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# APPLICATION OF THE INTERVAL LATTICE BOLTZMANN METHOD FOR A NUMERICAL MODELLING OF THIN METAL FILMS IRRADIATION BY ULTRA SHORT LASER PULSES

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***Abstract****. In the paper the one-dimensional numerical modelling of heat transfer in thin metal films irradiated by ultra short laser pulses is considered. In the mathematical description the relaxation times and the boundary conditions for phonons and electrons are given as interval numbers. The problem formulated has been solved by means of the interval lattice Boltzmann method using the rules of directed interval arithmetic. The examples of numerical computations are presented in the final part of the paper.*

**Keywords**: Boltzmann transport equation, interval lattice Boltzmann method, directed interval arithmetic

# ZASTOSOWANIE INTERWAŁOWEJ METODY SIATEK BOLTZMANNA DO NUMERYCZNEGO MODELOWANIA PROCESU NAŚWIETLANIA LASEREM PULSACYJNYM CIENKICH WARSTW METALOWYCH

***Streszczenie.*** *W artykule zaprezentowano jednowymiarowy model numeryczny przepływu ciepła w cienkich warstwach metalowych poddanych. naświetlaniu laserem pulsacyjnym. W opisie matematycznym czasy relaksacji oraz warunki brzegowe dla fononów i elektronów są zdefiniowane jako liczby przedziałowe. Sformułowane zagadnienie rozwiązano za pomocą interwałowej metody siatek Boltzmanna stosując skierowaną arytmetykę interwałową. W końcowej części artykułu przedstawione są przykłady obliczeń numerycznych.*

**Słowa kluczowe**: równanie transportu Boltzmanna, interwałowa metoda siatek Boltzmanna, skierowana arytmetyka interwałowa

## Introduction

In metals heat transport is mainly realized by electrons and phonons which are quanta of lattice vibrations. During this process these carriers transfer energy in the material. Energy transport in nanostructured materials can vary from a bulk. When dimensions are reduced properties predicted for the bulk phase, e.g., thermal conductivity, may not be suitable for modeling thermal transport and then we need some other nanoscale features.This phenomena of energy transport can be described by a system of two Boltzmann transport equations supplemented by the adequate boundary-initial conditions. The first equation is related to the electrons and the second one to the phonons. It is important to point out that both equations are connected by a so called coupled factor.

In the mathematical model describing the heat transfer in a thin gold film the interval values of relaxation times and boundary conditions for phonons and electrons have been assumed. The relaxation time is estimated experimentally and its actual value is still a subject of discussion [5]. So it seems natural to take the interval value of this parameter and this assumption is closer to the real physical conditions of the process analyzed. The external heat source is treated as ultra-short laser pulse [6, 9].

The problem analyzed has been solved using an interval version of the lattice Boltzmann method according to the rules of the directed interval arithmetic [7, 8].

## 1. Boltzmann transport equation

The Boltzmann transport equation (BTE) is one of the fundamental equation of solid physics. The BTE expressed in a carrier distribution function form [1, 2, 4] can be written as

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = \frac{f^{\,0} - f}{\tau_r} + g_{ef} \tag{1}$$

where $f$ is the carrier distribution function, $f^{\,0}$ is the equilibrium distribution function given by the Bose-Einstein or Fermi-Dirac statistics, $\mathbf{v}$ is the frequency-dependent carrier propagation speed, $\tau_r$ is the frequency-dependent carrier relaxation time and $g_{ef}$ is the electron generation rate due to electron-phonon scattering.

The Boltzmann transport equation can be transformed into an equivalent carrier energy density equation using the simplifying assumptions of the Debye model

$$\frac{\partial e}{\partial t} + \mathbf{v} \cdot \nabla e = -\frac{e - e^0}{\tau_r} + q_v \tag{2}$$

where $e$ is the carrier energy density, $e^{\,0}$ is the equilibrium carrier energy density and $q_v$ is the internal heat generation rate related to an unit of volume.

Using the Debye model the dependence between phonon and electron energy densities and their temperature can be calculated from the following formulas [1, 3]

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

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

where $\Theta_D$ is the Debye temperature of the solid, $k_b$ is the Boltzmann constant, $T_e$ and $T_{ph}$ are the carriers temperatures, $\varepsilon_F$ is the Fermi energy, $n_e$ is the electron density while $\eta$ is the number density of oscillators and can be calculated using the following formula [1]

$$\eta = \frac{1}{6\pi^2} \left( \frac{k_b \Theta_D}{\hbar\, \omega} \right)^3 \tag{5}$$

where ħ is the Planck constant divided by 2π and ω is the speed of sound in analysed material.

