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Heat transfer in thin metal film modeled by Boltzmann transport equation and a two-temperature model

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Contents:

Introduction

- The presentation concerns transient heat transport in 1D thin metal films.
- The Boltzmann transport equation and a two-temperature model supplemented by appropriate boundary and initial conditions are applied.
- The problem considered is solved by the lattice Boltzmann method and the finite difference method respectively.
- The internal heat source is given in two different ways: as a constant value and an exponential function which simulates irradiation of a laser.
- In the final part of the presentation numerical examples of comparison of two methods and conclusions are presented

The Boltzmann transport equation

The Boltzmann transport equation

In thin films heat transport can be described by **the Boltzmann transport equation** (BTE)

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

where:

f - the carrier distribution function,

$\mathbf{v}$ - the frequency-dependent carrier propagation speed,

τ_r - the frequency-dependent carrier relaxation time,

g_{ef} - the carrier generation rate due to electron-phonon scattering,

f^{eq} - the equilibrium distribution function given by the Bose-Einstein or Fermi-Dirac statistics.

The Boltzmann transport equation

The Boltzmann transport equation can be transformed into an equivalent carrier energy density equation using the simplifying assumptions of the Debye model

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

where:

- e - the carrier energy density,
- e^{eq} - the equilibrium carrier energy density
- q_v - the internal heat generation rate related to an unit of volume,
- τ_r - the relaxation time.

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

The Boltzmann transport equation

The dependence between electron energy density and electron temperature can be calculated from the following formula

$$e_e(T_e) = \left(n_e \frac{\pi^2}{2} \frac{k_b^2}{\varepsilon_F} \right) T_e^2$$

where:

ε_F - the Fermi energy,

n_e - the density of electrons.

The Boltzmann transport equation

The dependence between phonon energy density and lattice temperature can be calculated from the following formula

$$e_{ph}(T_{ph}) = \left(\frac{9\eta\, k_b}{\Theta_D^3} \int_0^{\Theta_D/T_{ph}} \frac{z^3}{\exp(z)-1} \mathrm{dz} \right) T_{ph}^4$$

where:

Θ_D - the Debye temperature of the solid,

η - the number density of oscillators

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

The lattice Boltzmann method – thin metal films

Energy transfer in thin metal film is the coupled problem with two relaxation times

$$\frac{\partial e_e}{\partial t} + \mathbf{v}_e \cdot \nabla e_e = -\frac{e_e - e_e^{eq}}{\tau_{re}} + Q_e$$

$$\frac{\partial e_{ph}}{\partial t} + \mathbf{v}_{ph} \cdot \nabla e_{ph} = -\frac{e_{ph} - e_{ph}^{eq}}{\tau_{rph}} + Q_{ph}$$

where:

$$Q_e = Q' - G(T_e - T_{ph})$$

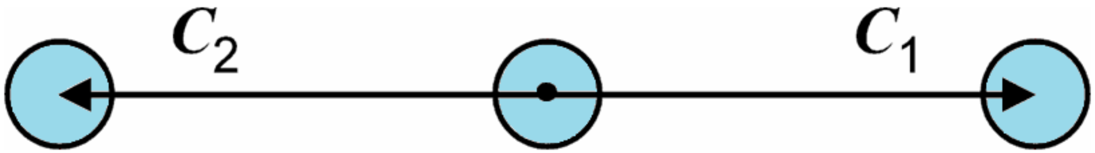
$$Q_{ph} = G(T_e - T_{ph})$$

The lattice Boltzmann method – thin metal film

Considered directions and values of velocities in 1D model

$$\mathbf{c}_{e1} = [c_e, 0] \quad \mathbf{c}_{e2} = [-c_e, 0]$$

$$\mathbf{c}_{ph1} = [c_{ph}, 0] \quad \mathbf{c}_{ph2} = [-c_{ph}, 0]$$



where:

Δx - the lattice distance from site to site,

$c = \Delta x / \Delta t$ - the component of velocity along the *x*-axis,

$\Delta t = t^{f+1} - t^{f}$ - the time step needed for a phonon to travel from one lattice site to the neighboring lattice site.

