MODELLING OF TRANSIENT HEAT TRANSPORT IN TWO-LAYERED CRYSTALLINE SOLID FILMS USING THE INTERVAL LATTICE BOLTZMANN METHOD

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Abstract. In the paper, the numerical modelling of heat transfer in one-dimensional crystalline solid films is considered. A generalized two-layer problem is described by the Boltzmann transport equations transformed in the phonon energy density equations supplemented by the adequate boundary-initial conditions. Such an approach in which the parameters appearing in the problem analysed are treated as the constant values is widely used, but in this paper the interval values of relaxation time and the boundary condition for silicon and diamond are taken into account. The problem formulated has been solved by means of the interval lattice Boltzmann method using the rules of directed interval arithmetic. In the final part of the paper the results of numerical computations are presented.

1. Introduction

In dielectric materials and semiconductors, the heat transport is mainly realized by a quanta of lattice vibrations called phonons. The phonons represent the conduction of heat and electricity through solids. In non-metals, phonons as heat carriers always "move" from the part with the higher temperature to the part with the lower temperature and, during this move, phonons carry energy. This kind of phenomena can be described by the Boltzmann transport equation (BTE). It should be pointed out that taking into account the extremely short duration and the domain dimensions expressed in nanometers, the macroscopic heat conduction equation based on the Fourier law cannot be used [1, 2]. Such an approach in which the parameters appearing in the mathematical model are treated as the constant values is widely used [3, 4]. Here, the interval values of relaxation times and boundary conditions

for successive sub-domains are taken into account. The relaxation time is estimated experimentally, and its actual value is still a subject of discussion [5]. In the paper the heat transport proceeding in a two-layered thin film is considered [6-9]. To solve the problem formulated, the interval version of the lattice Boltzmann method is applied using the rules of directed interval arithmetic [10, 11]. In the final part of the paper the examples of numerical computations are shown.

2. Boltzmann transport equation

The unsteady BTE in a phonon energy density formulation using the simplifying assumptions of the Debye model for one-dimensional two-layered analysis [3, 12] can be written as

$$\frac{\partial e_s}{\partial t} + \mathbf{v}_s \cdot \nabla e_s = -\frac{e_s - e_s^0}{\tau_{rs}} + q_{vs} \tag{1}$$

where $s = 1, 2$ corresponds to the successive layers of the thin film (silicon, diamond), e_s is the phonon energy density, e_s^0 is the equilibrium phonon energy density, $\mathbf{v}_s$ is the frequency-dependent phonon propagation speed, τ_{rs} is the frequency-dependent phonon relaxation time, t denotes the time and q_{vs} is the external heat generation rate related to a unit of volume.

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

$$e_s(T) = \left(\frac{9\eta_s k_b}{\Theta_{Ds}^3} \int_0^{\Theta_{Ds}/T_s} \frac{z^3}{\exp(z)-1} \mathrm{d}z \right) T_s^4 \tag{2}$$

where Θ_{Ds} is the Debye temperature of the solid, k_b is the Boltzmann constant, T_s is the lattice temperature while η_s is the number density of oscillators [3].

The equations (1) should be supplemented by the boundary and initial conditions.

3. Interval lattice Boltzmann equation

The lattice Boltzmann method (LBM) is a numerical technique for the simulation of heat transfer. The LBM solves a discretized set of the BTE known as the lattice Boltzmann equations. The phonon energy density is defined as the sum

$$\overline{e}_s(x, t) = \overline{e}_{1s}(x, t) + \overline{e}_{2s}(x, t) = \sum_{d=1}^{2} \overline{e}_{ds}(x, t) \tag{3}$$

where e_{1s} is the phonon energy density in the positive x direction for s^{th} layer while e_{2s} is the phonon energy density in the negative x direction and d signifies the lattice direction.

