

MODELING OF THERMAL PROCESSES PROCEEDING IN A 1D DOMAIN OF CRYSTALLINE SOLIDS USING THE LATTICE BOLTZMANN METHOD WITH AN INTERVAL SOURCE FUNCTION

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The interval lattice Boltzmann method (ILBM) with an uncertainly defined internal heat source function is used to simulate heat transfer in a thin silicone film. The solution to the interval Boltzmann transport equations has been obtained taking into account the rules of directed interval arithmetics. 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 heat source value. 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 (to some extent) correspond to the solution obtained under the assumption of the uncertainly defined source function. In the final part of the paper, numerical computations obtained for both methods are presented.

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

1. Introduction

The problem of heat transfer in nano-layers is frequently encountered in many fields of science and engineering such as mechanical engineering, thermal management of electronic cooling and improvement of performance of heat transfer systems (Escobar *et al.*, 2006; Huang *et al.*, 2005; Joshi and Majumdar, 1993; Mansoor and Yilbas, 2011, 2014). Heat transfer problems are usually solved using equations with deterministic thermophysical parameters (Eshraghi and Felicelli, 2012; Narumanchi *et al.*, 2003). However, in most cases of the engineering practice, values of these parameters cannot be defined with a high precision and, in such cases, it is much more convenient to define these parameters as interval numbers (Piasecka-Belkhat and Korczak, 2014, 2016).

In this paper, an interval version of the lattice Boltzmann method with the uncertainly defined heat source function has been presented with the application of the directed interval arithmetics. The solution obtained corresponds to $\pm 5\%$ perturbations of the heat source function. The results of numerical computations (energy and temperature heating curves at the selected points) have an interval form, of course. Additionally, the sensitivity analysis with respect to the constant heat source function has been done (Chonga *et al.*, 2016; Dems and Rousselet, 1999; Goethals *et al.*, 2011; Hwang *et al.*, 2016). The heat source value has been assumed as the middle value of the heat source interval. The application of the sensitivity function distribution and the Taylor formula with an increment of the source function equal to the half of the width of the heat source interval allows one to find the solution to the boundary-initial problem similar to the solution with some “uncertainties” appearing in the mathematical model. The aim of the paper is comparison of the results obtained using both methods.

2. Directed interval arithmetics

Let us consider a directed interval \bar{a} which can be defined as a set \mathbb{D} of all directed pairs of real numbers defined as follows (Neumaier, 1990; Piasecka-Belkhat, 2011a,b)

$$\bar{a} = [a^-, a^+] \quad \text{for } a^-, a^+ \in \mathbb{R} \quad (2.1)$$

where a^- and a^+ denote the beginning and the end of the interval, respectively.

The left or the right endpoint of the interval \bar{a} can be denoted as a^s , $s \in \{+, -\}$, where s is a binary variable. This variable can be expressed as a product of two binary variables and is defined as

$$\begin{aligned} ++ &= -- = + \\ +- &= -+ = - \end{aligned} \quad (2.2)$$

An interval is called proper if $a^- < a^+$, improper if $a^- > a^+$ and degenerate if $a^- = a^+$. The set of all directed interval numbers can be written as $\mathbb{D} = \mathbb{P} \cup \mathbb{I}$, where \mathbb{P} denotes a set of all directed proper intervals and \mathbb{I} denotes a set of all improper intervals.

Additionally, a subset $\mathbb{Z} = \mathbb{Z}_{\mathbb{P}} \cup \mathbb{Z}_{\mathbb{I}} \subset \mathbb{D}$ should be defined, where

$$\begin{aligned} \mathbb{Z}_{\mathbb{P}} &= \{\bar{a} \in \mathbb{P} \mid a^- \leq 0 \leq a^+\} \\ \mathbb{Z}_{\mathbb{I}} &= \{\bar{a} \in \mathbb{I} \mid a^+ \leq 0 \leq a^-\} \end{aligned} \quad (2.3)$$