The lattice Boltzmann method – thin metal film

After subsequent computations the approximate form of the interval Boltzmann transport equations for **1D coupled problem** is the following

$$
\begin{cases}
\left(e_{e1}\right)_{i+1}^{f+1} = \left(1 - \dfrac{\Delta t}{\tau_{re}}\right)\left(e_{e1}\right)_{i}^{f} + \dfrac{\Delta t}{\tau_{re}}\left(e_{e1}^{0}\right)_{i}^{f} + \Delta t\, Q_{e} \\
\left(e_{e2}\right)_{i-1}^{f+1} = \left(1 - \dfrac{\Delta t}{\tau_{re}}\right)\left(e_{e2}\right)_{i}^{f} + \dfrac{\Delta t}{\tau_{re}}\left(e_{e2}^{0}\right)_{i}^{f} + \Delta t\, Q_{e} \\
\left(e_{ph1}\right)_{i+1}^{f+1} = \left(1 - \dfrac{\Delta t}{\tau_{rph}}\right)\left(e_{ph1}\right)_{i}^{f} + \dfrac{\Delta t}{\tau_{rph}}\left(e_{ph1}^{0}\right)_{i}^{f} + \Delta t\, Q_{ph} \\
\left(e_{ph2}\right)_{i-1}^{f+1} = \left(1 - \dfrac{\Delta t}{\tau_{rph}}\right)\left(e_{ph2}\right)_{i}^{f} + \dfrac{\Delta t}{\tau_{rph}}\left(e_{ph2}^{0}\right)_{i}^{f} + \Delta t\, Q_{ph}
\end{cases}
$$

The lattice Boltzmann method – thin metal film

- upper and lower boundary conditions

$$
\begin{cases}
x=0: & q_{b1}^{e}(0,\,t)=c_e\left[e_e\left(T_e\right)_0-e_e\left(T_e\right)_1\right] \\
x=L: & q_{b2}^{e}(0,\,L)=c_e\left[e_e\left(T_e\right)_{n-1}-e_e\left(T_e\right)_n\right] \\
x=0: & q_{b1}^{ph}(0,\,t)=c_{ph}\left[e_{ph}\left(T_{ph}\right)_0-e_{ph}\left(T_{ph}\right)_1\right] \\
x=L: & q_{b2}^{ph}(0,\,t)=c_{ph}\left[e_{ph}\left(T_{ph}\right)_{n-1}-e_{ph}\left(T_{ph}\right)_n\right]
\end{cases}
$$

- the initial condition

$$
\begin{array}{ll}
t=0: & e_e(x,0)=e_e(T_0^{\,e}) \\
t=0: & e_{ph}(x,0)=e_{ph}(T_0^{\,ph})
\end{array}
$$

The lattice Boltzmann method – thin metal film

- The total interval electron and phonon energy density

$$e_e = e_{e1} + e_{e2} \qquad e_{ph} = e_{ph1} + e_{ph2}$$

- After subsequent computations the temperature of electrons and phonons are determined using the formula

$$T_e^f = \sqrt{e_e(T^f{}_e) \Big/ \left(n_e \frac{\pi^2}{2} \frac{k_b^2}{\varepsilon_F} \right)}$$

$$T_{ph}^f = \sqrt[4]{e(T_{ph}^f)\Theta_D^3 \Big/ 9\eta k_b \int_0^{\Theta_D/T_{ph}^{f-1}} \frac{z^3}{\exp(z)-1} dz}$$

A two-temperature model

A two-temperaturę model

Two-temperature model describing the temporal and spatial evolution of the lattice and electrons temperatures (T_l and T_e) in the irradiated metal can be written

$$C_e(T_e)\frac{\partial T_e(x,t)}{\partial t} = -\frac{\partial q_e(x,t)}{\partial t} - G\left[T_e(x,t) - T_l(x,t)\right] + Q(t)$$

$$C_l\frac{\partial T_l(x,t)}{\partial t} = -\frac{\partial q_l(x,t)}{\partial t} + G\left[T_e(x,t) - T_l(x,t)\right]$$

where $C_e(T_e)$, C_l are the volumetric specific heats, G is the electron-phonon coupling factor which characterizes the energy exchange between electrons and phonons, $Q(t)$ is the source function associated with the irradiation.

