

## NUMERICAL MODEL OF THIN METAL FILM HEATING USING THE BOUNDARY ELEMENT METHOD

EWA MAJCHRZAK<sup>1\*</sup>, BOHDAN MOCHNACKI<sup>2</sup>

<sup>1</sup> *Silesian University of Technology, Konarskiego 18a, 44-100 Gliwice*

<sup>2</sup> *University of Occupational Safety Management, Bankowa 8, 40-007 Katowice*

*\*Corresponding author: ewa.majchrzak@polsl.pl*

### Abstract

The subject of the paper is connected with the microscale heat transfer proceeding in the metal domain. In particular, the heating process of thin metal film subjected to an external heat flux is analysed. Thermal processes in the domain considered are described by the dual-phase lag equation (DPLE) supplemented by the appropriate boundary and initial conditions. At the stage of numerical modeling the variant of the boundary element method called the BEM using discretization in time is applied. So far, this method has not been used for the hyperbolic equations describing the micro-scale heat transfer. In the final part the example of computations is shown.

**Key words:** thin metal film heating, dual-phase lag equation, the BEM using discretization in time, numerical methods

### 1. INTRODUCTION

The subject of the paper is connected with the numerical modeling of thermal processes proceeding in the thin metal film subjected to an ultra-short heat pulse. From the practical point of view the analysis of heat conduction in the homogeneous or heterogeneous metal layers is of great importance in the designing of micro-scale technologies (Grigoropoulos et al., 2007; Zhang, 2007). So, the problems associated with the rapid heating of the solids become a very active research area especially during the last several years, for example (Al-Nimr, 1997; Tang & Araki, 1999; Chen & Beraun, 2001; Mochnecki & Paruch, 2013; Majchrzak et al., 2009a). The mathematical models of thin films heating based on the PDE are other than the classical equations describing the macroscale thermal diffusion. It results, among others, from the extremely short duration, extreme temperature gradients and very small geometrical dimensions of the domain considered (Hen et al., 2004; Smith & Norris, 2003; Tzou, 1997). In this

place the Cattaneo-Vernotte equation (Cattaneo, 1958; Özişik, 1994; Tamma & Zhou, 1998), the dual phase lag model (Chou & Yang, 2009; Majchrzak et al., 2009b; Majchrzak & Mochnecki, 2014; Ramadan et al., 2009), the two-temperature (parabolic or hyperbolic) models (Chen & Beraun, 2001; Anisimov et al., 1974) and the Boltzmann lattice method (Ho et al., 2003) can be mentioned. In this paper the mathematical model of the process is based on the dual phase lag equation supplemented by the appropriate boundary-initial conditions.

The typical practical problems in the area of microscale heat transfer can be effectively examined only by the using of numerical methods. So far, a large majority of numerical solutions have been obtained by use of the finite difference method – e.g. (Majchrzak et al., 2009c; Mochnecki & Paruch, 2013). Here, the algorithm based on the boundary element method is proposed. In particular the version of this method called the BEM using discretization in time is applied.

## 2. GOVERNING EQUATIONS

The dual phase lag equation results from the generalized form of the Fourier law containing two lag times, in particular the relaxation and thermalization ones (Chen & Beraun, 2001; Chen et al. 2004; Zhang 2007; Tzou 1997), namely

$$\mathbf{q}(X, t + \tau_q) = -\lambda \nabla T(X, t + \tau_T) \quad (1)$$

where  $\mathbf{q}$  is a heat flux,  $\lambda$  is a thermal conductivity,  $\tau_q$  and  $\tau_T$  are the phase lags (relaxation and thermalization times),  $X, t$  are the geometrical co-ordinates and time.

Using the Taylor series expansions, the following first-order approximation of equation (1) is obtained

$$\begin{aligned} \mathbf{q}(X, t) + \tau_q \frac{\partial \mathbf{q}(X, t)}{\partial t} = \\ -\lambda \left[ \nabla T(X, t) + \tau_T \frac{\partial \nabla T(X, t)}{\partial t} \right] \end{aligned} \quad (2)$$

Introducing this formula to the well known diffusion equation after the mathematical manipulations one has

$$\begin{aligned} c \left[ \frac{\partial T(X, t)}{\partial t} + \tau_q \frac{\partial^2 T(X, t)}{\partial t^2} \right] = \nabla [\lambda \nabla T(X, t)] + \\ \tau_T \frac{\partial \{ \nabla [\lambda \nabla T(X, t)] \}}{\partial t} + Q(X, t) + \tau_q \frac{\partial Q(X, t)}{\partial t} \end{aligned} \quad (3)$$

where  $c$  is a volumetric specific heat of material,  $Q$  is the capacity of internal heat sources.

