Modelling of thermal processes proceeding in a thin gold film using the lattice Boltzmann method with interval source function

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Abstract

The interval coupled lattice Boltzmann equations for electrons and phonons are used to analyze the heating process of thin metal films. The interval lattice Boltzmann method (ILBM) with the uncertainly defined internal source function associated with the laser irradiation is used to simulate the heat transfer. The solution of the interval Boltzmann transport equations has been obtained taking into account the rules of directed interval arithmetic. A similar analysis has been done using the sensitivity model where the Boltzmann transport equations and boundary-initial conditions have been differentiated with respect to the no-interval laser parameter. The knowledge of the sensitivity function distribution and the application of the Taylor formula allow one to find the border solutions of the problem analyzed which correspond to the solution obtained assuming the uncertainly defined source function. In the final part of the paper the results of numerical computations obtained using both methods are presented.

Keywords: lattice Boltzmann method, directed interval arithmetic, sensitivity analysis

1. Introduction

In the paper the interval version of the lattice Boltzmann method with the heat source specified as an uncertainly defined function in the mathematical model has been presented [3]. Additionally, the application of the directed interval arithmetic is applied. The solution obtained takes into account $\pm 5\%$ perturbations in the heat source function. The results of numerical computations such as energy and temperature heating curves at the selected points have the interval form. The sensitivity analysis with respect to the constant heat source function has been done. The heat source value has been assumed as the central value of the heat source interval.

2. The Boltzmann transport equation

The unsteady BTEs transformed into equivalent energy density equations for the 1D coupled model with two kinds of carriers (*e*-electrons and *ph*-phonons) can be written using the formulas [2]

$$\frac{\partial e_e}{\partial t} + \mathbf{v}_e \cdot \nabla e_e = -\frac{e_e - e_e^0}{\tau_{re}} + Q_e \tag{1}$$

$$\frac{\partial e_{ph}}{\partial t} + \mathbf{v}_{ph} \cdot \nabla e_{ph} = -\frac{e_{ph} - e_{ph}^0}{\tau_{r\,ph}} + Q_{ph} \tag{2}$$

where e_e, e_{ph} are the energies densities, e_e^0, e_{ph}^0 are the equilibrium energies densities, $\mathbf{v}_e, \mathbf{v}_{ph}$ are the frequency-dependent propagation speed, $\tau_{re}, \tau_{r\,ph}$ are the relaxation times, t denotes the time and Q_e, Q_{ph} are the energies source related to an unit of volume for electrons and phonons respectively.

The electron and phonon energy densities at their equivalent nonequilibrium temperatures are given by the formulas

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

and

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

where Θ_D is the Debye temperature of the solid, k_b is the Boltzmann constant, T_e, T_{ph} are the lattice temperature for electrons and phonons respectively, while n_e is the electron density and η_{ph} is the phonon density.

The electron and phonon energy sources are calculated using the following expressions [2]

$$Q_e = Q' - G(T_e - T_{ph}) \tag{5}$$

$$Q_{ph} = G(T_e - T_{ph}) \tag{6}$$

where Q' is the power density deposited by the external source function and G is the electron-phonon coupling factor which characterizes the energy exchange between electrons and phonons. The equations (1) and (2) should be supplemented by the initial and boundary conditions.

The temporal variation of laser output pulse is treated as source term in the energy equation and may be approximated by a form of exponential function [1]

$$Q'(x,t) = I_0 \delta e^{-\delta x - \beta t} \tag{7}$$

where I_0 is the peak power intensity of the laser pulse, δ is the absorption coefficient, β is the laser pulse parameter.

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3. Sensitivity analysis

In order to analyze the sensitivity of electron and phonon energy densities field, the governing equations should be differentiated with respect to the chosen parameter. In the paper the sensitivity analysis is presented with respect to the value of laser parameter β.

To the differentiated equations (1), (2) the sensitivity functions $U_e(x,t,\beta) = \partial e_e(x,t) / \partial \beta$ and $U_{ph}(x,t,\beta) = \partial e_{ph}(x,t) / \partial \beta$ are introduced and then

$$\frac{\partial U_e(x,t,\beta)}{\partial t} + v_e \frac{\partial U_e(x,t,\beta)}{\partial x} = -\frac{1}{2\tau_{re}} U_e(x,t,\beta) + \frac{\partial Q_e}{\partial \beta}$$
$$\frac{\partial U_{ph}(x,t,\beta)}{\partial t} + v_{ph} \frac{\partial U_{ph}(x,t,\beta)}{\partial x} = -\frac{1}{2\tau_{r\,ph}} U_{ph}(x,t,\beta) + \frac{\partial Q_{ph}}{\partial \beta} \tag{8}$$

