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MODELLING OF TRANSIENT HEAT TRANSPORT IN CRYSTALLINE SOLIDS USING THE INTERVAL LATTICE BOLTZMANN METHOD (TWO-DIMENSIONAL MODEL)

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Abstract. *In the paper the two-dimensional numerical modelling of heat transfer in crystalline solids is considered. In the mathematical description the relaxation time and the boundary conditions 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.*

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

MODELOWANIE PRZEPŁYWU CIEPŁA W DWUWYMIAROWYM CIELE KRYSTALICZNYM ZA POMOCĄ INTERWAŁOWEJ METODY SIATEK BOLTZMANNA

Streszczenie. *W artykule zaprezentowano dwuwymiarowy model numeryczny przepływu ciepła w ciele krystalicznym. W opisie matematycznym czas relaksacji i warunki brzegowe są zdefiniowane jako liczby przedziałowe. Sformułowane zagadnienie rozwiązano za pomocą interwałowej metody siatek Boltzmanna stosując skierowaną arytmetykę interwałową.*

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

Introduction

In dielectric materials and also semiconductors the heat transport is mainly realized by quanta of lattice vibrations called phonons. Phonons always "move" from the part with the higher temperature to the part with the lower temperature. During this process phonons carry energy. This phenomena can be described by the Boltzmann transport equation transformed in the phonon energy density [4].

Such approach in which the parameters appearing in the problem analyzed are treated as constant values is widely used. Here, in the mathematical model describing the heat transfer in a thin silicon film the interval values of relaxation time and boundary conditions have been assumed.

The problem analyzed has been solved using an interval version of the lattice Boltzmann method using the rules of directed interval arithmetic.

1. Directed interval arithmetic

Let us consider a directed interval $\bar{a}$ which can be defined as a set $\mathbf{D}$ of all directed pairs of real numbers defined as [3, 6]

$$\bar{a} = \left[a^-,\, a^+\right] := \left\{\bar{a} \in \mathbf{D} \,\middle|\, a^-,\, a^+ \in \mathbf{R}\right\} \tag{1}$$

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 follows

$$\begin{aligned} &++ = -- = + \\ &+- = -+ = - \end{aligned} \tag{2}$$

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

Additionally a subset $\mathbf{Z} = \mathbf{Z_P} \cup \mathbf{Z_I} \in \mathbf{D}$ should be defined, where

$$\begin{aligned} \mathbf{Z_P} &= \left\{\bar{a} \in \mathbf{P} \middle| a^- \le 0 \le a^+\right\} \\ \mathbf{Z_I} &= \left\{\bar{a} \in \mathbf{I} \middle| a^+ \le 0 \le a^-\right\} \end{aligned} \tag{3}$$

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

$$\tau(\bar{a}) = \begin{cases} +, & if \;\; a^- \le a^+ \\ -, & if \;\; a^- > a^+ \end{cases} \tag{4}$$

and the other is the sign variable

$$\sigma(\bar{a}) = \begin{cases} +, & if \;\; a^- > 0,\, a^+ > 0 \\ -, & if \;\; a^- < 0,\, a^+ < 0 \end{cases}, \qquad \bar{a} \in \mathbf{D} \setminus \mathbf{Z} \tag{5}$$

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

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

$$\bar{a} + \bar{b} = \left[a^- + b^-,\, a^+ + b^+\right], \quad \bar{a},\, \bar{b} \in \mathbf{D} \tag{6}$$

The difference is of the form

$$\bar{a} - \bar{b} = \left[a^- - b^+,\, a^+ - b^-\right], \quad \bar{a},\, \bar{b} \in \mathbf{D} \tag{7}$$