The heating process of the thin metal film can be described by the one dimensional DPLE (taking into account the geometrical properties of domain considered, the 1D model  $x \in [0, G]$  is quite acceptable), at the same time the function describing the internal heat sources is equal to 0. So, for the constant values of thermophysical parameters the following energy equation should be considered

$$\begin{aligned} c \frac{\partial T(x, t)}{\partial t} + c \tau_q \frac{\partial^2 T(x, t)}{\partial t^2} = \\ \lambda \frac{\partial^2 T(x, t)}{\partial x^2} + \lambda \tau_T \frac{\partial^3 T(x, t)}{\partial t \partial x^2} \end{aligned} \quad (4)$$

The equation (4) is supplemented by the modified Neumann boundary conditions for  $x = 0$  and  $x = G$

$$q_b(x, t) + \tau_q \frac{\partial q_b(x, t)}{\partial t} = -\lambda \left[ \frac{\partial T(x, t)}{\partial x} + \tau_T \frac{\partial^2 T(x, t)}{\partial t \partial x} \right] \quad (5)$$

where  $q_b$  is the boundary heat flux (for  $x = G$ :  $q_b = 0$ ). The initial conditions (the initial temperature and initial heating rate  $v(x, 0)$ ) are also given.

## 3. THE BEM USING DISCRETIZATION IN TIME

To solve the problem considered, the BEM using discretization in time called also the combined variant of the BEM (Brebbia et al., 1984; Curran et al., 1980; Szopa, 1999) in the extended version corresponding to the hyperbolic PDE is applied.

Let us introduce the temporal mesh

$$\Omega_t : \{t^0, t^1, \dots, t^{f-2}, t^{f-1}, t^f, \dots, t^S < \infty\} \quad (6)$$

with the constant step  $\Delta t$ . To use the method proposed, the equation (4) is transformed to the form

$$\begin{aligned} c \frac{T(x, t^f) - T(x, t^{f-1})}{\Delta t} + c \tau_q \frac{T(x, t^f) - 2T(x, t^{f-1}) + T(x, t^{f-2})}{(\Delta t)^2} = \\ \lambda \frac{\partial^2 T(x, t^f)}{\partial x^2} + \frac{\lambda \tau_T}{\Delta t} \left[ \frac{\partial^2 T(x, t^f)}{\partial x^2} - \frac{\partial^2 T(x, t^{f-1})}{\partial x^2} \right] \end{aligned} \quad (7)$$

After the mathematical manipulations one has

$$\begin{aligned} \frac{\partial^2 T(x, t^f)}{\partial x^2} - \frac{c(\Delta t + \tau_q)}{\lambda \Delta t (\Delta t + \tau_T)} T(x, t^f) - \frac{\tau_T}{\Delta t + \tau_T} \frac{\partial^2 T(x, t^{f-1})}{\partial x^2} + \\ \frac{c(\Delta t + 2\tau_q)}{\lambda \Delta t (\Delta t + \tau_T)} T(x, t^{f-1}) - \frac{c \tau_q}{\lambda \Delta t (\Delta t + \tau_T)} T(x, t^{f-2}) = 0 \end{aligned} \quad (8)$$

or

$$\begin{aligned} \frac{\partial^2 T(x, t^f)}{\partial x^2} - BT(x, t^f) + C \frac{\partial^2 T(x, t^{f-1})}{\partial x^2} \\ + DT(x, t^{f-1}) + ET(x, t^{f-2}) = 0 \end{aligned} \quad (9)$$

where

$$\begin{aligned} B = \frac{c(\Delta t + \tau_q)}{\lambda \Delta t (\Delta t + \tau_T)}, \quad C = -\frac{\tau_T}{\Delta t + \tau_T}, \\ D = \frac{c(\Delta t + 2\tau_q)}{\lambda \Delta t (\Delta t + \tau_T)}, \quad E = -\frac{c \tau_q}{\lambda \Delta t (\Delta t + \tau_T)} \end{aligned} \quad (10)$$



