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THE INTERVAL LATTICE BOLTZMANN METHOD FOR TRANSIENT HEAT TRANSPORT

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Abstract. In this paper an application of the interval lattice Boltzmann method for solving one-dimensional problems is presented. The Boltzmann transport equation transformed in the phonon energy density equation is considered. Such approach in which the parameters appearing in the problem analyzed are treated as the constant values is widely used. Here, the model with interval value of relaxation time is analyzed. In the final part of the paper, results of numerical computations are shown.

Introduction

Heat transport in dielectric materials and semiconductors is mainly realized by quanta of crystal vibrational energy called phonons. The study of phonons is an important part of solid state physic, because phonons play a major role in many of the physical properties of solids, especially a material's thermal conductivity. The crystal can be considered as a container filled with a gas of phonons. Phonons always “move” from the part with the higher temperature to the part with the lower temperature. During this move phonons carry energy. This kind of phenomena can be described by the Boltzmann transport equation in which the relaxation time appears. The relaxation time is estimated experimentally and its actual value is still a subject of discussion [3, 4]. In such conditions it seems natural to define the relaxation time as an interval value. In the paper the heat transport proceeding in a thin silicon film is considered.

1. Boltzmann transport equation

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

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

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 in a phonon energy density equation of the form [1]

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

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 (2) must be supplemented by the boundary initial conditions.

Using the Debye model the relation between phonon energy and lattice temperature can be calculated using the formula

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

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 is defined using the formula

$$\eta = \frac{1}{6\pi^2} \left(\frac{k_b \Theta_D}{\hbar \omega} \right)^3 \tag{4}$$

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

2. The Interval Lattice Boltzmann Method

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

$$\frac{\partial e}{\partial t} + v_x \frac{\partial e}{\partial x} = -\frac{e - e^0}{\left[\underline{\tau}_r, \overline{\tau}_r \right]} + q_v \tag{5}$$

where v_x is the component of velocity along the x-axis and $\left[\underline{\tau}_r, \overline{\tau}_r \right]$ is the interval relaxation time.

All mathematical computations must be calculated according to the rules of an interval arithmetic [5, 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. Phonons can travel only to neighboring lattice sites by ballistically traveling with the certain velocity and collide with other phonons residing at these sites [1].

The time step needed for a phonon to travel from one lattice site to the neighboring lattice site is denoted by Δt, while $\boldsymbol{c}_k$ (k = 1, 2) is a discrete set of propagation velocities in the main lattice directions, this means

$$\boldsymbol{c}_1 = (c, 0) \qquad \boldsymbol{c}_2 = (-c, 0) \tag{6}$$

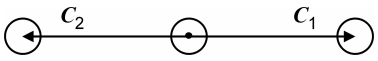

Fig. 1. Velocity vectors in a 1D lattice

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

$$\begin{aligned} \frac{\partial e_1}{\partial t} + v\frac{\partial e_1}{\partial x} &= -\frac{e_1 - e_1^{\,0}}{\left[\underline{\tau}_r, \overline{\tau}_r\right]} + q_v \\ \frac{\partial e_2}{\partial t} - v\frac{\partial e_2}{\partial x} &= -\frac{e_2 - e_2^{\,0}}{\left[\underline{\tau}_r, \overline{\tau}_r\right]} + q_v \end{aligned} \tag{7}$$

where e_1 and e_2 denote the phonon energy for two main lattice directions and $v = \Delta x / \Delta t$ where Δx is the lattice distance from site to site. The equations (7) must be supplemented by the following boundary-initial conditions

$$\begin{cases} x = 0: & e_1(0, t) = e(T_1) \\ x = L: & e_2(L, t) = e(T_2) \\ t = 0: & e(x, 0) = e(T_0) \end{cases} \tag{8}$$

where T_1, T_2 denote the boundary temperatures and T_0 is the initial temperature.

The approximation of the first derivatives using right-hand side differential quotients is the following

$$\begin{aligned} \frac{\partial e_1}{\partial t} &= \frac{e_1(x, t + \Delta t) - e_1(x, t)}{\Delta t} \\ \frac{\partial e_1}{\partial x} &= \frac{e_1(x + \Delta x, t + \Delta t) - e_1(x, t + \Delta t)}{\Delta x} \end{aligned} \tag{9}$$

and using left-hand side differential quotients is of the form

$$\frac{\partial e_2}{\partial t} = \frac{e_2(x, t+\Delta t) - e_2(x, t)}{\Delta t}$$
$$\frac{\partial e_2}{\partial x} = \frac{e_2(x, t+\Delta t) - e_2(x-\Delta x, t+\Delta t)}{\Delta x} \tag{10}$$

Thus one obtains the approximate form of the equations (7)

$$\left[\underline{e}_1, \overline{e}_1\right]_{i+1}^{f+1} = \left(1 - \left[\underline{b}, \overline{b}\right]\right)\left[\underline{e}_1, \overline{e}_1\right]_i^f + \left[\underline{b}, \overline{b}\right]\left[\underline{e}_1{}^0, \overline{e}_1{}^0\right]_i^f + \Delta t\, q_v$$
$$\left[\underline{e}_2, \overline{e}_2\right]_{i-1}^{f+1} = \left(1 - \left[\underline{b}, \overline{b}\right]\right)\left[\underline{e}_2, \overline{e}_2\right]_i^f + \left[\underline{b}, \overline{b}\right]\left[\underline{e}_2{}^0, \overline{e}_2{}^0\right]_i^f + \Delta t\, q_v \tag{11}$$

where $\left[\underline{b}, \overline{b}\right] = \Delta t / \left[\underline{\tau}_r, \overline{\tau}_r\right]$.

