Numerical modelling of transient heat transport in a two-layered metal film using the fuzzy lattice Boltzmann method with α-cuts

Alicja Piasecka-Belkhayat* and Anna Korczak

Institute of Computational Mechanics and Engineering
Silesian University of Technology, Konarskiego 18A, 44-100 Gliwice, Poland
e-mail: alicja.piasecka@polsl.pl, anna.korczak@polsl.pl

Abstract

In the paper a description of heat transfer in a one-dimensional two-layered metal film is considered. The fuzzy coupled lattice Boltzmann equations for electrons and phonons supplemented by appropriate boundary and initial conditions are applied to analyze the thermal process in a thin metal film. The model with fuzzy values of relaxation times and boundary-initial conditions for gold and titanium is proposed. A problem considered is solved by the fuzzy lattice Boltzmann method using α-cuts and the rules of directed interval arithmetic. The application of α-cuts allows one to avoid complicated arithmetical operations in the fuzzy numbers set. In the final part of the paper an example for a numerical solution is presented.

Keywords: Boltzmann transport equation, fuzzy lattice Boltzmann method, α-cuts, directed interval arithmetic

1. Introduction

In metals the heat transport is mainly realized by two kinds of heat carriers: electrons and quanta of lattice vibrations called phonons. Electrons and phonons as heat carriers always "move" from the part with the higher temperature to the part with the lower temperature and during this move they carry energy. This kind of phenomena can be described by the Boltzmann transport equation (BTE) which is difficult to solve. For this reason, the lattice Boltzmann method (LBM) is applied to find a solution of a discretized set of the Boltzmann transport equations. In the paper the coupled lattice Boltzmann equations for electrons and phonons have been assumed. The coupled model contains two energy equations determining the heat exchange in the electron gas and the metal lattice [1, 5, 6]. Such an approach in which the physical parameters appearing in the mathematical model are treated as constant values is widely used. In this paper, fuzzy values of relaxation times and boundary-initial 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 [7]. In the paper the heat transport proceeding in a two-layered thin film is considered [9]. To solve the problem formulated the fuzzy lattice Boltzmann method using α-cuts and the rules of directed interval arithmetic is applied [3, 4]. In the final part of the paper the examples of numerical computations are shown.

2. The fuzzy Boltzmann transport equation

The unsteady fuzzy BTEs transformed into equivalent fuzzy energy density equations for the 1D coupled model with two kinds of carriers (*e*-electrons and *ph*-phonons) can be written as follows [2]

$$\frac{\partial \tilde{e}_{es}}{\partial t} + \mathbf{v}_{es} \cdot \nabla \tilde{e}_{es} = -\frac{\tilde{e}_{es} - \tilde{e}_{es}^{0}}{\tilde{\tau}_{res}} + \tilde{Q}_{es} \tag{1}$$

$$\frac{\partial \tilde{e}_{phs}}{\partial t} + \mathbf{v}_{phs} \cdot \nabla \tilde{e}_{phs} = -\frac{\tilde{e}_{phs} - \tilde{e}_{phs}^{0}}{\tilde{\tau}_{rphs}} + \tilde{Q}_{phs} \tag{2}$$

where $s = 1, 2$ corresponds to the successive layers of the thin film (gold, titanium), $\tilde{e}_s$ is the fuzzy energy density, $\tilde{e}_s^0$ is the equilibrium fuzzy energy density, $\mathbf{v}_s$ is the frequency-dependent propagation speed, $\tilde{\tau}_{rs}$ is the fuzzy relaxation time, t denotes the time and $\tilde{Q}_s$ is the fuzzy internal energy source related to an unit of volume for electrons and phonons respectively.

The electron and phonon energy densities at their equivalent nonequilibrium temperatures are given by the formulas

$$\tilde{e}_{es}(\tilde{T}_{es}) = \left(n_{es} \frac{\pi^2}{2} \frac{k_b^2}{\varepsilon_{Fs}} \right) \tilde{T}_{es}^{2} \tag{3}$$

$$\tilde{e}_{phs}(\tilde{T}_{phs}) = \left(\frac{9\eta_{phs} k_b}{\Theta_{Dphs}^3} \int_0^{\Theta_{Dphs}/\tilde{T}_{phs}} \frac{z^3}{\exp(z) - 1} \mathrm{d}z \right) \tilde{T}_{phs}^{4} \tag{4}$$

where Θ_{Ds} is the Debye temperature of the solid, k_b is the Boltzmann constant, ε_{Fs} is the Fermi energy, $\tilde{T}_{es}$, $\tilde{T}_{phs}$ are the fuzzy lattice temperatures for electrons and phonons respectively, while n_{es} is the electron density and η_{phs} is the phonon density.

The fuzzy electron and phonon energy sources are calculated using the following expressions [2]

$$\tilde{Q}_{es} = Q'_s - G_s(\tilde{T}_{es} - \tilde{T}_{phs}) \tag{5}$$

$$\tilde{Q}_{phs} = G_s(\tilde{T}_{es} - \tilde{T}_{phs}) \tag{6}$$

where Q'_s is the power density deposited by the external source function and G_s is the electron-phonon coupling factor which characterizes the energy exchange between electrons and phonons. The equations (1) and (2) should be supplemented by the initial condition and fuzzy boundary conditions.

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3. Fuzzy lattice Boltzmann equation

The fuzzy lattice Boltzmann method (LBM) is a numerical technique for the simulation of heat transfer.