To apply the weighted residual method criterion (WRMC) the difference  $R$  between the left- and right-hand side of equation (9) must be introduced. In the case considered  $R$  corresponds to the left-hand side of equation (9), of course. The WRMC for the 1D problem takes a form (Brebbia et al., 1984)

$$\int_0^G R \cdot T^*(\xi, x) dx = 0 \quad (11)$$

where  $T^*(\xi, x)$  is the fundamental solution and for the 1D objects oriented in rectangular co-ordinate system it is a function of the form

$$T^*(\xi, x) = \frac{1}{2\sqrt{B}} \exp(-|x - \xi|\sqrt{B}) \quad (12)$$

while  $\xi \in (0, G)$  is called the observation point.

One can check that the fundamental solution fulfils the equation

$$\frac{\partial^2 T^*(\xi, x)}{\partial x^2} - BT^*(\xi, x) = -\delta(\xi, x) \quad (13)$$

where  $\delta(\xi, x)$  is the Dirac function.

The formula determining the heat flux resulting from the fundamental solution  $q^*(\xi, x) = -\lambda \partial T^*(\xi, x) / \partial x$  should be calculated, this means

$$q^*(\xi, x) = \frac{\lambda \operatorname{sgn}(x - \xi)}{2} \exp(-|x - \xi|\sqrt{B}) \quad (14)$$

where  $\operatorname{sgn}(\cdot)$  is the sign function.

Integrating twice by parts the first component of equation (11) and taking into account the property of fundamental solution (13), one obtains

$$\int_0^G \left[ \frac{\partial^2 T(x, t^f)}{\partial x^2} - BT(x, t^f) \right] T^*(\xi, x) dx = \left[ T^*(\xi, x) \frac{\partial T(x, t^f)}{\partial x} \right]_{x=0}^{x=G} - \left[ T(x, t^f) \frac{\partial T^*(\xi, x)}{\partial x} \right]_{x=0}^{x=G} - T(\xi, t^f) \quad (15)$$

Finally, the equation (15) takes the form

$$T(\xi, t^f) + \frac{1}{\lambda} \left[ T^*(\xi, x) W(x, t^f) \right]_{x=0}^{x=G} = \frac{1}{\lambda} \left[ q^*(\xi, x) T(x, t^f) \right]_{x=0}^{x=G} + Z(\xi, t^f) \quad (16)$$

where

$$Z(\xi, t^f) = \int_0^G \left[ C \frac{\partial^2 T(x, t^{f-1})}{\partial x^2} + DT(x, t^{f-1}) + ET(x, t^{f-2}) \right] T^*(\xi, x) dx$$

$$W(x, t^f) = -\lambda \frac{\partial T(x, t^f)}{\partial x} \quad (17)$$

To calculate the integral  $Z(\xi, t^f)$ , the domain  $[0, G]$  is divided into  $n$  internal cells, and next this integral is substituted by the sum of integrals from  $x_{j-1}$  to  $x_j$ . These integrals are calculated using the 6-points Gauss quadratures. The constant internal cells are used here and then the nodes 0 and  $n+1$  are located on the boundaries  $x = 0$  and  $x = L$ .

For  $\xi \rightarrow 0$  and  $\xi \rightarrow G$  one obtains the system of equations which can be written in the matrix form

$$\mathbf{A} \cdot \mathbf{W}^f = \mathbf{B} \cdot \mathbf{T}^f + \mathbf{Z}^f \quad (18)$$

where

$$\mathbf{A} = \begin{bmatrix} -\frac{1}{2\lambda\sqrt{B}} & \frac{1}{2\lambda\sqrt{B}} \exp(-G\sqrt{B}) \\ -\frac{1}{2\lambda\sqrt{B}} \exp(-G\sqrt{B}) & \frac{1}{2\lambda\sqrt{B}} \end{bmatrix} \quad (19)$$

$$\mathbf{B} = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} \exp(-G\sqrt{B}) \\ \frac{1}{2} \exp(-G\sqrt{B}) & -\frac{1}{2} \end{bmatrix} \quad (20)$$

$$\mathbf{W}^f = \begin{bmatrix} W(0, t^f) \\ W(G, t^f) \end{bmatrix}, \quad \mathbf{T}^f = \begin{bmatrix} T(0, t^f) \\ T(G, t^f) \end{bmatrix},$$

$$\mathbf{Z}^f = \begin{bmatrix} Z(0, t^f) \\ Z(G, t^f) \end{bmatrix} \quad (21)$$