The product of the directed intervals is described by the formula

$$\bar{a} \cdot \bar{b} = \begin{cases} \left[a^{-\sigma(\bar{b})} \cdot b^{-\sigma(\bar{a})},\, a^{\sigma(\bar{b})} \cdot b^{\sigma(\bar{a})}\right] & \bar{a},\, \bar{b} \in \mathbf{D} \setminus \mathbf{Z} \\ \left[a^{\sigma(\bar{a})\tau(\bar{b})} \cdot b^{-\sigma(\bar{a})},\, a^{\sigma(\bar{a})\tau(\bar{b})} \cdot b^{\sigma(\bar{a})}\right], & \bar{a} \in \mathbf{D} \setminus \mathbf{Z},\, \bar{b} \in \mathbf{Z} \\ \left[a^{-\sigma(\bar{b})} \cdot b^{\sigma(\bar{b})\tau(\bar{a})},\, a^{\sigma(\bar{b})} \cdot b^{\sigma(\bar{b})\tau(\bar{a})}\right], & \bar{a} \in \mathbf{Z},\, \bar{b} \in \mathbf{D} \setminus \mathbf{Z} \\ \left[\min\left(a^- \cdot b^+, a^+ \cdot b^-\right), \max\left(a^- \cdot b^-, a^+ \cdot b^+\right)\right], & \bar{a},\, \bar{b} \in \mathbf{Z_P} \\ \left[\max\left(a^- \cdot b^-, a^+ \cdot b^+\right), \min\left(a^- \cdot b^+, a^+ \cdot b^-\right)\right], & \bar{a},\, \bar{b} \in \mathbf{Z_I} \\ 0, & \left(\bar{a} \in \mathbf{Z_P},\, \bar{b} \in \mathbf{Z_I}\right) \cup \left(\bar{a} \in \mathbf{Z_I},\, \bar{b} \in \mathbf{Z_P}\right) \end{cases} \tag{8}$$

The quotient of two directed intervals can be written using the formula

$$\bar{a} / \bar{b} = \begin{cases} \left[a^{-\sigma(\bar{b})} / b^{\sigma(\bar{a})},\, a^{\sigma(\bar{b})} / b^{-\sigma(\bar{a})}\right], & \bar{a},\, \bar{b} \in \mathbf{D} \setminus \mathbf{Z} \\ \left[a^{-\sigma(\bar{b})} / b^{-\sigma(\bar{b})\tau(\bar{a})},\, a^{\sigma(\bar{b})} / b^{-\sigma(\bar{b})\tau(\bar{a})}\right], & \bar{a} \in \mathbf{Z},\, \bar{b} \in \mathbf{D} \setminus \mathbf{Z} \end{cases} \tag{9}$$

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

$$-_{\mathbf{D}}\, \bar{a} = \left[-a^-,\, -a^+\right], \quad \bar{a} \in \mathbf{D} \tag{10}$$

and inversion of multiplication

$$1/_{\mathbf{D}}\, \bar{a} = \left[1/a^-,\, 1/a^+\right], \quad \bar{a} \in \mathbf{D} \setminus \mathbf{Z} \tag{11}$$

So, two additional mathematical operations can be defined as follows

$$\bar{a} -_{\mathbf{D}} \bar{b} = \left[a^- - b^-,\ a^+ - b^+ \right], \quad \bar{a}, \bar{b} \in \mathbf{D} \tag{12}$$

and

$$\bar{a} /_{\mathbf{D}} \bar{b} = \begin{cases} \left[a^{-\sigma(\bar{b})} / b^{-\sigma(\bar{a})},\ a^{\sigma(\bar{b})} / b^{\sigma(\bar{a})} \right], & \bar{a}, \bar{b} \in \mathbf{D} \setminus \mathbf{Z} \\ \left[a^{-\sigma(\bar{b})} / b^{\sigma(\bar{b})},\ a^{\sigma(\bar{b})} / b^{\sigma(\bar{b})} \right], & \bar{a} \in \mathbf{Z}, \bar{b} \in \mathbf{D} \setminus \mathbf{Z} \end{cases} \tag{13}$$

Now, it is possible to obtain the number zero by subtraction of two identical intervals $\bar{a} -_{\mathbf{D}} \bar{a} = 0$ and the number one as the result of the division $\bar{a} /_{\mathbf{D}} \bar{a} = 1$, which was impossible when applying classical interval arithmetic [5].

2. Boltzmann transport equation

One of the fundamental equations of solid state physic is the Boltzmann transport equation (BTE) which takes the following form [1, 2]

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = \frac{f^0 - f}{\tau_r} + g_{ef} \tag{14}$$

where f is the phonon distribution function, f^0 is the equilibrium distribution function given by the Bose-Einstein statistic, $\mathbf{v}$ 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 to an equation on carrier energy density of the form [1]

$$\frac{\partial e}{\partial t} + \mathbf{v} \cdot \nabla e = -\frac{e - e^0}{\tau_r} + q_v \tag{15}$$

where e is the phonon energy density, e^0 is the equilibrium phonon energy density and q_v is the internal heat generation rate related to an unit of volume. The equation (15) must be supplemented by the boundary initial conditions.