The interval Boltzmann transport equations for the one-dimensional problem take the form [13]

$$\frac{\partial \overline{e}_{ds}}{\partial t} + v \frac{\partial \overline{e}_{ds}}{\partial x} = -\frac{\overline{e}_{ds} - \overline{e}_{ds}^{\;0}}{\left[\tau_{rs}^-, \tau_{rs}^+ \right]} + \overline{q}_{vs} \tag{4}$$

where $v_s = \Delta x_s / \Delta t$ is the component of velocity along the x-axis, Δx_s 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, $\overline{\tau}_{rs} = \left[\tau_{rs}^-, \tau_{rs}^+ \right]$ is the interval relaxation time and $\overline{e}_{ds}^{\;0} = \overline{e}_s(x, t)/d$.

The set of equations (4) must be supplemented by the boundary-initial conditions [6, 9]

$$\begin{cases} x = 0: & \overline{e}_{11}(0, t) = \overline{e}_1(\overline{T}_{b1}) \\ x = L: & \overline{e}_{22}(L, t) = \overline{e}_2(\overline{T}_{b2}) \\ t = 0: & e_s(x, 0) = e_s(T_{0s}) \end{cases} \tag{5}$$

where $\overline{T}_{b1}$ and $\overline{T}_{b2}$ are the interval boundary temperatures and T_{0s} is the initial temperature. Between the successive sub-domains the continuity condition can be taken into account [9]

$$x = L/2: \;\; \overline{e}_1(x, t) = \overline{e}_2(x, t) \tag{6}$$

The interval LBM algorithm has been used to solve the problem analysed [6, 10]. The approximate form of the equations (4) is of the following form

$$\begin{cases} \left(\overline{e}_{1s} \right)_{i+1}^{f+1} = \left(1 - \Delta t / \overline{\tau}_{rs} \right) \left(\overline{e}_{1s} \right)_i^f + \Delta t / \overline{\tau}_{rs} \cdot \left(\overline{e}_{1s}^{\;0} \right)_i^f + \Delta t \, \overline{q}_{vs} \\ \left(\overline{e}_{2s} \right)_{i-1}^{f+1} = \left(1 - \Delta t / \overline{\tau}_{rs} \right) \left(\overline{e}_{2s} \right)_i^f + \Delta t / \overline{\tau}_{rs} \cdot \left(\overline{e}_{2s}^{\;0} \right)_i^f + \Delta t \, \overline{q}_{vs} \end{cases} \tag{7}$$

Taking into account the assumption that

$$\overline{a} /_{\mathbf{D}} \overline{b} = \begin{cases} \left[a^{-\sigma(\overline{b})} / b^{-\sigma(\overline{a})}, \, a^{\sigma(\overline{b})} / b^{\sigma(\overline{a})} \right], & \overline{a}, \overline{b} \in \mathbf{D} \setminus \mathbf{Z} \\ \left[a^{-\sigma(\overline{b})} / b^{\sigma(\overline{b})}, \, a^{\sigma(\overline{b})} / b^{\sigma(\overline{b})} \right], & \overline{a} \in \mathbf{Z}, \, \overline{b} \in \mathbf{D} \setminus \mathbf{Z} \end{cases} \tag{8}$$