The formulation of the heat transport problem in metals demand system of two equations which in an equivalent carrier energy density equations has the following form

$$\frac{\partial e_e}{\partial t} + \mathbf{v}_e \cdot \nabla e_e = \frac{e_e^{\,0} - e_e}{\tau_e} + Q_e \tag{6}$$

$$\frac{\partial e_{ph}}{\partial t} + \mathbf{v}_{ph} \cdot \nabla e_{ph} = \frac{e_{ph}^{\,0} - e_{ph}}{\tau_{ph}} + Q_{ph} \tag{7}$$

where $e_e$, $e_{ph}$ are the carrier energy densities, $e_e^{\,0}$, $e_{ph}^{\,0}$ are the equilibrium carrier energy densities and $Q_e$, $Q_{ph}$ are the carrier energy sources related to an unit of volume.

## 2. The interval lattice Boltzmann method

The lattice Boltzmann method (LBM) is a numerical technique for the simulation of heat transfer. The LBM solves a discretized set of the Boltzmann transport equations known as the lattice Boltzmann equations. The Boltzmann transport equations for the coupled problem with two relaxation times can be written in the following form [1, 3]

$$\frac{\partial \bar{e}_e}{\partial t} + \mathbf{v}_e \cdot \nabla \bar{e}_e = \frac{\bar{e}_e^{\,0} - \bar{e}_e}{\bar{\tau}_e} + \bar{Q}_e \tag{8}$$

$$\frac{\partial \bar{e}_{ph}}{\partial t} + \mathbf{v}_{ph} \cdot \nabla \bar{e}_{ph} = \frac{\bar{e}_{ph}^{\,0} - \bar{e}_{ph}}{\bar{\tau}_{ph}} + \bar{Q}_{ph} \tag{9}$$

where $\bar{e}_e, \bar{e}_{ph}$ are the interval values of carrier energy densities for electrons and phonons respectively, $\bar{e}_e^{\,0}, \bar{e}_{ph}^{\,0}$ are the interval equilibrium carrier energy densities and $\bar{\tau}_e, \bar{\tau}_{ph}$ are the interval relaxation times of electrons and phonons, $\bar{Q}_e$ is the interval electron energy source

$$\bar{Q}_e = Q' - G(\bar{T}_e - \bar{T}_{ph}) \tag{10}$$

and $\bar{Q}_{ph}$ is the interval phonon energy source which is calculated using the formula

$$\bar{Q}_{ph} = G(\bar{T}_e - \bar{T}_{ph}) \tag{11}$$

where $Q'$ is the power density function deposited by the external source associated with the laser irradiation, $G$ is the electron-phonon coupling factor which characterizes the energy exchange between electrons and phonons, $\bar{T}_e$ and $\bar{T}_{ph}$ are the interval temperature values of electrons and phonons.

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 [5, 11, 12]

$$Q'(x,t) = I_0 \delta e^{-\delta x - \beta t} \tag{12}$$

where $I_0$ is the peak power intensity of the laser pulse, $\delta$ is the absorption coefficient, $\beta$ is the laser pulse parameter. The absorption coefficient is given by [12]

$$\delta = \frac{4\pi k_{ext}}{\lambda} \tag{13}$$

where $k_{ext}$ is the imaginary parts of the refractive index ($k_{ext}$ = 1.49 for Au) and $\lambda$ is the wavelength of the laser.

The discrete set of propagation velocities in the main lattice directions for one-dimensional model is defined as follows (see Fig. 1)

$$\begin{aligned} \mathbf{c}_{e1} &= [c_e, 0] \\ \mathbf{c}_{e2} &= [-c_e, 0] \\ \mathbf{c}_{ph1} &= [c_{ph}, 0] \\ \mathbf{c}_{ph2} &= [-c_{ph}, 0] \end{aligned} \tag{14}$$

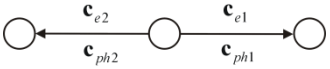


*Fig. 1. One-dimensional 2-speed lattice Boltzmann model*

The vectors $\mathbf{c}_{e1}$ and $\mathbf{c}_{e2}$ represent the velocities of the electrons, while the vectors $\mathbf{c}_{ph1}$ and $\mathbf{c}_{ph2}$ represent the velocity of the phonons in the horizontal direction [1].