A two-temperaturę model

Instead of the classical Fourier law the following formulas are introduced

$$C_e(T_e)\frac{\partial T_e(x,t)}{\partial t} = -\frac{\partial q_e(x,t)}{\partial t} - G\left[T_e(x,t) - T_l(x,t)\right] + Q(t)$$

$$C_l\frac{\partial T_l(x,t)}{\partial t} = -\frac{\partial q_l(x,t)}{\partial t} + G\left[T_e(x,t) - T_l(x,t)\right]$$

where $\lambda_e(T_e, T_l)$, λ_l are the thermal conductivities of electrons and lattice, respectively, τ_e is the relaxation time of free electrons in metals, τ_l is the relaxation time in phonon collisions.

A two-temperaturę model

For low laser intensity the following relationships describing the electrons thermal capacity and volumetric specific heat are widely used

$$\lambda_e(T_e, T_l) = \lambda_0 \frac{T_e}{T_l}, \; C_e(T_e) = AT_e$$

where λ_0 and *A* are the material constants. For low laser intensity λ_l , C_l, and G are also constant values depended on material.

Results of computations

As a numerical example heat transport in a gold film of the hight 200 nm has been analyzed.

The following input data have been introduced for:

- the relaxation times $\tau_{re} = 0.04\,\text{ps}$

  $\tau_{rph} = 0.8\,\text{ps}$
- the Debye'a temperature $\Theta_D = 170\,\text{K}$
- the initial temperature $T_0 = 300\,\text{K}$
- the lattice step $\Delta x = 1\text{nm}$
- the time step $\Delta t = 0.001\text{ps}$
- the coupling factor $G = 2.3 \times 10^{16}\ \text{W/m}^3\text{K}$

Results of computations

Examples of the internal heat source Q(t):

- Constant:

$Q(t) = 10^{13}$ W/m^3

- Exponential:

$$Q(t) = I_0\, e^{-\beta t}\ \mathrm{W/m^3}$$

$$I_0 = 2 \cdot 10^{13}\ \mathrm{W/m^3}$$

β:

1) $0.5 \cdot 10^{13}\ 1/\mathrm{s}$

2) $10^{13}\ 1/\mathrm{s}$

3) $1.5 \cdot 10^{13}\ 1/\mathrm{s}$

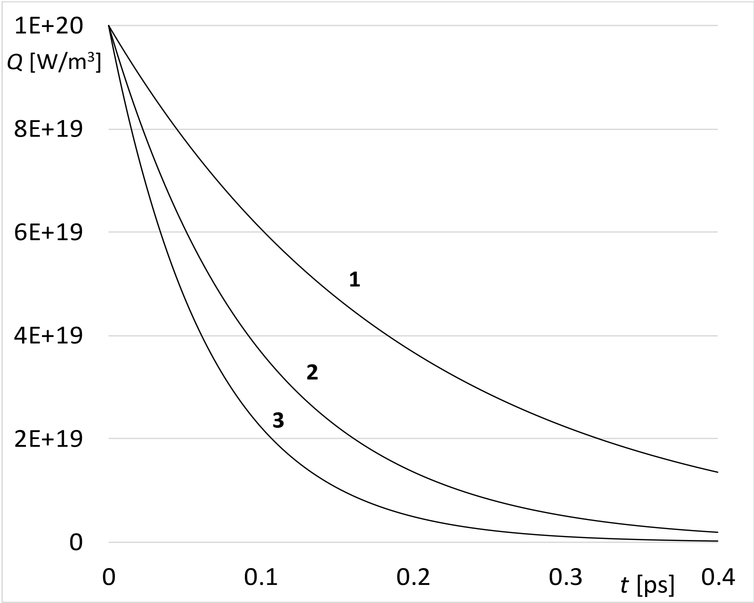


Fig. 1. Exponential heat source function

Results of computations

Example 1.

