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THE INTERVAL LATTICE BOLTZMANN METHOD FOR TRANSIENT HEAT TRANSFER IN A SILICON THIN FILM

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Abstract In this paper the numerical modelling of heat transfer in a two-dimensional crystalline solid is considered. It is assumed that some parameters (the relaxation time and the boundary conditions) appearing in the mathematical model of the problem analyzed are given as interval numbers. The problem discussed has been solved using the interval form of the lattice Boltzmann method using the rules of the directed interval arithmetic [2].

Keywords: interval lattice Boltzmann method, directed interval arithmetic, heat transport.
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1. INTRODUCTION

Microscale heat transfer is a new field of study which arises from the need to understand the mechanisms of the energy transport in thin films. Microscale heat transfer can be defined as the study of thermal energy transfer with taking into account individual carriers. The classical diffusion-based model for transient heat transfer cannot be used for analyzing small length scale. In semiconductors and dielectric materials, the heat transfer is carried mainly by vibrations in the crystal lattice called phonons. The more common method to analyze this kind of phenomena is the application of the Boltzmann transport equation.

In the mathematical model describing this process some parameters as the relaxation time are estimated experimentally, so it seems natural to take the values of these parameters as interval numbers [5]. This assumption is closer to the real physical conditions of the problem analyzed. In the paper the interval lattice Boltzmann method for solving non-steady transient heat transfer with interval thermophysical parameters has been presented.

2. DIRECTED INTERVAL ARITHMETIC

Let us consider a directed interval $\bar{a}$ which can be defined as a set D of all directed pairs of real numbers defined as

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

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

$$\begin{array}{c} + \ + \ = \ - \ - \ = \ + \\ + \ - \ = \ - \ + \ = \ - \end{array}$$

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 $D = P \cup I$, where P denotes a set of all directed proper intervals and I denotes a set of all improper intervals. Additionally a subset $Z = Z_P \cup Z_I \in D$ should be defined, where

$$\begin{array}{l} Z_P = \{\bar{a} \in\ P | \, a^- \le 0 \le a^+\} \\ Z_I = \{\bar{a} \in\ I | \, a^+ \le 0 \le a^-\} \end{array}$$

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

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

and the other is the sign variable

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

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

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

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

The difference is of the form

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

The product of the directed intervals is described by the formula

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

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

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

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

$$-_D\bar{a} = \left[-a^-,\ -a^+\right], \quad \bar{a} \in D$$

and inversion of multiplication

$$1/_D\bar{a} = \left[1/a^-,\ 1/a^+\right], \quad \bar{a} \in D\backslash Z$$

So, two additional mathematical operations can be defined as follows

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

and

$$\bar{a}/_D\bar{b} = \begin{cases} \left[a^{-\sigma(\bar{b})}/b^{-\sigma(\bar{a})},\ a^{\sigma(\bar{b})}/b^{\sigma(\bar{a})}\right], & \bar{a},\ \bar{b} \in D\backslash Z \\ \left[a^{-\sigma(\bar{b})}/b^{\sigma(\bar{b})},\ a^{\sigma(\bar{b})}/b^{\sigma(\bar{b})}\right], & \bar{a} \in Z,\ \bar{b} \in D\backslash Z \end{cases}$$

Now, it is possible to obtain the number zero by subtraction of two identical intervals $\bar{a} -_D \bar{a} = 0$ and the number one as the result of the division $\bar{a}/_D\bar{a} = 1$, which was impossible when applying classical interval arithmetic [2].

3. THE INTERVAL LATTICE BOLTZMANN METHOD

In dielectric materials and 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 process can be described by the Boltzmann transport equation (BTE)

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

where f is the phonon distribution function, f^0 is the equilibrium distribution function given by the Bose-Einstein statistic, **v** is the frequency-dependent phonon propagation speed, τ_r is the frequency-dependent phonon relaxation time and g_{ef} is the phonon generation rate due to electron-phonon scattering.

The BTE is one of the fundamental equations of solid state physics. In order to take advantage of the simplifying assumption of the Debye model, the Boltzmann

transport equation can be transformed to an equivalent phonon energy density equation [1]

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

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. This equation must be supplemented by the adequate boundary-initial conditions.

The dependence between phonon energy and lattice temperature can be calculated from the following formula using the Debye model

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

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.

The interval lattice Boltzmann method (ILBM) is a discrete representation of the interval Boltzmann transport equation [6]. 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.