For directed interval numbers, two binary variables are defined. The first of them is the direction variable

$$\tau(\bar{a}) = \begin{cases} + & \text{if } a^- \leq a^+ \\ - & \text{if } a^- > a^+ \end{cases} \quad (2.4)$$

and the other is the sign variable

$$\sigma(\bar{a}) = \begin{cases} + & \text{if } a^- > 0, a^+ > 0 \\ - & \text{if } a^- < 0, a^+ < 0 \end{cases} \quad \bar{a} \in \mathbb{D} \setminus \mathbb{Z} \quad (2.5)$$

For the zero argument $\sigma([0, 0]) = \sigma(0) = +$, for all intervals including the zero element $\bar{a} \in \mathbb{Z}$, $\sigma(\bar{a})$ is not defined.

The sum of two directed intervals $\bar{a} = [a^-, a^+]$ and $\bar{b} = [b^-, b^+]$ can be written as

$$\bar{a} + \bar{b} = [a^- + b^-, a^+ + b^+] \quad \bar{a}, \bar{b} \in \mathbb{D} \quad (2.6)$$

The difference is of the form

$$\bar{a} - \bar{b} = [a^- - b^+, a^+ - b^-] \quad \bar{a}, \bar{b} \in \mathbb{D} \quad (2.7)$$

The product of the directed intervals is described by the formula

$$\bar{a}\bar{b} = \begin{cases} [a^{-\sigma(\bar{b})}b^{-\sigma(\bar{a})}, a^{\sigma(\bar{b})}b^{\sigma(\bar{a})}] & \bar{a}, \bar{b} \in \mathbb{D} \setminus \mathbb{Z} \\ [a^{\sigma(\bar{a})}\tau(\bar{b})b^{-\sigma(\bar{a})}, a^{\sigma(\bar{a})}\tau(\bar{b})b^{\sigma(\bar{a})}] & \bar{a} \in \mathbb{D} \setminus \mathbb{Z}, \bar{b} \in \mathbb{Z} \\ [a^{-\sigma(\bar{b})}b^{\sigma(\bar{b})}\tau(\bar{a}), a^{\sigma(\bar{b})}b^{\sigma(\bar{b})}\tau(\bar{a})] & \bar{a} \in \mathbb{Z}, \bar{b} \in \mathbb{D} \setminus \mathbb{Z} \\ [\min(a^-b^+, a^+b^-), \max(a^-b^-, a^+b^+)] & \bar{a}, \bar{b} \in \mathbb{Z}_{\mathbb{P}} \\ [\max(a^-b^-, a^+b^+), \min(a^-b^+, a^+b^-)] & \bar{a}, \bar{b} \in \mathbb{Z}_{\mathbb{I}} \\ 0 & (\bar{a} \in \mathbb{Z}_{\mathbb{P}}, \bar{b} \in \mathbb{Z}_{\mathbb{I}}) \vee (\bar{a} \in \mathbb{Z}_{\mathbb{I}}, \bar{b} \in \mathbb{Z}_{\mathbb{P}}) \end{cases} \quad (2.8)$$

The quotient of two directed intervals can be written as

$$\bar{a}/\bar{b} = \begin{cases} [a^{-\sigma(\bar{b})}/b^{\sigma(\bar{a})}, a^{\sigma(\bar{b})}/b^{-\sigma(\bar{a})}] & \bar{a}, \bar{b} \in \mathbb{D} \setminus \mathbb{Z} \\ [a^{-\sigma(\bar{b})}/b^{-\sigma(\bar{b})\tau(\bar{a})}, a^{\sigma(\bar{b})}/b^{-\sigma(\bar{b})\tau(\bar{a})}] & \bar{a} \in \mathbb{Z}, \bar{b} \in \mathbb{D} \setminus \mathbb{Z} \end{cases} \quad (2.9)$$