Q(t) = const

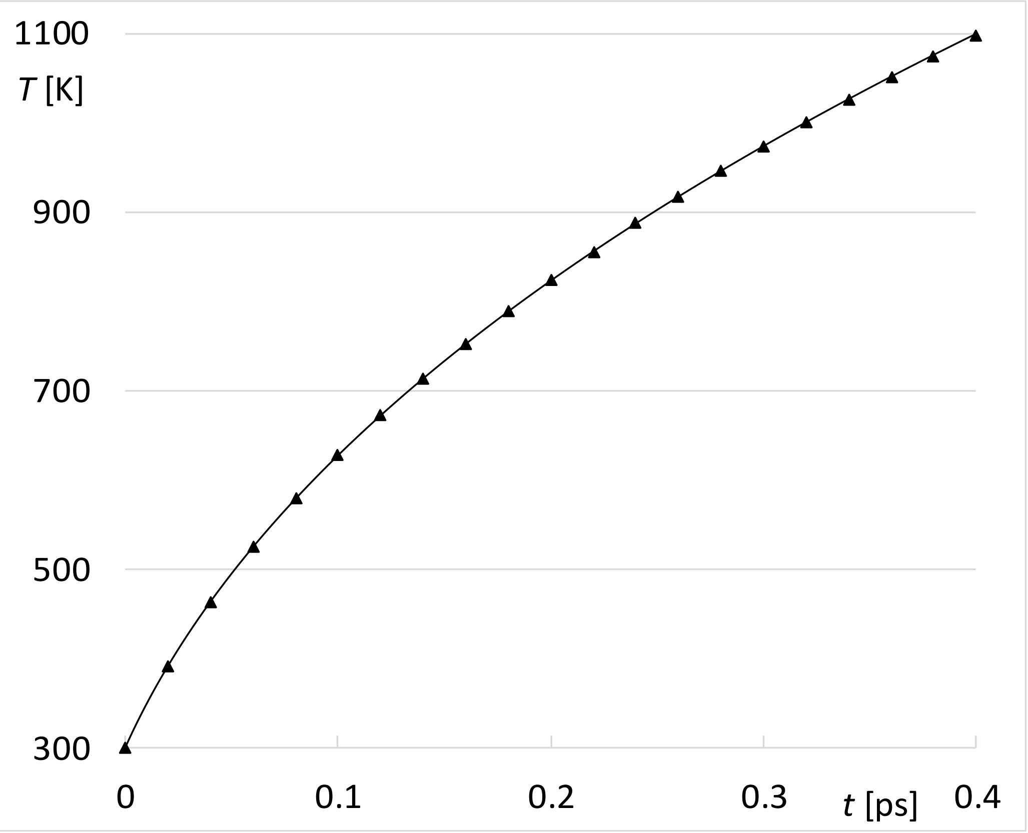


Fig. 2. The interval heating curves at internal nodes

Results of computations

Example 2.

$$Q(t) = I_0 \, e^{-\beta t}$$

$$I_0 = 2 \cdot 10^{13} \, \mathrm{W/m^3}$$

β :

