Solution of heat transfer inverse problem in thin film irradiated by laser

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Abstract: *The presented paper deals with an inverse problem in nanoscale heat transfer simulation. A thin metal film irradiated by the ultrashort laser pulse is modeled using the Boltzmann transport equation. Heat transfer parameters of the model arheat transfer, Boltzmann transport equation, identification, evolutionary algorithme identified using evolutionary algorithm an optimization algorithm inspired on biological evolution of species, where the difference between obtained and expected results is minimized.*

1 INTRODUCTION

In the presented research, identification of short-pulse laser parameters was carried out. In the discussed example thin metal film was influenced by a laser beam. The process was modelled numerically. In the identification, experimental data was used, in order to minimize the error between numerical and experimental results.

Heat flow in solids can be modelled using various models. When dealing with objects of small dimensions, of the order of nanometres, and with fast heating processes, comparable to relaxation times, then it is reasonable to use molecular dynamics or the Boltzmann transport equation (BTE). The presented coupled system of Boltzmann transport equations has the advantage over molecular dynamics that it has a less complicated mathematical apparatus and calculations proceed faster. This is an important advantage considering inverse problems, where computations are performed repeatedly for different possible combinations of identified parameters.

The goal of the identification presented in this paper is to obtain three parameters of the laser irradiation, such as the laser intensity, the optical penetration depth, the reflectivity and the laser pulse duration. The base of result evaluation is the outcome of the experiment described in [3] where experimental data are shown for electron temperatures in chosen node in a function of time. Proposed identification finds parameters of a numerical model that would recreate the real process flow as exactly as possible.

2 THE BOLTZMANN TRANSPORT EQUATION

In the presented problem as the governing equation is used the Boltzmann transport equation (BTE). According to the Debye simplifications the equivalent transformed form of energy density equation is analysed. This paper considers the one-dimensional heat transfer model in metals. As it is a coupled problem, then both types of energy carriers must be taken into account. The coupled system of equations can be written using the differential equation (subscript: e-electrons and ph-phonons) [4]

$$\frac{\partial e_e}{\partial t} + \mathbf{c}_e \frac{\partial e_e}{\partial x} = -\frac{e_e - e_e^0}{\tau_e} + Q_e \tag{1}$$

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$$\frac{\partial e_{ph}}{\partial t} + \mathbf{c}_{ph}\frac{\partial e_{ph}}{\partial x} = -\frac{e_{ph} - e_{ph}^{0}}{\tau_{ph}} + Q_{ph} \tag{2}$$

where $e_e = e_e\left(t, x\right)$, $e_{ph} = e_{ph}\left(t, x\right)$ are the energy densities, $e_e^0 = \frac{e_e}{2}$, $e_{ph}^0 = \frac{e_{ph}}{2}$ are the equilibrium energies densities, $\mathbf{c}_e$, $\mathbf{c}_{ph}$ are the propagation speed, τ_e, τ_{ph} are the relaxation times, t is the time and $Q_e = Q_e\left(t, x\right)$, $Q_{ph} = Q_{ph}\left(t, x\right)$ are the energies sources for electrons and lattice respectively.

Since the system of governing equations is formulated for energy densities there is a need for formulas that allow to recalculate energy density to temperature and vice versa. Such conversion can be made using presented formulas [2]

$$e_e\left(T_e\right) = \left(n_e\frac{\pi^2}{2}\frac{k_b^2}{\varepsilon_F}\right)T_e^2 \tag{3}$$

$$e_{ph}\left(T_{ph}\right) = \left(\frac{9\eta_{ph}k_b}{\Theta_D^3}\int_0^{\frac{\Theta_D}{T_{ph}}}\frac{x^3}{exp(x) - 1}dx\right)T_{ph}^4 \tag{4}$$

where k_b is the Boltzmann constant, Θ_D is the Debye temperature of the metal, T_e, T_{ph} are the temperatures for electrons and phonons respectively, while n_e and η_{ph} are densities of these carriers. The electrons and the phonons energy sources depend on temperature of both carriers, the electron-phonon coupling factor which vary for deferent materials and can be calculated using the following expressions [1, 5]

$$Q_e\left(t, x\right) = Q\left(t, x\right) - G\left(T_e\left(t, x\right) - T_{ph}\left(t, x\right)\right) \tag{5}$$

$$Q_{ph}\left(t, x\right) = G\left(T_e\left(t, x\right) - T_{ph}\left(t, x\right)\right) \tag{6}$$

The electron-phonon coupling factor is a coefficient which characterizes the energy exchange between both carriers. To make model complete the equations (1) and (2), should be supplemented by the boundary-initial conditions. In the paper are considered the 2nd type of the boundary conditions (BC) on both edges, particularly adiabatic condition, because the laser heating lasts for a short period and then the heat losses from the both surfaces of the thin film can be neglected. To solve direct problem based on presented system of equations (1) and (2) the lattice Boltzmann method (LBM) was applied. For D1Q2 model in the LBM the discrete set of two propagation directions with appropriate velocities for electrons and phonons (Figure 1) are defined.