In the directed interval arithmetics, two extra operators are defined, the inversion of summation

$$-_{\mathbb{D}}\bar{a} = [-a^-, -a^+] \quad \bar{a} \in \mathbb{D} \quad (2.10)$$

and the inversion of multiplication

$$1/_{\mathbb{D}}\bar{a} = [1/a^-, 1/a^+] \quad \bar{a} \in \mathbb{D} \setminus \mathbb{Z} \quad (2.11)$$

So, two additional mathematical operations can be defined as follows

$$\bar{a} -_{\mathbb{D}} \bar{b} = [a^- - b^-, a^+ - b^+] \quad \bar{a}, \bar{b} \in \mathbb{D} \quad (2.12)$$

and

$$\bar{a}/_{\mathbb{D}}\bar{b} = \begin{cases} [a^{-\sigma(\bar{b})}/b^{-\sigma(\bar{a})}, a^{\sigma(\bar{b})}/b^{\sigma(\bar{a})}] & \bar{a}, \bar{b} \in \mathbb{D} \setminus \mathbb{Z} \\ [a^{-\sigma(\bar{b})}/b^{\sigma(\bar{b})}, a^{\sigma(\bar{b})}/b^{\sigma(\bar{b})}] & \bar{a} \in \mathbb{Z}, \bar{b} \in \mathbb{D} \setminus \mathbb{Z} \end{cases} \quad (2.13)$$

Now, it is possible to obtain the number zero by subtraction of two identical intervals $\bar{a} -_{\mathbb{D}} \bar{a} = \bar{0}$ and the number one as the result of division $\bar{a}/_{\mathbb{D}}\bar{a} = \bar{1}$, which is impossible when applying classical interval arithmetics (Markov, 1995).

3. Boltzmann transport equation

The Boltzmann transport equation (BTE) is one of the fundamental equations of solid state physics and takes the following form (Escobar *et al.*, 2006)

$$\frac{\partial f}{\partial t} + v\nabla f = \frac{f^0 - f}{\tau_r} + g_{ef} \quad (3.1)$$

where f is the phonon distribution function, f^0 is the equilibrium distribution function given by the Bose-Einstein statistics, v is the phonon group velocity, τ_r is the relaxation time and g_{ef} is the phonon generation rate due to electron-phonon scattering.

In order to take advantage of the simplifying assumption of the Debye model, the BTE can be transformed into an equation of the carrier energy density, and for a one-dimensional problem has the following form (Escobar *et al.*, 2006)

$$\frac{\partial e}{\partial t} + v\nabla e = -\frac{e - e^0}{\tau_r} + q_v \quad (3.2)$$

where e is the phonon energy density, e^0 is the equilibrium phonon energy density and q_v is the internal heat source related to a unit of volume. Equation (3.2) must be supplemented by the adequate boundary-initial conditions.

Using the Debye model, the relation between the phonon energy density and lattice temperature is given by the following formula (Escobar *et al.*, 2006)

$$e(T) = \left(\frac{9\eta k_b}{\Theta_{\mathbb{D}}^3} \int_0^{\Theta_{\mathbb{D}}/T} \frac{z^3}{\exp(z) - 1} dz \right) T^4 \quad (3.3)$$

where $\Theta_{\mathbb{D}}$ is the Debye temperature of the solid, k_b is the Boltzmann constant, T is the lattice temperature while η is the number density of phonons, and can be calculated using the formula (Escobar *et al.*, 2006)

$$\eta = \frac{1}{6\pi^2} \left(\frac{k_b \Theta_{\mathbb{D}}}{\hbar \omega} \right)^3 \quad (3.4)$$

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

4. Interval lattice Boltzmann method

The lattice Boltzmann method (LBM) is a numerical technique for simulation of fluid flows and heat transfer. Here LBM has been successfully applied to simulate heat transfer in nano layers. Unlike the conventional numerical methods based on discretizations of macroscopic continuum equations, the LBM is based on nanoscale models and heat transfer equations.