In the interval lattice Boltzmann method is needed to solve a system of four partial differential equations allowing to compute phonon and electron energy densities in different lattice nodes according to the following equations

$$\begin{cases} \dfrac{\partial \bar{e}_{e1}}{\partial t} + c\dfrac{\partial \bar{e}_{e1}}{\partial x} = -\dfrac{\bar{e}_{e1} - \bar{e}_{e1}^{\,0}}{\bar{\tau}_e} + \bar{Q}_e \\ \dfrac{\partial \bar{e}_{e2}}{\partial t} - c\dfrac{\partial \bar{e}_{e2}}{\partial x} = -\dfrac{\bar{e}_{e2} - \bar{e}_{e2}^{\,0}}{\bar{\tau}_e} + \bar{Q}_e \\ \dfrac{\partial \bar{e}_{ph1}}{\partial t} + c\dfrac{\partial \bar{e}_{ph1}}{\partial x} = -\dfrac{\bar{e}_{ph1} - \bar{e}_{ph1}^{\,0}}{\bar{\tau}_{ph}} + \bar{Q}_{ph} \\ \dfrac{\partial \bar{e}_{ph2}}{\partial t} - c\dfrac{\partial \bar{e}_{ph2}}{\partial x} = -\dfrac{\bar{e}_{ph2} - \bar{e}_{ph2}^{\,0}}{\bar{\tau}_{ph}} + \bar{Q}_{ph} \end{cases} \tag{15}$$

where $c = \Delta x / \Delta t$ is the component of velocity along the $x$-axis, $\Delta x$ is the lattice distance from site to site, $\Delta t = t^{f+1} - t^f$ is the time step. The set of equations (15) must be supplemented by the boundary conditions of the following form

$$\begin{cases} x = 0: & \bar{q}_b^e(0, t) = c_e\left[e_e\left(\bar{T}_e\right)_0 - e_e\left(\bar{T}_e\right)_1\right] \\ x = L: & \bar{e}_e(L, t) = e_e\left(\bar{T}_{b2}^e\right) \\ x = 0: & \bar{q}_b^{ph}(0, t) = c_{ph}\left[e_{ph}\left(\bar{T}_{ph}\right)_0 - e_{ph}\left(\bar{T}_{ph}\right)_1\right] \\ x = L: & \bar{e}_{ph}(L, t) = e_{ph}\left(\bar{T}_{b2}^{ph}\right) \end{cases} \tag{16}$$

and the initial condition

$$t = 0: \quad e_e(x, 0) = e_e(T_0^e), \quad e_{ph}(x, 0) = e_{ph}(T_0^{ph}) \tag{17}$$

where $\bar{T}_{b2}^e$ and $\bar{T}_{b2}^{ph}$ are the interval boundary temperatures of electrons and phonons, $T_0^e$ and $T_0^{ph}$ are the initial temperatures of electrons and phonons, $\bar{q}_b^e$, $\bar{q}_b^{ph}$ are the interval boundary heat fluxes of electrons and phonons.

The approximation of the first derivatives using right-hand and left-hand sides differential quotients for electrons and phonons is defined as

$$\frac{\partial \bar{e}_i}{\partial t} = \frac{\bar{e}_i(x, t + \Delta t) - \bar{e}_i(x, t)}{\Delta t}, \quad i = e1, e2, ph1, ph2 \tag{18}$$

and

$$\begin{aligned} \frac{\partial \bar{e}_{e1}}{\partial x} &= \frac{\bar{e}_{e1}(x + \Delta x, t + \Delta t) - \bar{e}_{e1}(x, t + \Delta t)}{\Delta x} \\ \frac{\partial \bar{e}_{e2}}{\partial x} &= \frac{\bar{e}_{e2}(x - \Delta x, t + \Delta t) - \bar{e}_{e2}(x, t + \Delta t)}{\Delta x} \\ \frac{\partial \bar{e}_{ph1}}{\partial x} &= \frac{\bar{e}_{ph1}(x + \Delta x, t + \Delta t) - \bar{e}_{ph1}(x, t + \Delta t)}{\Delta x} \\ \frac{\partial \bar{e}_{ph2}}{\partial x} &= \frac{\bar{e}_{ph2}(x - \Delta x, t + \Delta t) - \bar{e}_{ph2}(x, t + \Delta t)}{\Delta x} \end{aligned} \tag{19}$$