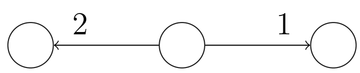

Figure 1: Directions of propagation energy carriers

Moreover, in the mathematical model the internal heat source $Q\left(t, x\right)$ is applied. It takes into account the temporal variation of the laser pulse approximated by a form of exponential function

$$Q\left(t, x\right) = \sqrt{\frac{\beta}{\pi}}\frac{1 - R}{t_p\delta_s}I_0 e^{\frac{-x}{\delta_s} - \beta\frac{t - 2t_p}{t_p}} \tag{7}$$

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, $\beta = 4\ln\left(2\right)$.

3 INVERSE PROBLEM SOLUTION

The considered inverse problem consists of identification of four model parameters, describing the laser irradiation. The performed identification is defined as an optimization problem where the goal is to minimize the differences between the results obtained from model with given parameters, and the expected values. The problem is solved using an evolutionary algorithm.

3.1 Evolutionary algorithm

Evolutionary algorithm (Figure 2) is a metaheuristic optimization algorithm that is inspired by the mechanisms of biological evolution of species. It operates on a set (population) of potential solutions (individuals) to a given problem. The quality of each individual is evaluated by the minimized goal function, that determines the adaptation of the individual to the environment. The higher the adaptation is, the bigger are the chances of the individual to survive. Genetic operators such as crossover (mixing genes from more than one individual) or mutation (random changes in genes) are applied in order to create populations for subsequent generations [6][8].

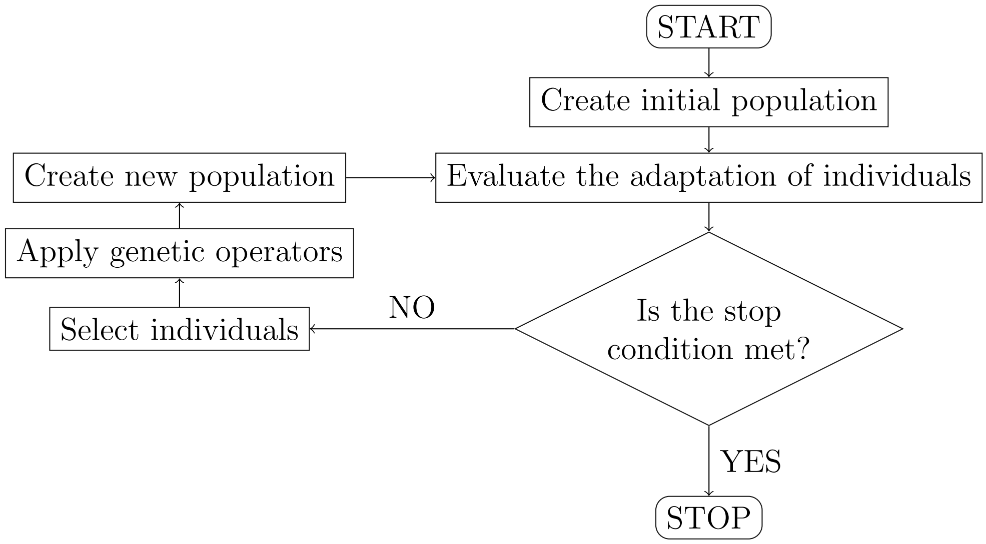

Figure 2: Evolutionary algorithm

3.2 Identification problem parameters

The goal is to adjust the numerical model, described using BTE, to fit experimental results published in [1], as accurate as possible. The considered results are electron temperatures in a chosen node in the function of time. The identified model parameters are: (a) laser intensity I_0, (b) optical penetration depth δ_s, (c) reflectivity R, and (d) laser pulse duration t_p. The boundaries of the parameters' values assumed in the identification are presented in Table 1.