Using the Debye model the relation between phonon energy density and lattice temperature is given by

$$e(T) = \left(\frac{9\eta\, k_b}{\Theta_D^3} \int_0^{\Theta_D/T} \frac{z^3}{\exp(z) - 1} \mathrm{d}z \right) T^4 \tag{16}$$

where Θ_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 oscillators and can be calculated using the formula

$$\eta = \frac{1}{6\pi^2} \left(\frac{k_b \Theta_D}{\hbar\,\omega} \right)^3 \tag{17}$$

where $\hbar$ is the Planck constant divided by 2π and ω is the phonon frequency.

3. Interval lattice Boltzmann method

The interval lattice Boltzmann method (ILBM) is a discrete representation of the Boltzmann transport equation. For two-dimensional problems the interval Boltzmann transport equation can be written as

$$\frac{\partial \bar{e}}{\partial t} + \mathbf{v} \cdot \nabla \bar{e} = -\frac{\bar{e} - \bar{e}^0}{\bar{\tau}_r} + q_v \tag{18}$$

where $\bar{e}$ is the interval phonon energy density, $\bar{e}^0$ is the interval equilibrium phonon energy density, $\mathbf{v}$ is the phonon group velocity, q_v is the internal heat generation rate related to an unit of volume and $\bar{\tau}_r = \left[\tau_r^-,\ \tau_r^+ \right]$ is the interval relaxation time.

For two-dimensional model the discrete phonon velocities are expressed as [2]

$$\boldsymbol{c}_d = \begin{cases} (0,0) & d = 0 \\ \left(\cos\left[(2d-1)\pi/2\right],\ \sin\left[(2d-1)\pi/2\right] \right) c & d = 1,\ldots,4 \end{cases} \tag{19}$$

where $c = \Delta x / \Delta t = \Delta y / \Delta t$ is the lattice speed, Δx and Δy are the lattice distances 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 d is the direction.

The interval lattice Boltzmann method algorithm has been used to solve the problem analyzed [1, 7].

The ILBM discretizes the space domain considered by defining lattice sites where the phonon energy density is calculated.

The lattice is a network of discrete points arranged in a regular mesh with phonons located in lattice sites. Phonons can travel only to neighboring lattice sites by ballistically traveling with the certain velocity and collide with other phonons residing at these sites according to Fig. 1 [1].

The discrete set of propagation velocities in the main lattice directions can be defined as (see eq. 19)

$$\begin{gathered} \boldsymbol{c}_0 = (0,\ 0) \quad \boldsymbol{c}_1 = (c,\ 0) \quad \boldsymbol{c}_2 = (0,\ c) \\ \boldsymbol{c}_3 = (-c,\ 0) \quad \boldsymbol{c}_4 = (0, -c) \end{gathered} \tag{20}$$

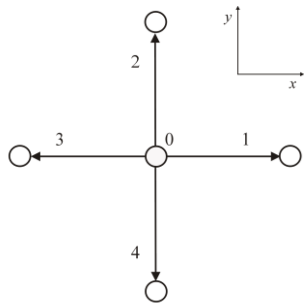

Fig. 1. Two dimensional 5-speed (D2Q5) lattice Boltzmann model

In the ILBM it is needed to solve five equations allowing to compute phonon energy in different lattice nodes according to the following equations

$$\begin{aligned} &\frac{\partial \bar{e}_0}{\partial t} = -\frac{\bar{e}_0 - \bar{e}_0{}^0}{\left[\tau_r^-,\ \tau_r^+\right]} + q_v \\ &\frac{\partial \bar{e}_1}{\partial t} + c\frac{\partial \bar{e}_1}{\partial x} = -\frac{\bar{e}_1 - \bar{e}_1{}^0}{\left[\tau_r^-,\ \tau_r^+\right]} + q_v \\ &\frac{\partial \bar{e}_2}{\partial t} + c\frac{\partial \bar{e}_2}{\partial y} = -\frac{\bar{e}_2 - \bar{e}_2{}^0}{\left[\tau_r^-,\ \tau_r^+\right]} + q_v \\ &\frac{\partial \bar{e}_3}{\partial t} - c\frac{\partial \bar{e}_3}{\partial x} = -\frac{\bar{e}_3 - \bar{e}_3{}^0}{\left[\tau_r^-,\ \tau_r^+\right]} + q_v \\ &\frac{\partial \bar{e}_4}{\partial t} - c\frac{\partial \bar{e}_4}{\partial y} = -\frac{\bar{e}_4 - \bar{e}_4{}^0}{\left[\tau_r^-,\ \tau_r^+\right]} + q_v \end{aligned} \tag{21}$$