In this paper, it is shown how the LBM solves a discretized set of the Boltzmann transport equation (BTE) in the case of interval values appearing in the mathematical model. Then the interval Boltzmann transport equation for a one-dimensional problem has the following form (Piasecka-Belkhat and Korczak, 2014)

$$\frac{\partial \bar{e}(x, t)}{\partial t} + v \frac{\partial \bar{e}(x, t)}{\partial x} = -\frac{\bar{e}(x, t) - \bar{e}^0(x, t)}{\tau_r} + \bar{q}_v(x, t) \quad (4.1)$$

where $\bar{e}(x, t)$ is the interval phonon energy density, $\bar{e}^0(x, t)$ is the interval equilibrium phonon energy density, τ_r is the relaxation time, $v_1 = v$ and $v_2 = -v$ (see Fig. 1) and $\bar{q}_v(x, t)$ is the interval heat source, x is the spatial coordinate and t is the time.

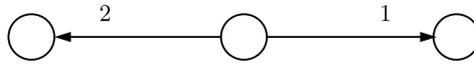


Fig. 1. Directions of the lattice vibrations

The interval total phonon energy density is defined as the sum of phonon energy densities in all directions. In the paper, a one-dimensional model with two directions of the phonon velocities is assumed (Piasecka-Belkhat and Korczak, 2014, 2016)

$$\bar{e}(x, t) = \bar{e}_1(x, t) + \bar{e}_2(x, t) = \sum_{d=1}^2 \bar{e}_d(x, t) \quad (4.2)$$

where $\bar{e}_1(x, t)$ is the phonon energy density in the positive x direction while $\bar{e}_2(x, t)$ is the phonon energy density in the negative x direction, d means the lattice direction (see Fig. 1).

In the interval lattice Boltzmann method it is needed to solve system of two partial differential equations allowing one to compute phonon energy in different lattice nodes according to the following equations (Piasecka-Belkhat and Korczak, 2014)

$$\frac{\partial \bar{e}_d(x, t)}{\partial t} + (-1)^{d-1} v \frac{\partial \bar{e}_d(x, t)}{\partial x} = -\frac{\bar{e}_d(x, t) - \bar{e}_d^0(x, t)}{\tau_r} + \bar{q}_v(x, t) \quad d = 1, 2 \quad (4.3)$$

where $v = \Delta x / \Delta t$ is the component of velocity along the x -axis, Δx is the lattice distance from site to site, $\Delta t = t^{f+1} - t^f$ is the time step needed for a phonon to travel from one lattice site to the neighboring lattice site and

$$\bar{e}_d^0(x, t) = \bar{e}(x, t) / d \quad (4.4)$$

The set of equations (4.3) must be supplemented by the boundary-initial conditions (Goethals *et al.*, 2011)

$$\begin{aligned}
 x = 0 : \quad & e_1(0, t) = e(T_{b1}) \\
 x = L : \quad & e_2(L, t) = e(T_{b2}) \\
 t = 0 : \quad & e(x, 0) = e(T_0)
 \end{aligned} \tag{4.5}$$

where T_{b1} and T_{b2} are the boundary temperatures, T_0 is the initial temperature.

The approximate form of equations (4.3) is of the following form

$$\begin{aligned}
 (\bar{e}_1)_{i+1}^{f+1} &= \left(1 - \frac{\Delta t}{\tau_r}\right) (\bar{e}_1)_i^f + \frac{\Delta t}{\tau_r} (\bar{e}_1^0)_i^f + \Delta t \bar{q}_v \\
 (\bar{e}_2)_{i-1}^{f+1} &= \left(1 - \frac{\Delta t}{\tau_r}\right) (\bar{e}_2)_i^f + \frac{\Delta t}{\tau_r} (\bar{e}_2^0)_i^f + \Delta t \bar{q}_v
 \end{aligned} \tag{4.6}$$

After subsequent computations, the interval lattice temperature is determined according to the rules of directed interval arithmetics using the formula (see Eq. (3.3))

$$\bar{T}^f = \sqrt[4]{\bar{e}^f \Theta_{\mathbb{D}}^3 \left(9\eta k_b \int_0^{\Theta_{\mathbb{D}}/\bar{T}^{f-1}} \frac{z^3}{\exp(z) - 1} dz \right)^{-1}} \tag{4.7}$$

5. Sensitivity analysis

In order to analyze the sensitivity of the phonon energy density field, the governing equations should be differentiated with respect to the chosen parameter (Kleiber, 1997). In the paper, the sensitivity analysis is presented with respect to the value of the internal heat source.