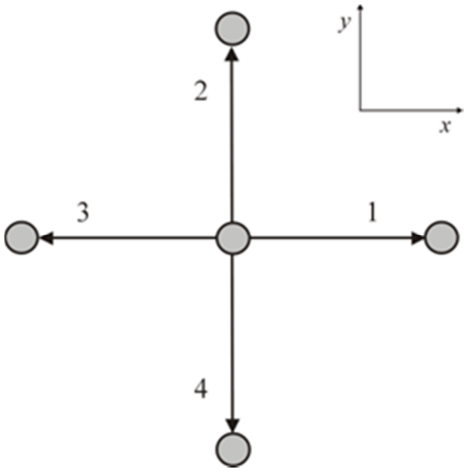

Fig. 1. Two dimensional 4-speed (D2Q4) lattice Boltzmann model

There are a few possibilities for spatial position of the particles. In the paper the D2Q4 lattice, which has two dimensions and four velocities, has been applied. Phonons can travel only to neighboring lattice sites by ballistically travelling with a certain velocity and collide with other phonons residing at these sites (see Fig. 1).

The discrete set of propagation velocities in the main lattice directions can be defined as

$$c_1 = (c, 0) \quad c_2 = (0, c) \quad c_3 = (-c,\ 0) \quad c_4 = (0, -c)$$

In the ILBM it is needed to solve four interval equations supplemented by the boundary and initial conditions allowing to compute interval phonon energy in different lattice nodes. The interval Boltzmann transport equations for a two-dimensional problem take the following form [1, 3, 4]

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

This set of equations must be supplemented by the boundary conditions

$$\begin{cases}
x = 0, & 0 \le y \le L: \quad \overline{e}(0, y, t) = \overline{e}(\overline{T}_{b1}) \\
x = L, & 0 \le y \le L: \quad \overline{e}(L, y, t) = \overline{e}(\overline{T}_{b2}) \\
y = 0, & 0 \le x \le L: \quad \overline{e}(x, 0, t) = \overline{e}(\overline{T}_{b3}) \\
y = L, & 0 \le x \le L: \quad \overline{e}(x, L, t) = \overline{e}(\overline{T}_{b4})
\end{cases}$$

and the initial condition of the following form

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

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

$$\bar{e} = \sum_{d=1}^{4} \bar{e}_d$$

After subsequent computations the interval lattice temperature is determined using the formula describing the relation between interval phonon energy and interval lattice temperature

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

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 $\bar{\tau}_r = [6.36675,\ 6.69325]$ ps, the Debye temperature $\Theta_D = 640$ K, the boundary conditions $\bar{T}_{b1} = [780,\ 820]$ K and $\bar{T}_{b2} = \bar{T}_{b3} = \bar{T}_{b4} = [292.5,\ 307.5]$ K, the initial temperature $T_0 = 300$ K. The lattice step $\Delta x = \Delta y = 20$ nm and the time step $\Delta t = 5$ ps have been assumed.
Calculations were carry out at the three internal nodes (40, 20) - 1, (160, 40) - 2 and (100, 100) - 3 (see fig. 2).

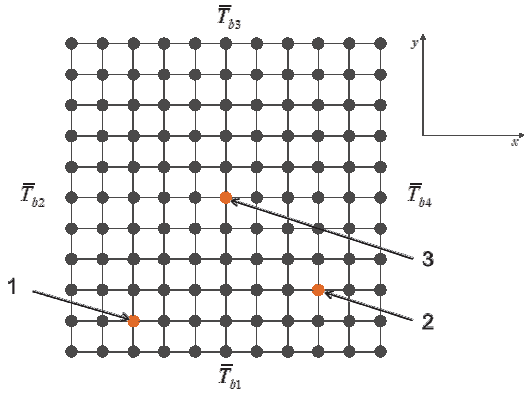

Fig. 2. Discretized domain

Figures 3 and 4 present the courses of the temperature function at chosen internal nodes for the heat source $q_v = 0$ and $q_v = 10^{18}$ W/m^3 respectively.

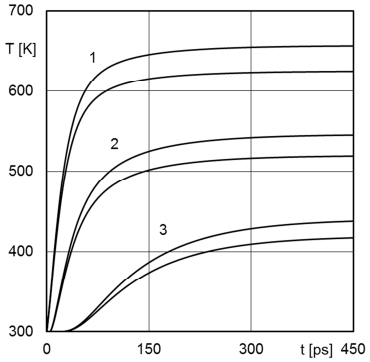

Fig. 3. The interval heating curves for $q_v = 0$

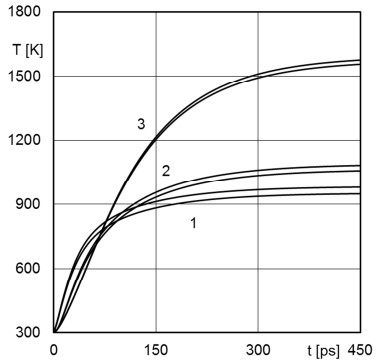

Fig. 4. The interval heating curves for $q_v = 10^{18}\ W/m^3$

5. CONCLUSIONS

The interval lattice Boltzmann method is an effective tool to numerical simulation of the heat transfer in crystalline solids. 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. In the paper the Boltzmann transport equation with the interval values of the relaxation time and the boundary conditions has been considered.

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