and

$$
\overline{a} \cdot \overline{b} =
\begin{cases}
\left[a^{-\sigma(\overline{b})} \cdot b^{-\sigma(\overline{a})},\, a^{\sigma(\overline{b})} \cdot b^{\sigma(\overline{a})} \right] & \overline{a}, \overline{b} \in \mathbf{D} \setminus \mathbf{Z} \\[2mm]
\left[a^{\sigma(\overline{a})\tau(\overline{b})} \cdot b^{-\sigma(\overline{a})},\, a^{\sigma(\overline{a})\tau(\overline{b})} \cdot b^{\sigma(\overline{a})} \right], & \overline{a} \in \mathbf{D} \setminus \mathbf{Z}, \overline{b} \in \mathbf{Z} \\[2mm]
\left[a^{-\sigma(\overline{b})} \cdot b^{\sigma(\overline{b})\tau(\overline{a})},\, a^{\sigma(\overline{b})} \cdot b^{\sigma(\overline{b})\tau(\overline{a})} \right], & \overline{a} \in \mathbf{Z}, \overline{b} \in \mathbf{D} \setminus \mathbf{Z} \\[2mm]
\left[\min\left(a^- \cdot b^+, a^+ \cdot b^- \right), \max\left(a^- \cdot b^-, a^+ \cdot b^+ \right) \right], & \overline{a}, \overline{b} \in \mathbf{Z_P} \\[2mm]
\left[\max\left(a^- \cdot b^-, a^+ \cdot b^+ \right), \min\left(a^- \cdot b^+, a^+ \cdot b^- \right) \right], & \overline{a}, \overline{b} \in \mathbf{Z_I} \\[2mm]
0, & \left(\overline{a} \in \mathbf{Z_P}, \overline{b} \in \mathbf{Z_I} \right) \text{ or } \left(\overline{a} \in \mathbf{Z_I}, \overline{b} \in \mathbf{Z_P} \right)
\end{cases}
\tag{9}
$$

the product $\Delta t / \overline{\tau}_{rs} \cdot \left(\overline{e}_{1s}{}^0 \right)_i^f$ ($s = 1$, $i = 3$, $f = 4$) is calculated using the rules of directed interval arithmetic according to the following formula

$$
\Delta t / \overline{\tau}_{rs} \cdot \left(\overline{e}_{1s}{}^0 \right)_i^f = \left([5,\, 5] / [6.37,\, 6.69] \right) \cdot \left[1.49 \cdot 10^8,\, 1.53 \cdot 10^8 \right] =
$$
$$
\left[0.78,\, 0.75 \right] \cdot \left[1.49 \cdot 10^8,\, 1.53 \cdot 10^8 \right] = \left[1.16 \cdot 10^8,\, 1.15 \cdot 10^8 \right]
\tag{10}
$$

As a result, the interval obtained is improper.

After subsequent computations the interval lattice temperature is determined using the formula (see eq. (2))

$$
\overline{T}_s^{f+1} = \sqrt[4]{ \overline{e}_s(\overline{T}^f) \Theta_{Ds}^3 \Big/ \left(9\eta_s k_b \int_0^{\Theta_{Ds}/\overline{T}_s^f} \frac{z^3}{\exp(z) - 1} \, dz \right) }
\tag{11}
$$

4. Results of computations

As a numerical example, the heat transport in a silicon-diamond film of the dimension $L = 200$ nm has been analysed. The following input data have been introduced for a silicon-diamond film respectively: $\overline{\tau}_{r1} = [6.37,\, 6.69]$ ps, $\overline{\tau}_{r2} = [20.38,\, 21.42]$ ps, $\Theta_{D1} = 640$ K, $\Theta_{D2} = 2200$ K, $\overline{T}_{b1} = [575,\, 615]$ K, $\overline{T}_{b2} = [292.5,\, 307.5]$ K, $T_{0s} = 300$ K, $q_{vs} = 0$ W/m^3, $\Delta x_s = 20$ nm and $\Delta t = 5$ ps.

Figure 1 illustrates the interval temperature distribution in the domain considered for the chosen times. Figure 2 presents the courses of the temperature function at the internal nodes $x_1 = 60$ nm (1) and $x_2 = 160$ nm (2) for the silicon and diamond layer respectively.
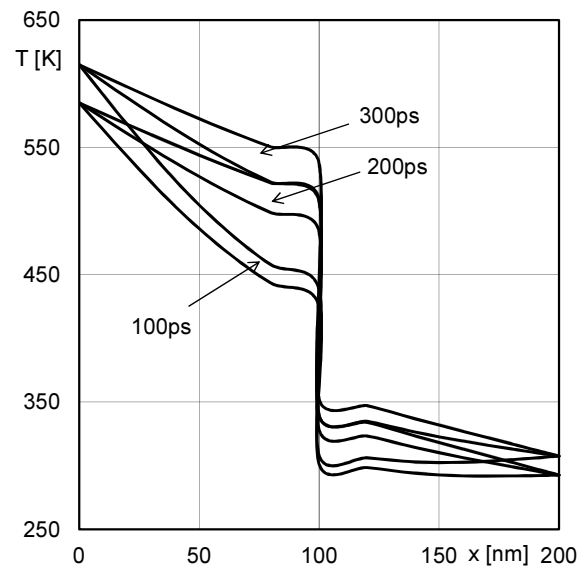
Fig. 1. The interval temperature distribution