The Boltzmann transport equation for the one-dimensional problem and the constant value of the heat source q_v has the following form (Kałuza *et al.*, 2016; Majchrzak and Mochnacki, 2014; Mochnacki and Majchrzak, 2007; Mohebbi and Sellier, 2016)

$$\frac{\partial e_d(x, t)}{\partial t} + (-1)^{d-1} v \frac{\partial e_d(x, t)}{\partial x} = -\frac{e_d(x, t) - e_d^0(x, t)}{\tau_r} + q_v \quad d = 1, 2 \tag{5.1}$$

with the boundary-initial conditions

$$\begin{aligned}
 x = 0 : \quad & e_1(0, t) = e(T_{b1}) \\
 x = L : \quad & e_2(L, t) = e(T_{b2}) \\
 t = 0 : \quad & e(x, 0) = e(T_0)
 \end{aligned} \tag{5.2}$$

Using the direct approach of sensitivity analysis, equation (5.1) is differentiated with respect to q_v (Jasiński, 2014; Mochnacki and Majchrzak, 2007; Mohebbi and Sellier, 2016)

$$\frac{\partial}{\partial q_v} \left(\frac{\partial e_d(x, t)}{\partial t} \right) + (-1)^{d-1} v \frac{\partial}{\partial q_v} \left(\frac{\partial e_d(x, t)}{\partial x} \right) = -\frac{1}{2\tau_r} \frac{\partial e_d(x, t)}{\partial q_v} + \frac{\partial q_v}{\partial q_v} \quad d = 1, 2 \tag{5.3}$$

Next, differentiation of boundary-initial conditions (5.2) leads to the following formulas

$$\begin{aligned}
 x = 0 : \quad & \frac{\partial e_1(0, t)}{\partial q_v} = \frac{\partial e(T_{b1})}{\partial q_v} = 0 \\
 x = L : \quad & \frac{\partial e_2(L, t)}{\partial q_v} = \frac{\partial e(T_{b2})}{\partial q_v} = 0 \\
 t = 0 : \quad & \frac{\partial e(x, 0)}{\partial q_v} = \frac{\partial e(T_0)}{\partial q_v} = 0
 \end{aligned} \tag{5.4}$$

To equation (5.3) and boundary-initial conditions (5.4), the sensitivity functions $U_d(x, t, q_v) = \partial e_d(x, t)/\partial q_v$ are introduced

$$\begin{aligned} \frac{\partial U_d(x, t, q_v)}{\partial t} + (-1)^{d-1} v \frac{\partial U_d(x, t, q_v)}{\partial x} &= -\frac{1}{2\tau_r} U_d(x, t, q_v) + 1 & d = 1, 2 \\ x = 0 : \quad U_1(0, t, q_v) &= 0 \\ x = L : \quad U_2(L, t, q_v) &= 0 \\ t = 0 : \quad U(x, 0, q_v) &= 0 \end{aligned} \quad (5.5)$$