The set of equations (21) must be supplemented by the boundary conditions

$$\begin{cases} x = 0,\ 0 \le y \le L: & \bar{e}(0,\ y,\ t) = \bar{e}\left(\bar{T}_{b1}\right) \\ x = L,\ 0 \le y \le L: & \bar{e}(L,\ y, t) = \bar{e}\left(\bar{T}_{b2}\right) \\ y = 0,\ 0 < x < L: & \bar{e}(x,\ 0,\ t) = \bar{e}\left(\bar{T}_{b3}\right) \\ y = L,\ 0 < x < L: & \bar{e}(x,\ L,\ t) = \bar{e}\left(\bar{T}_{b4}\right) \end{cases} \tag{22}$$

and the initial condition

$$t = 0: \quad \bar{e}(x,\ y,\ 0) = \bar{e}(T_0) \tag{23}$$

where $\bar{T}_{b1} = [T_{b1}^-, T_{b1}^+]$, $\bar{T}_{b2} = [T_{b2}^-, T_{b2}^+]$, $\bar{T}_{b3} = [T_{b3}^-, T_{b3}^+]$ and $\bar{T}_{b4} = [T_{b4}^-, T_{b4}^+]$ are the interval boundary temperatures, T_0 is the initial temperature.

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

$$\frac{\partial \bar{e}_i}{\partial t} = \frac{\bar{e}_i(x,\, y,\, t+\Delta t) - \bar{e}_i(x,\, y,\, t)}{\Delta t} \qquad \text{i} = 0, 1, ..., 4 \tag{24}$$

and

$$\begin{aligned}
\frac{\partial \bar{e}_1}{\partial x} &= \frac{\bar{e}_1(x+\Delta x,\, y,\, t+\Delta t) - \bar{e}_1(x,\, y,\, t+\Delta t)}{\Delta x} \\
\frac{\partial \bar{e}_2}{\partial y} &= \frac{\bar{e}_2(x,\, y+\Delta y,\, t+\Delta t) - \bar{e}_2(x,\, y,\, t+\Delta t)}{\Delta y} \\
\frac{\partial \bar{e}_3}{\partial x} &= \frac{\bar{e}_3(x,\, y,\, t+\Delta t) - \bar{e}_3(x-\Delta x,\, y,\, t+\Delta t)}{\Delta x} \\
\frac{\partial \bar{e}_4}{\partial y} &= \frac{\bar{e}_4(x,\, y,\, t+\Delta t) - \bar{e}_4(x,\, y-\Delta y,\, t+\Delta t)}{\Delta y}
\end{aligned} \tag{25}$$

Thus one obtains the approximate form of the interval Boltzmann transport equations for 2D problem in five directions of the lattice [1, 2]