In the second analysed example it is assumed that the external heat generation rate related to an unit of volume is the interval number $\overline{q}_{vs} = \left[0.975 \cdot 10^{18}, \ 1.025 \cdot 10^{18} \right]$ W/m^3.
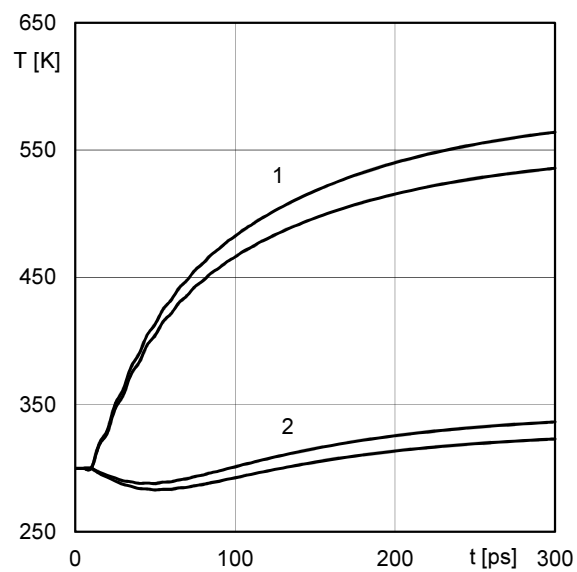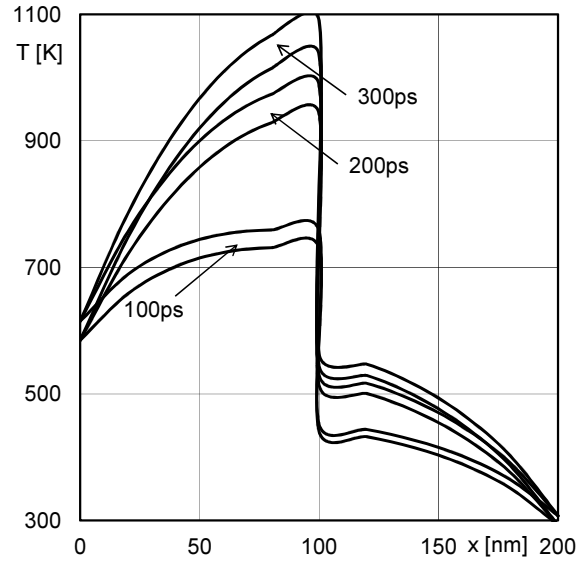
Fig. 2. The interval heating curves at internal nodes

Similar to the previous example, Figure 3 illustrates the interval temperature distribution in the domain considered for the chosen times, and Figure 4 presents the courses of the temperature function at the same internal nodes.

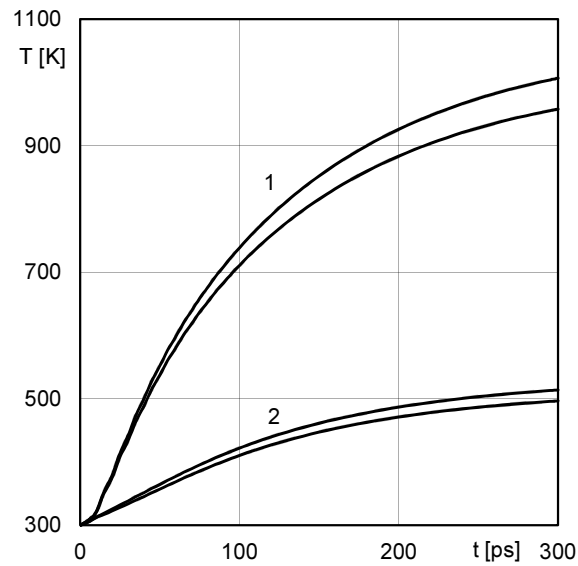Fig. 3. The interval temperature distribution