The electron and the phonon energy densities functions $e_e(x,t,q_v \pm \Delta q_v)$ and $e_{ph}(x,t,q_v \pm \Delta q_v)$ are expanded into the Taylor series taking into account the first two components according to the formulas

$$e_e(x,t,\beta+\Delta\beta) \approx e_{eb}(x,t) + \frac{\partial e_e(x,t)}{\partial \beta} \cdot \Delta\beta$$
$$e_e(x,t,\beta-\Delta\beta) \approx e_{eb}(x,t) - \frac{\partial e_e(x,t)}{\partial \beta} \cdot \Delta\beta \tag{9}$$

where $\Delta\beta$ is a certain increment of the laser parameter and the starting points $e_{eb}(x,t)$ and $e_{phb}(x,t)$ correspond to the basic solution.

Taking into account the sensitivity functions and after some simplification one obtains certain increments of the energy functions Δe_e and Δe_{ph} which can be calculated using the formulae

$$\Delta e_e(x,t) \approx 2U_e(x,t,\beta) \cdot \Delta\beta$$
$$\Delta e_{ph}(x,t) \approx 2U_{ph}(x,t,\beta) \cdot \Delta\beta \tag{10}$$

4. Results of computations

Heat transfer in one-dimensional gold film of the thickness L=200 nm has been analyzed. The following input data have been introduced: the electron relaxation time $\tau_e = 0.04$ ps, the phonon relaxation time $\tau_{ph} = 0.8$ ps, the Debye temperature $\Theta_D = 170$ K, the absorption coefficient $\delta = 7.55 \cdot 10^7$ 1/m, the initial temperature $T_0^e = T_0^{ph} = 300$ K, the boundary conditions $T_{b1}^e = T_{b1}^{ph} = 300$ K, $q_{b2}^e = q_{b2}^{ph} = 0$ W/m^2, coupling factor G = $2.3 \cdot 10^{16}$ W/m^{3}K, the lattice distance $\Delta x = 20$ nm and the time step $\Delta t = 0.01$ ps. To the modelling internal heat source was taken into account the KrF laser with the wavelength of $\lambda = 248$ nm and the peak power intensity of the pulse I_0 = $2 \cdot 10^{13}$ W/m^2.

In the first example the interval value of the laser parameter has been considered $\overline{\beta} = \left(0.5 \cdot 10^{13} - 0.05 \cdot 0.5 \cdot 10^{13},\ 0.5 \cdot 10^{13} + 0.05 \cdot 0.5 \cdot 10^{13}\right)$ 1/s.

In the second example the no-interval value of the laser parameter has been introduced $\beta = 0.5 \cdot 10^{13}$ 1/s and the sensitivity analysis with respect to the laser parameter has been applied. In this model an increment of the laser parameter has been introduced as $\Delta\beta = 0.05 \cdot 0.5 \cdot 10^{13}$ W/m^3.

Figures 1 and 2 present the courses of the electrons temperature history taking into account the same internal nodes for the first and the second example, respectively.

As one can see, both results are similar.

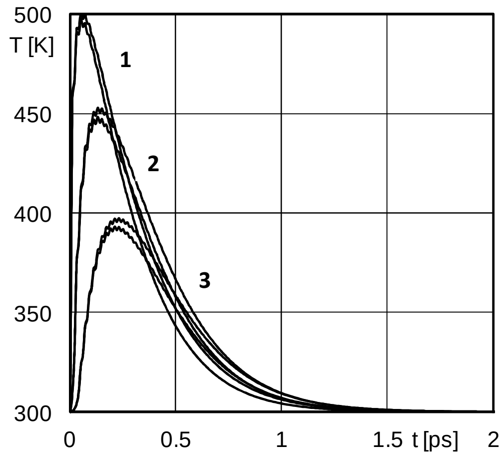

Figure 1: Electrons temperature history – first method

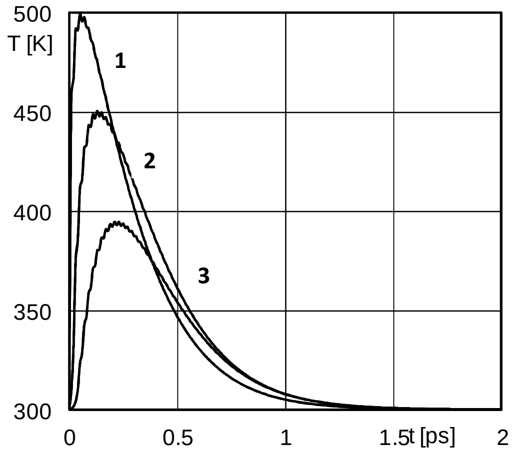

Figure 2: Electrons temperature history – second method

References

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