Then equations (5.3) are the following

$$\frac{\partial U_d(x, t, q_v)}{\partial t} + (-1)^{d-1} v \frac{\partial U_d(x, t, q_v)}{\partial x} = -\frac{U_d(x, t, q_v) - U_d^0(x, t, q_v)}{\tau_r} + 1 \quad d = 1, 2 \quad (5.6)$$

where

$$U_d^0(x, t, q_v) = \frac{\partial e_d^0(x, t)}{\partial q_v} = \frac{\partial}{\partial q_v} \left(\frac{e(x, t)}{2} \right) = \frac{U(x, t, q_v)}{2} \quad (5.7)$$

while

$$U(x, t, q_v) = \sum_{d=1}^2 U_d(x, t, q_v) \quad (5.8)$$

The phonon energy density function $e(x, t, q_v \pm \Delta q_v)$ is expanded into the Taylor series taking into account the first two components according to the formulas

$$\begin{aligned} e(x, t, q_v + \Delta q_v) &\approx e_b(x, t) + \frac{\partial e(x, t)}{\partial q_v} \Delta q_v \\ e(x, t, q_v - \Delta q_v) &\approx e_b(x, t) - \frac{\partial e(x, t)}{\partial q_v} \Delta q_v \end{aligned} \quad (5.9)$$

where Δq_v is a certain increment of the source function, and the starting point $e_b(x, t)$ corresponds to the basic solution.

Taking into account the sensitivity function $U(x, t, q_v) = \partial e(x, t)/\partial q_v$, one obtains

$$\begin{aligned} e(x, t, q_v + \Delta q_v) &\approx e_b(x, t) + U(x, t, q_v) \Delta q_v \\ e(x, t, q_v - \Delta q_v) &\approx e_b(x, t) - U(x, t, q_v) \Delta q_v \end{aligned} \quad (5.10)$$

and a certain increment of the energy function Δe can be calculated using the formula

$$\Delta e(x, t) \approx 2U(x, t, q_v) \Delta q_v \quad (5.11)$$

6. Numerical example

In the paper, heat transfer in a one-dimensional silicon film of dimension $L = 200$ nm has been analyzed. The following input data have been introduced: relaxation time $\tau_r = 6.53$ ps, Debye temperature $\Theta_D = 640$ K, initial temperature $T_0 = 300$ K, boundary conditions $T_{b1} = T_{b2} = 300$ K, lattice distance $\Delta x = 20$ nm and the time step $\Delta t = 5$ ps.

In the first example, the interval value of the heat source function has been considered $\bar{q}_v = [10^{18} - 0.05 \cdot 10^{18}, 10^{18} + 0.05 \cdot 10^{18}]$ W/m³. Figure 2a illustrates the interval heating curves of the phonon energy at the internal nodes 1 (20 nm), 2 (80 nm) and 3 (140 nm).