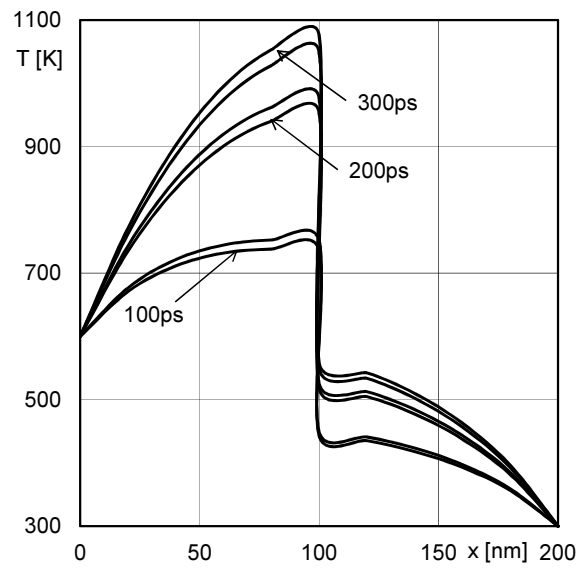Fig. 4. The interval heating curves at internal nodes
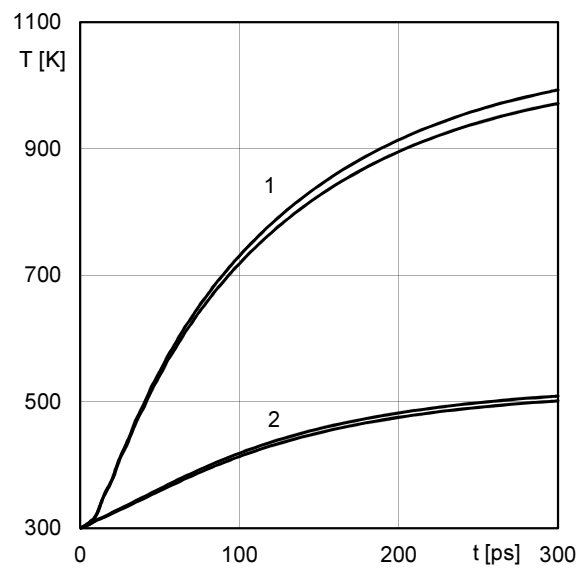
Fig. 5. The interval temperature distribution

Fig. 6. The interval heating curves at internal nodes

In the last numerical example, accurate boundary temperatures $\overline{T}_{b1} = 600$ K and $\overline{T}_{b2} = 300$ K have been introduced. In Figure 5, the interval temperature distribution in the domain considered for the chosen times are shown and Figure 6 presents the courses of the temperature function at the same internal nodes.

It should be pointed out, that for each node of the domain considered there are two curves representing the beginning and end of temperatures intervals. The interval solution is illustrated by the area between these two curves.

Additionally one can see, that for longer calculation time, the temperature intervals are wider (see Figs. 2, 4 and 6). It is visible that a greater number of operations in the set of interval numbers impacts on the increase of the width of the obtained intervals.

5. Conclusions

In the paper a interval version of the lattice Boltzmann method for solving 1D problems in two-layered crystalline solid films has been presented. A model with interval values of relaxation times, boundary conditions and the external heat generation rate related to a unit of volume for a silicon-diamond film has been proposed.

The generalization of LBM allows one to find the numerical solution in the interval form, and such information may be important, especially for the parameters that are estimated experimentally, for example the relaxation time. The problem analysed can be extended to multi-layered thin films.

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