$$\begin{cases}
\left(\bar{e}_0\right)^{f+1}_{i,\,j} = \left(1-\Delta t/\bar{\tau}_r\right)\left(\bar{e}_0\right)^{f}_{i,\,j} + \Delta t/\bar{\tau}_r \cdot \left(\bar{e}^0_0\right)^{f}_{i,\,j} + \Delta t\, q_v \\
\left(\bar{e}_1\right)^{f+1}_{i+1,\,j} = \left(1-\Delta t/\bar{\tau}_r\right)\left(\bar{e}_1\right)^{f}_{i,\,j} + \Delta t/\bar{\tau}_r \cdot \left(\bar{e}^0_1\right)^{f}_{i,\,j} + \Delta t\, q_v \\
\left(\bar{e}_2\right)^{f+1}_{i,\,j+1} = \left(1-\Delta t/\bar{\tau}_r\right)\left(\bar{e}_2\right)^{f}_{i,\,j} + \Delta t/\bar{\tau}_r \cdot \left(\bar{e}^0_2\right)^{f}_{i,\,j} + \Delta t\, q_v \\
\left(\bar{e}_3\right)^{f+1}_{i-1,\,j} = \left(1-\Delta t/\bar{\tau}_r\right)\left(\bar{e}_3\right)^{f}_{i,\,j} + \Delta t/\bar{\tau}_r \cdot \left(\bar{e}^0_3\right)^{f}_{i,\,j} + \Delta t\, q_v \\
\left(\bar{e}_4\right)^{f+1}_{i,\,j-1} = \left(1-\Delta t/\bar{\tau}_r\right)\left(\bar{e}_4\right)^{f}_{i,\,j} + \Delta t/\bar{\tau}_r \cdot \left(\bar{e}^0_4\right)^{f}_{i,\,j} + \Delta t\, q_v
\end{cases} \tag{26}$$

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

$$\bar{e} = \sum_{d=0}^{4} \bar{e}_d \tag{27}$$

After subsequent computations the lattice temperature is determined using the formula

$$\bar{T}^{\,f+1} = \sqrt[4]{\bar{e}(\bar{T}^{\,f})\,\Theta_D^3 \Bigg/ \left(9\eta\, k_b \int\limits_0^{\Theta_D/\bar{T}^{f}} \frac{z^3}{\exp(z)-1}\,\mathrm{d}z\right)} \tag{28}$$

4. Results of computations

As a numerical example the heat transport in a silicon thin film of the dimensions 200 nm × 200 nm has been analyzed. The following input data have been introduced: the relaxation time $\bar{\tau}_r = [6.36675,\, 6.69325]\,\text{ps}$, the Debye temperature $\Theta_D = 640\,\text{K}$, the boundary conditions $\bar{T}_{b1} = [780,\, 820]\,\text{K}$ and $\bar{T}_{b2} = \bar{T}_{b3} = \bar{T}_{b4} = [292.5,\, 307.5]\,\text{K}$, the initial temperature $T_0 = 300\,\text{K}$. The lattice step $\Delta x = \Delta y = 20\,\text{nm}$ and the time step $\Delta t = 5\,\text{ps}$ have been assumed.

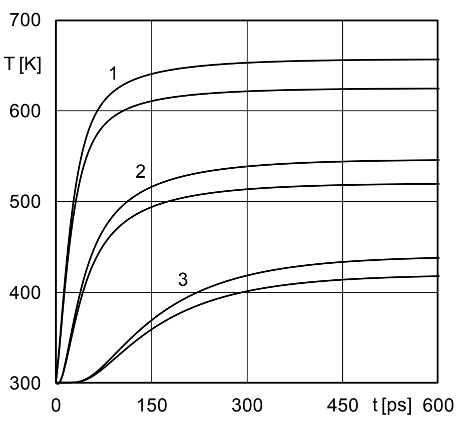

Fig. 2. The interval heating curves at internal nodes for q_v=0

Figure 2 presents the courses of the temperature function at the internal nodes (40, 20) – 1, (160, 40) – 2 and (100, 100) – 3 for the heat source $q_v = 0$. Figure 3 shows the courses of the temperature function at the same nodes like in Fig. 2 but for the heat source $q_v = 10^{18}$ W/m^3.

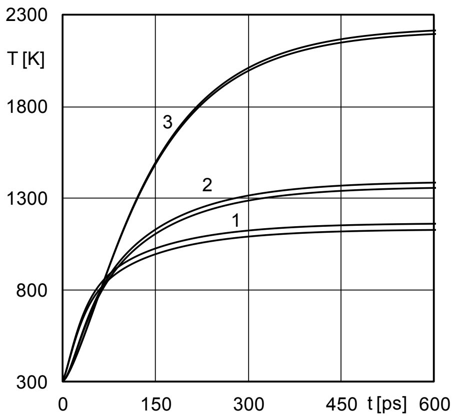

Fig. 3. The interval heating curves at internal nodes for q_v=10^{18}W/m^3

5. Conclusions

In the paper the Boltzmann transport equation with the interval values of the relaxation time and the boundary conditions has been considered. The interval version of the lattice Boltzmann method for solving 2D problems has been presented. The generalization of LBM 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.

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