1) $0.5 \cdot 10^{13} \, 1/\mathrm{s}$

2) $10^{13} \, 1/\mathrm{s}$

3) $1.5 \cdot 10^{13} \, 1/\mathrm{s}$

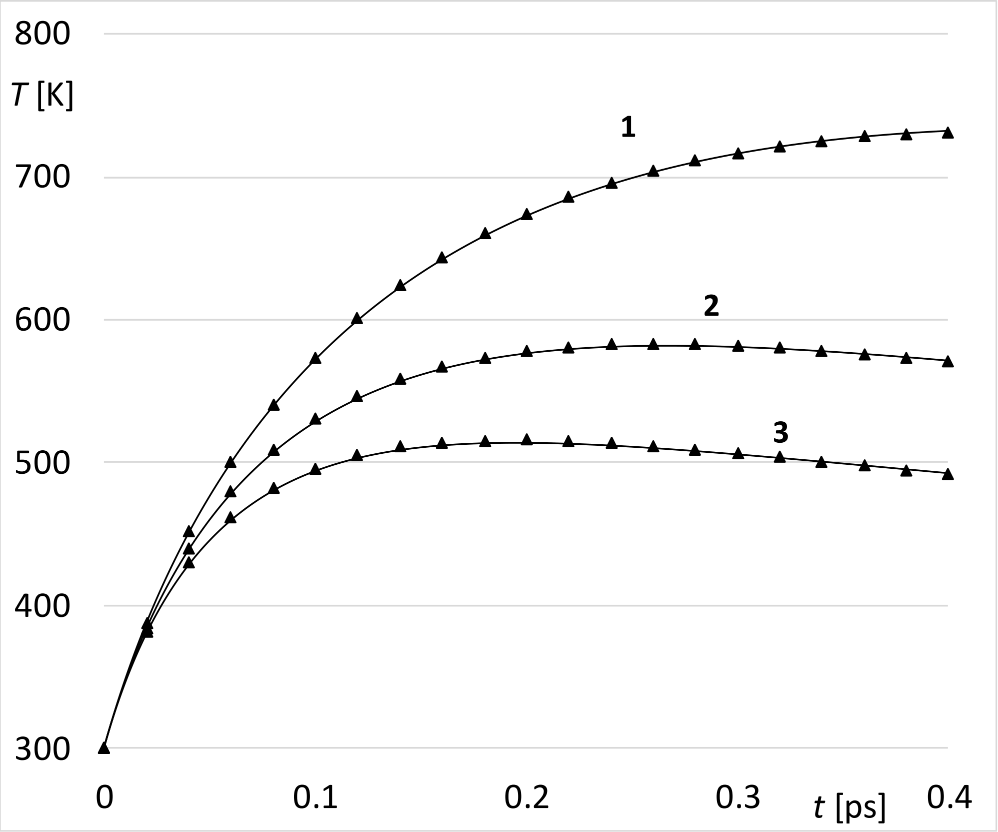


Fig. 3. The interval heating curves at internal nodes

Results of computations

Example 2.

The relative error δ:

$$\delta = \left| \frac{\mathbf{FDM} - \mathbf{LBM}}{\mathbf{FDM}} \right| \cdot 100\%$$

time	FDM	LBM	δ [%]	time	FDM	LBM	δ [%]
0.04	440.0907	438.3789	0.38897	0.24	582.5611	580.8897	0.28691
0.08	508.7353	506.5825	0.42317	0.28	582.7515	581.5039	0.21409
0.12	546.5965	544.3312	0.41444	0.32	580.2610	579.5346	0.12519
0.16	567.5201	565.3244	0.38689	0.36	576.0237	575.9115	0.01948
0.2	578.2466	576.2557	0.3443	0.4	570.6550	571.2458	0.1035

Estimated error between presented two methods in node *x=0,* for $\beta = 10^{13}\,1/s$

Conclusions

Conclusions

- In the paper the temperatures obtained using two different mathematical models: the Boltzmann transport equation and the two-temperature model were compared.
- Numerical methods: the lattice Boltzmann method and the finite difference method respectively were used to solve them.
- The results obtained when applying the two types of heat sources are comparable with **the relative error less than 0.5%**.

Thank you for attention