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

$$\left[\underline{e}(x,t), \overline{e}(x,t)\right]_i = \left[\underline{e}_1(x,t), \overline{e}_1(x,t)\right]_i + \left[\underline{e}_2(x,t), \overline{e}_2(x,t)\right]_i \tag{12}$$

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

$$\left[\underline{e}^0(x,t), \overline{e}^0(x,t)\right]_i = \left[\underline{e}(x,t), \overline{e}(x,t)\right]_i / 2 \tag{13}$$

The ILBM algorithm is an expansion of the algorithm presented in the paper [1] being equivalent method for constant value of the relaxation time.

The lattice temperature is determined using the formula describing the relation between phonon energy and lattice temperature (see equation (3))

$$T^{f+1} = \sqrt[4]{\frac{e(T^f)\Theta_D^3}{9\eta k_b \int_0^{\Theta_D/T^f} \frac{z^3}{\exp(z)-1}\,\mathrm{d}z}} \tag{14}$$

3. Example of computations

As an numerical example the transient heat transport in a silicon film of the dimension L = 200 nm has been analyzed. The following input data have been introduced: the Debye temperature $\Theta_D = 640\,\mathrm{K}$, the relaxation time $\tilde{\tau}_r = [6.3994, 6.6606]$ ps, the boundary conditions $T_1 = 800\,\mathrm{K}$, $T_2 = 300\,\mathrm{K}$, the initial temperature $T_0 = 300\,\mathrm{K}$

and $q_v = 0$. The lattice step $\Delta x = 20\,\text{nm}$ and the time step $\Delta t = 5\,\text{ps}$ have been assumed.

Figure 2 illustrates the interval temperature distribution for time $t = 25\,\text{ps}$, $t = 50\,\text{ps}$ and $t = 150\,\text{ps}$ in the silicon film. The solid line denotes the upper bound of the temperature interval while the dotted line denotes the lower bound of the temperature interval.

Figure 3 shows the interval courses of the temperature function obtained at the internal nodes $x_1 = 20\,\text{nm}$ (1), $x_2 = 100\,\text{nm}$ (2), $x_3 = 180\,\text{nm}$ (3).

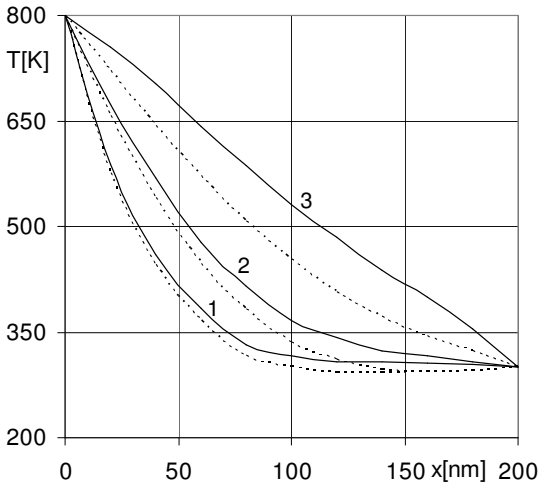

Fig. 2. The interval temperature distribution (1 - 25 ps, 2 - 50 ps and 3 - 150 ps)

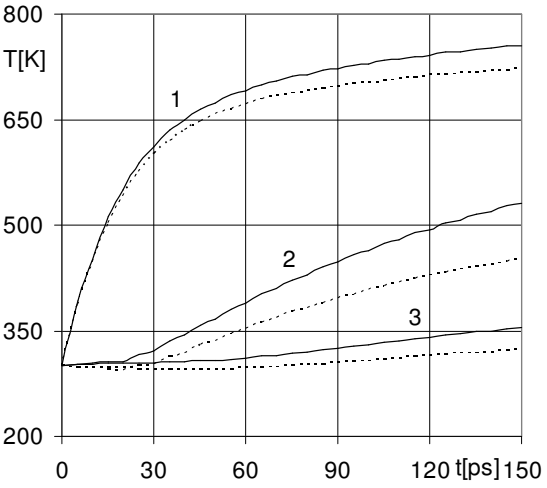

Fig. 3. The interval heating curves at internal nodes

Conclusions

In the paper the Boltzmann transport equation with the interval relaxation time has been considered. The ILBM for solving 1D problems has been presented. This application should be extended to 2D and 3D problems and take into account the boundary conditions of the 2nd and 3rd type.

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