Then after introduction time and position derivatives the discretized form of (15) is as follows

$$\begin{cases} \left(\bar{e}_{e1}\right)_{i+1}^{f+1} = \left(1 - \dfrac{\Delta t}{\bar{\tau}_e}\right)\left(\bar{e}_{e1}\right)_i^f + \dfrac{\Delta t}{\bar{\tau}_e}\left(\bar{e}_{e1}^0\right)_i^f + \Delta t \bar{Q}_e \\ \left(\bar{e}_{e2}\right)_{i-1}^{f+1} = \left(1 - \dfrac{\Delta t}{\bar{\tau}_e}\right)\left(\bar{e}_{e2}\right)_i^f + \dfrac{\Delta t}{\bar{\tau}_e}\left(\bar{e}_{e2}^0\right)_i^f + \Delta t \bar{Q}_e \\ \left(\bar{e}_{ph1}\right)_{i+1}^{f+1} = \left(1 - \dfrac{\Delta t}{\bar{\tau}_{ph}}\right)\left(\bar{e}_{ph1}\right)_i^f + \dfrac{\Delta t}{\bar{\tau}_{ph}}\left(\bar{e}_{ph1}^0\right)_i^f + \Delta t \bar{Q}_{ph} \\ \left(\bar{e}_{ph2}\right)_{i-1}^{f+1} = \left(1 - \dfrac{\Delta t}{\bar{\tau}_{ph}}\right)\left(\bar{e}_{ph2}\right)_i^f + \dfrac{\Delta t}{\bar{\tau}_{ph}}\left(\bar{e}_{ph2}^0\right)_i^f + \Delta t \bar{Q}_{ph} \end{cases} \tag{20}$$

The equilibrium electron energy density and phonon energy density is the same in all lattice directions and can be calculated using the formula

$$\left(\overline{e}_e^0\right)_i^{f+1} = \frac{\left(\overline{e}_e\right)_i^{f+1}}{2} \tag{21}$$

$$\left(\overline{e}_{ph}^0\right)_i^{f+1} = \frac{\left(\overline{e}_{ph}\right)_i^{f+1}}{2} \tag{22}$$

The total energy density is defined as the sum of discrete electron and phonon energy densities in two directions of the lattice

$$\overline{e}_e = \overline{e}_{e1} + \overline{e}_{e2} \tag{23}$$

$$\overline{e}_{ph} = \overline{e}_{ph1} + \overline{e}_{ph2} \tag{24}$$

After subsequent computations the temperature of electrons and phonons are determined using the following formulas (see eq. 3 and 4)

$$\overline{T}_e^{\,f+1} = \sqrt{\overline{e}_e(\overline{T}_e^{\,f}) \Big/ \left( n_e \frac{\pi^2}{2} \frac{k_b^2}{\varepsilon_F} \right)} \tag{25}$$

$$\overline{T}_{ph}^{\,f+1} = \sqrt[4]{\overline{e}(\overline{T}_{ph}^{\,f})\Theta_D^3 \Big/ 9\eta\, k_b \int_0^{\Theta_D/\overline{T}_{ph}^{\,f}} \frac{z^3}{\exp(z)-1}\mathrm{d}z} \tag{26}$$

## 1. Results of computations

As a numerical example the heat transport in a gold thin film of the dimension 200 nm has been analyzed. To the modelling internal heat source was taken into account the KrF laser with the wavelength of $\lambda$ = 248 nm [7].

The following input data have been introduced: the relaxation time $\overline{\tau}_{re} = [0.038, 0.042]$ps, $\overline{\tau}_{rph} = [0.76, 0.84]$ps, the Debye temperature $\Theta_D = 170$K, the peak power intensity of the laser pulse $I_0 = 2\cdot10^{13}$ W/m$^2$, the absorption coefficient $\delta = 7.55\cdot10^7$ 1/m, the laser pulse parameter $\beta = 0.5\cdot10^{13}$ 1/s, the coupling factor G = $2.3\cdot10^{16}$ W/m$^3$K, the boundary conditions of the 2$^{nd}$ type on the left boundary $\overline{q}_b^e(0, t) = \overline{q}_b^{ph}(0, t) = \overline{0}$ and the 1$^{st}$ type on the right boundary with the interval temperature $\overline{T}_{b2}^e = \overline{T}_{b2}^{ph} = [285, 315]$K, the initial temperature $T_0 = 300$K. The lattice step $\Delta x = 20$nm and the time step $\Delta t = 0.01$ps have been assumed.

Figure 2 presents the courses of the temperature functions at the internal nodes 1 – 20 nm, 2 – 80 nm and 3 – 140 nm. For interval values of the electron and phonon relaxation times and the boundary conditions we obtain two curves for each internal node which denote the first and the second endpoints of the temperature interval. The application of the interval version of the LBM allows one to find the numerical solution in the interval form.