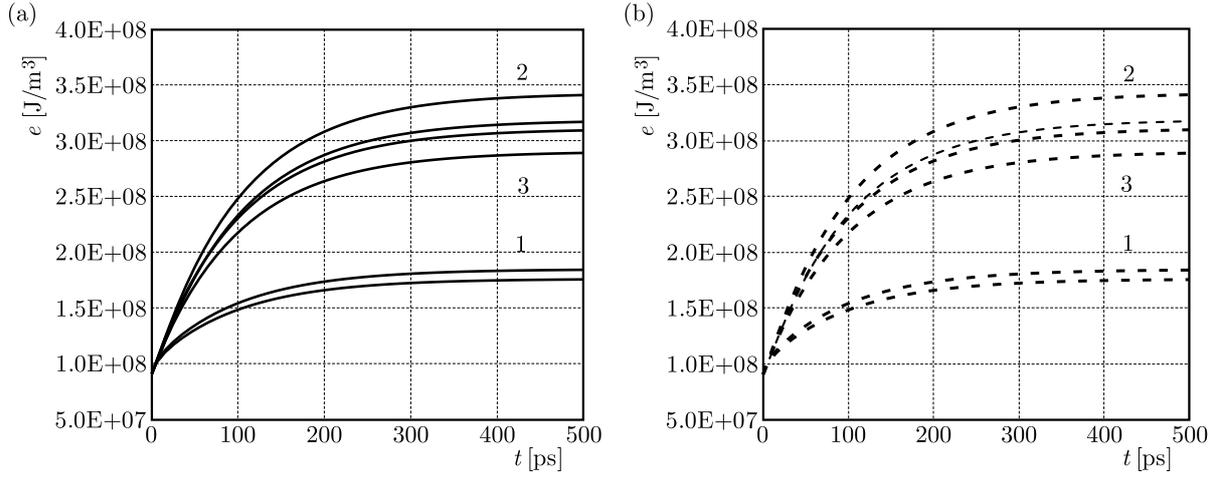


Fig. 2. Energy heating curves: (a) – first method, (b) – second method

In the second example, the no-interval value of the heat source function has been introduced $q_v = 10^{18} \text{ W/m}^3$ and the sensitivity analysis with respect to the heat source parameter has been applied. In this model, an increment of the heat source parameter has been introduced as $\Delta q_v = 0.05 \cdot 10^{18} \text{ W/m}^3$. In Fig. 2b, the courses of heating curves of the phonon energy at the same internal nodes are presented. One can see that the both results are similar.

Figures 3a and 3b present the courses of heating curves taking into account the same internal nodes for the first and second example, respectively.

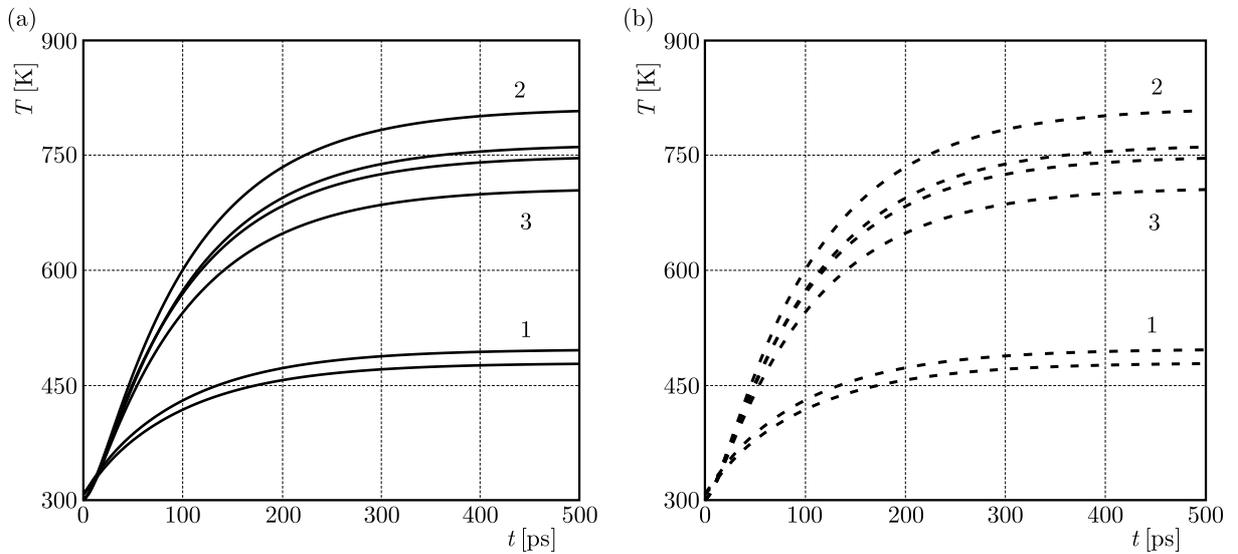


Fig. 3. Temperature heating curves: (a) – first method, (b) – second method

7. Conclusions

In the paper, heat transfer in one-dimensional crystalline solids is considered. The main subject of the paper is the comparison of the results obtained using two methods. In the first method, the interval lattice Boltzmann method with an uncertainly defined internal heat source function is used. The solution to the interval Boltzmann transport equations has been obtained taking into account the rules of directed interval arithmetics. In the second method, the sensitivity

analysis with respect to the internal heat source parameter has been done. The application of the sensitivity functions and the Taylor formula enables one to find a solution similar to the solution received using the interval lattice Boltzmann method.

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