3}{\exp(z)-1} \mathrm{d}z \right) T_l^4 \tag{5}$$

where Θ_D is the Debye temperature of the solid, k_b is the Boltzmann constant, T_e, T_l are the temperature for electrons and phonons respectively, while n_e is the electron density, η_{ph} is the phonon density and ε_F the Fermi energy. By successively transforming relations (4) and (5) one can calculate the temperatures of phonons and electrons depending on their energy density, which provides a basis for comparing results obtained by other methods.

3. A two-temperature model

In this chapter two-temperature model is presented. This model describes the temporal and spatial evolution of the lattice and electrons temperatures (T_l and T_e) in the irradiated metal can be written (Chen, 2001) (1D problem)

$$C_e(T_e) \frac{\partial T_e(x,t)}{\partial t} = -\frac{\partial q_e(x,t)}{\partial t} - G\left[T_e(x,t) - T_l(x,t)\right] + Q(t) \tag{6}$$

$$C_l \frac{\partial T_l(x,t)}{\partial t} = -\frac{\partial q_l(x,t)}{\partial t} + G\left[T_e(x,t) - T_l(x,t)\right] \tag{7}$$

where $T_e(x, t)$, $T_l(x, t)$ are the temperatures of electrons and lattice, respectively, $C_e(T_e)$, C_l are the volumetric specific heats, G is the electron-phonon coupling factor which characterizes the energy exchange between electrons and phonons, $Q(t)$ is the source function associated with the irradiation. In a place of the classical Fourier law we use the Maxwell – Cattaneo relation for heat conduction

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

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

where $\lambda_e(T_e, T_l)$, λ_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 thermophysical parameters are highly nonlinear and are determined according to formulas presented in (Majchrzak, 2012).

An algorithm based on the finite difference method is used to solve the formulated problem (Majchrzak, 2012). 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 introduced. I means that $T_i^f = T(ih, f\Delta t)$ 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.

4. Calculations

As a numerical example, the heat transport in a gold thin film of the thickness L=100 nm has been analysed. The following input data have been introduced: the relaxation times $\tau_e = 0.04\,\text{ps}$, $\tau_{ph} = 0.8\,\text{ps}$, the Debye temperature $\Theta_D = 170\,\text{K}$, the Fermi energy $\varepsilon_F = 5.53\,\text{eV}$, the peak power intensity of the laser pulse I_0 = 13.4 J/m^2, the reflectivity R = 0.95, the optical penetration depth $\delta_s = 15.3 \cdot 10^{-9}$ m, the laser pulse duration $t_p = 0.1 \cdot 10^{-12}$ s, the coupling factor G = 2.3·10^{16} W/m^{3}K, the boundary conditions of the 2nd type on the both edges $q_{b1}^k(0, t) = q_{b2}^k(L, t) = 0$, the initial temperature $T_0 = 300\,\text{K}$. The lattice step $\Delta x = 1\text{nm}$ and the time step $\Delta t = 0.0001\text{ps}$ have been assumed. Heating curves for x = 0 that were obtained using both methods compared to experimental data are depicted in Figure 1.

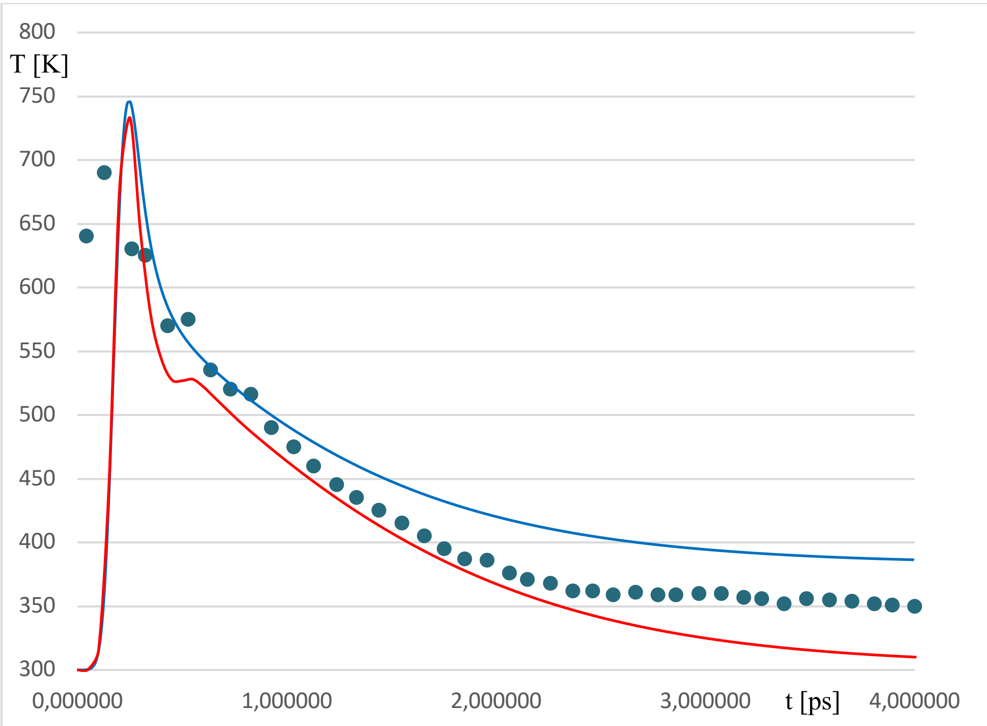

Fig. 1: Heating curves for x = 0.

The red line presents electron temperature obtained for two-temperature model. Blue line expresses the Boltzmann transport equation result and the dotet line represents the experimental data (Chen, 2001). It can be seen that both methods accurately reflect the results of the experiment.

Table 1 shows the relative error between the experimental results and both methods presented in the article. Convergence of results and a similar level of deviation can be noticed.

Tab. 1: Relative error.

Boltzmann transport equation	Two-temperature model
0,53	0,53
0,30	0,18
0,20	0,06
0,14	0,03
0,04	0,03
0,06	0,01
0,01	0,01
0,04	0,02
0,04	0,12
0,05	0,10
0,06	0,08
0,07	0,06
0,07	0,05
0,10	0,02

5. Conclusions

In the presented problem, calculations of heat transfer in the use of two methods and experimental data were compared. Numerical results that were taken into account were supposed to give electron temperature distribution for $x = 0$, so the surface that were irradiated, that fit experimental results.

The accuracy of obtained temperatures using both models can be considered as satisfying, as can be observed in Fig. 1 where comparison with experimental data is presented. During the initial laser exposure, both numerical methods show good agreement, with a slight shift of the maximum temperature in relation to the experimental data. Further, the results obtained by the two-temperature model take values below those obtained by experiment, in contrast to the Boltzmann transport equation, which take higher values, but still keeping the same trend. In the course of the temperature obtained by the two-temperature model, the wave character can be seen, which results from the hyperbolic model.

Additionally, an error analysis was performed, the results of which can be found in Table 1.

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