Table 1: Boundaries of the identified parameters

Parameter	Lower bound	Upper bound	Unit
I_0	5	100	J/m^2
δ_s	10^{-11}	50×10^{-9}	m
R	0.01	1	-
t_p	10^{-14}	10^{-12}	ps

The goal (fitness) function F in the identification (optimization) problem was formulated as follows:

$$F(I_0, \delta_s, R, t_p) = \sum_{i=1}^{n} (T_i^{exp} - T_i^{num})^2 \quad (8)$$

where T_i^{exp} and T_i^{num} are the experimentally measured and numerically computed nodal electron temperatures at time sample i.

The parameters of the evolutionary algorithm were adapted as follows: population size 50, scattered crossover with probability of 0.8, and Gaussian mutation. The stop conditions were maximum number of generations 400 and 50 stall generations.

3.3 Obtained results

The convergence of the algorithm can be observed in Figure 3 as the mean fitness function value F of the population, over subsequent generations. The algorithm converged in 218 generation, after 50 stall generations. The fitness function value F for the best individual was 6.9964×10^4, while the mean value for whole final population was 7.0549×10^4.

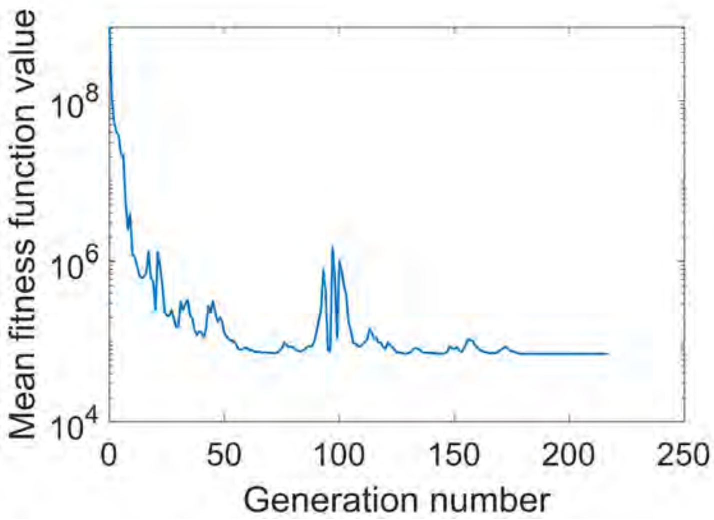

Figure 3: Convergence of the evolutionary algorithm

The identified parameters of the model are: $I_0 = 18.8843 J/m^2$, $\delta_s = 18.386 \times 10^{-9} m$, $R = 0.9619$ and $t_p = 0.0259 \times 10^{-12} s$. The time plot of the electron temperature of the source experimental data and that obtained from the identified numerical model are compared in Figure 4.

4 CONCLUSIONS

In the presented identification problem, the values of four model parameters (laser intensity I_0, optical penetration depth δ_s, reflectivity R, and laser pulse duration t_p) were searched. These parameter values introduced to the numerical model based on BTE were supposed to give electron temperature distribution that fit experimental results. Evolutionary algorithm was implemented to the identification problem. As indicated by Figure 3, the convergence process was successful, minimum value of fitness function was reached in 218 generations, after 50 stall generations. The accuracy of the BTE model with identified parameters values can be considered as satisfying, as can be observed in Figure 4 where comparison with experimental data is presented.

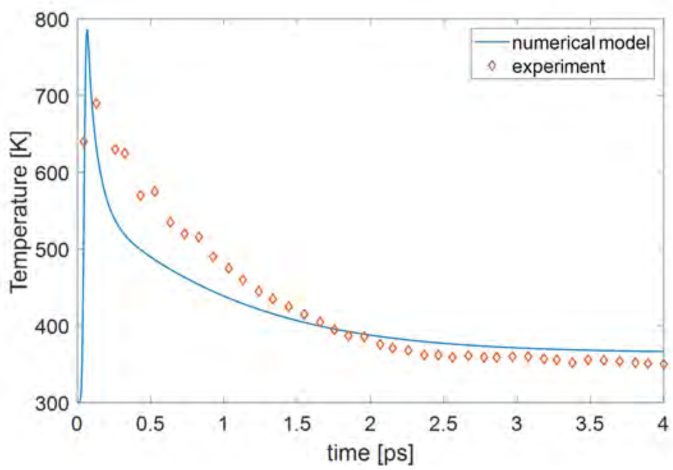

Figure 4: Comparison of experimental and numerical results

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