Figure 3 shows the courses of the temperature function at the same internal nodes but for wider intervals of the boundary conditions ($\overline{T}_{b2}^e = \overline{T}_{b2}^{ph} = [270, 330]$K) and the relaxation times ($\overline{\tau}_{re} = [0.036, 0.044]$ps, $\overline{\tau}_{rph} = [0.72, 0.88]$ps). The interval temperatures are, of course, wider.

Figure 4 presents the interval temperature distribution in the domain considered for the chosen times: 0.6, 0.8 and 1 ps. Figure 5 also shows the interval temperature distribution in the domain but for wider intervals of the boundary conditions and the relaxation times. We can see that the temperature intervals are also wider.

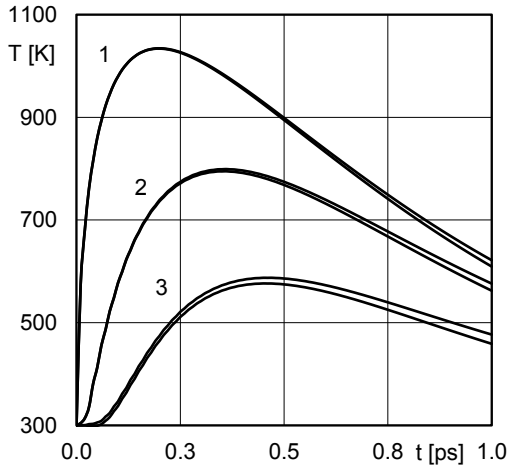


*Fig. 2. The interval heating curves at internal nodes*

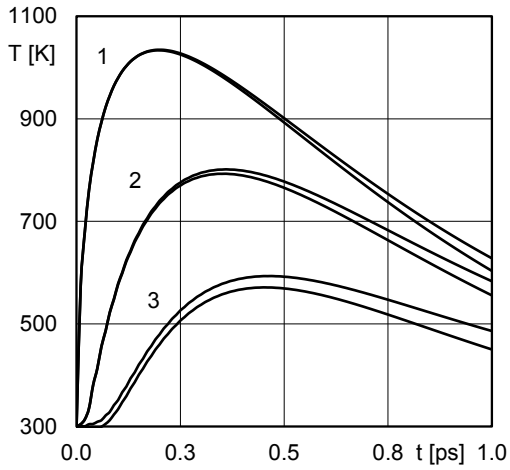


*Fig. 3. The interval heating curves at internal nodes for wider parameters*

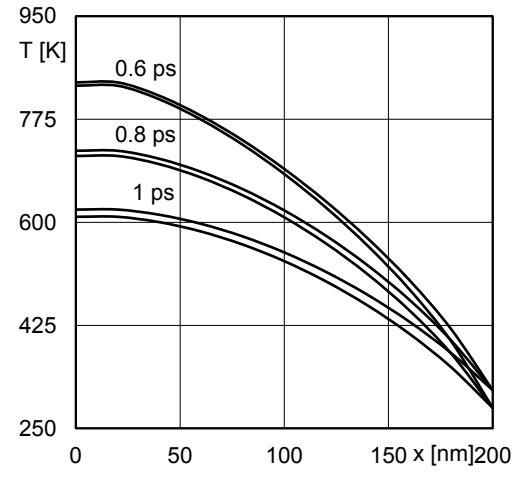


*Fig. 4. The interval temperature distribution in gold film*

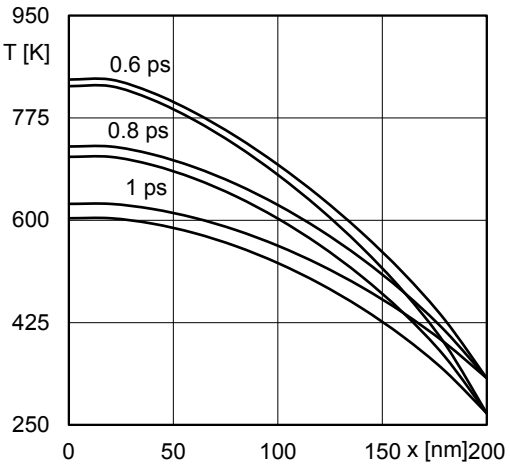


*Fig. 5. The interval temperature distribution in gold film for wider parameters*

## 2. Conclusions

In the paper the coupled Boltzmann transport equation with the interval values of the relaxation times and the boundary conditions for electrons and phonons has been considered. The generalization of lattice Boltzmann method allows one to find the numerical solution in the interval form and such an information may be important especially for the parameters which are estimated experimentally, for example the relaxation time. The main advantage of the directed interval arithmetic upon the classical interval arithmetic is that the obtained temperature intervals are much narrower. The problem analyzed can be extended to multi-layered domains.

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