In the problem analyzed a set of eight fuzzy differential equations is obtained [8]

$$\begin{cases} \left(\tilde{e}_{e1s}\right)_{i+1}^{f+1} = \left(1-\Delta t/\tilde{\tau}_{es}\right)\left(\tilde{e}_{e1s}\right)_i^f + \dfrac{\Delta t}{\tilde{\tau}_e}\left(\tilde{e}_{e1s}^0\right)_i^f + \Delta t\,\tilde{Q}_{es} \\ \left(\tilde{e}_{e2s}\right)_{i-1}^{f+1} = \left(1-\Delta t/\tilde{\tau}_{es}\right)\left(\tilde{e}_{e2s}\right)_i^f + \dfrac{\Delta t}{\tilde{\tau}_{es}}\left(\tilde{e}_{e2s}^0\right)_i^f + \Delta t\,\tilde{Q}_{es} \\ \left(\tilde{e}_{ph1s}\right)_{i+1}^{f+1} = \left(1-\Delta t/\tilde{\tau}_{phs}\right)\left(\tilde{e}_{ph1s}\right)_i^f + \dfrac{\Delta t}{\tilde{\tau}_{ph}}\left(\tilde{e}_{ph1s}^0\right)_i^f + \Delta t\,\tilde{Q}_{phs} \\ \left(\tilde{e}_{ph2s}\right)_{i-1}^{f+1} = \left(1-\Delta t/\tilde{\tau}_{phs}\right)\left(\tilde{e}_{ph2s}\right)_i^f + \dfrac{\Delta t}{\tilde{\tau}_{ph}}\left(\tilde{e}_{ph2s}^0\right)_i^f + \Delta t\,\tilde{Q}_{phs} \end{cases} \tag{7}$$

where $\Delta t = t^{f+1} - t^f$ is the time step needed for electron/ phonon to travel from one lattice site to the neighboring lattice site.
The total fuzzy energy density for electrons and phonons is defined as the sum of discrete fuzzy energy densities in all the lattice directions and takes the form

$$\left(\tilde{e}_{es}\right)_i^{f+1} = \left(\tilde{e}_{e1s}\right)_i^{f+1} + \left(\tilde{e}_{e2s}\right)_i^{f+1} = \sum_{d=1}^{2}\left(\tilde{e}_{eds}(x,\,t)\right)_i^{f+1} \tag{8}$$

$$\left(\tilde{e}_{phs}\right)_i^{f+1} = \left(\tilde{e}_{ph1s}\right)_i^{f+1} + \left(\tilde{e}_{ph2s}\right)_i^{f+1} = \sum_{d=1}^{2}\left(\tilde{e}_{phds}(x,\,t)\right)_i^{f+1} \tag{9}$$

where $d = 1, 2$ corresponds to the positive and negative x direction [2].
The equilibrium fuzzy electron energy density and phonon energy density is the same in all lattice directions and can be calculated using the following formula [8]

$$\left(\tilde{e}_{es}^0\right)_i^{f+1} = \left(\tilde{e}_{es}\right)_i^{f+1}/2 \tag{10}$$

$$\left(\tilde{e}_{phs}^0\right)_i^{f+1} = \left(\tilde{e}_{phs}\right)_i^{f+1}/2 \tag{11}$$

After subsequent computations the fuzzy lattice temperatures for electrons and phonons are determined using the formulas (3) and (4).

4. Results of computations

As a numerical example the heat transport in a gold-titanium film of the thickness L=200 nm has been analyzed. The following input data have been introduced for the film respectively: $\tilde{q}_{b1} = \tilde{0}\,\mathrm{W/m^2}$, $\tilde{T}_{b2} = (285, 300, 315)\,\mathrm{K}$, $T_{0s} = 300\,\mathrm{K}$, $Q_s' = 10^{20}\,\mathrm{W/m^3}$, $\Delta x_s = 20\,\mathrm{nm}$, $\Delta t = 0.01\,\mathrm{ps}$, fuzzy relaxation times for phonons and electrons $\tilde{\tau}_{phs} = (\tau_{phs} - 0.05\tau_{phs}, \tau_{phs}, \tau_{phs} + 0.05\tau_{phs})$, $\tilde{\tau}_{es} = (\tau_{es} - 0.05\tau_{es}, \tau_{es}, \tau_{es} + 0.05\tau_{es})$ and other material properties that are defined in Table 1.

Table1: Material properties

	τ_{phs}	τ_{es}	Θ_D	$n_e\ (\times 10^{28})$	$\varepsilon_F\ (\times 10^{-19})$
Au	0.8	0.04	170	5.9	8.86
Ti	0.5	0.01	420	13.80	15.61

Figure 1 illustrates the fuzzy electrons temperature distribution in the domain considered for the chosen times.

The generalization of LBM allows one to find the numerical solution in the fuzzy form and such an information may be important especially for the parameters which are estimated experimentally, for example the relaxation time.

The problem analyzed can be extended to multi-layered thin films.

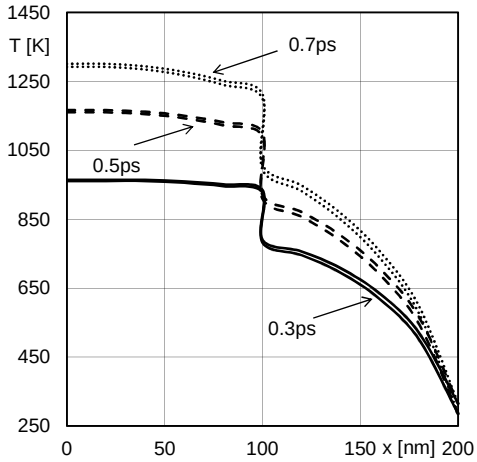

Figure 1: The fuzzy electrons temperature distribution

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