At the end of this part of considerations, the problem of matrix  $\mathbf{W}^f$  elements computations should be explained. So, the modified Neumann condition (5) can be written in the form

$$q_b(x, t^f) + \tau_q \frac{\partial q_b(x, t^f)}{\partial t} = -\lambda \frac{\partial T(x, t^f)}{\partial x} - \lambda \frac{\tau_T}{\Delta t} \left[ \frac{\partial T(x, t^f)}{\partial x} - \frac{\partial T(x, t^{f-1})}{\partial x} \right] \quad (22)$$

and next



$$W(x, t^f) = \frac{\Delta t}{\Delta t + \tau_T} \left[ q_b(x, t^f) + \tau_q \frac{\partial q_b(x, t^f)}{\partial t} \right] - \frac{\lambda \tau_T}{\Delta t + \tau_T} \frac{\partial T(x, t^{f-1})}{\partial x} \quad (23)$$

If for  $x = 0$  the boundary heat flux is a constant value (as in the examples presented below) then

$$W(0, t^f) = \frac{\Delta t}{\Delta t + \tau_T} q_b - \frac{\lambda \tau_T}{\Delta t + \tau_T} \frac{T_1^{f-1} - T_0^{f-1}}{h/2} \quad (24)$$

while for  $x = G$  (the no-flux condition) one has

$$W(G, t^f) = -\frac{\lambda \tau_T}{\Delta t + \tau_T} \frac{T_{n+1}^{f-1} - T_n^{f-1}}{h/2} \quad (25)$$

where  $h$  is the length of internal cell. The knowledge of the boundary values allows one to calculate the values of temperatures for time  $t^f$  at the set of internal points  $\xi_j$

$$T(\xi_j, t^f) = \frac{1}{\lambda} q^*(\xi_j, G) T(G, t^f) - \frac{1}{\lambda} q^*(\xi_j, 0) T(0, t^f) - \frac{1}{\lambda} T^*(\xi_j, G) W(G, t^f) + \frac{1}{\lambda} T^*(\xi_j, 0) W(0, t^f) + Z(\xi_j, t^f) \quad (26)$$

The obtained temperature field constitutes the pseudo-initial condition for the next loop of computations.

#### 4. EXAMPLE OF COMPUTATIONS

At the stage of preliminary studies the simple example having the analytical solution (Dai & Nassar, 2001) has been considered. In particular, the heating of the single layer ( $G = 10^{-4}$ ) and the thermophysical parameters equal to  $\lambda = 1$ ,  $c = 1$ ,  $\tau_q = 1/\pi^2 + 100$ ,  $\tau_T = 1/\pi^2 + 10^{-6}$  is analyzed. The process is described by the following hyperbolic PDE

$$\frac{\partial T(x, t)}{\partial t} + \left( \frac{1}{\pi^2} + 100 \right) \frac{\partial^2 T(x, t)}{\partial t^2} = \frac{\partial^2 T(x, t)}{\partial x^2} + \left( \frac{1}{\pi^2} + 10^{-6} \right) \frac{\partial^3 T(x, t)}{\partial t \partial x^2} \quad (27)$$

The boundary – initial conditions are of the form

$$T(0, t) = 0, \quad T(G, t) = 0 \quad (28)$$

$$T(x, 0) = \sin(10^4 \pi x),$$

$$\left. \frac{\partial T(x, t)}{\partial t} \right|_{t=0} = -\pi^2 \sin(10^4 \pi x) \quad (29)$$

One can check that the analytical solution of the problem formulated above is the following (Dai & Nassar, 2001)

$$T(x, t) = \exp(-\pi^2 t) \sin(10^4 \pi x) \quad (30)$$

In figure 1 the comparison of analytical and numerical solutions at the points  $x = G/4$  and  $x = G/2$  is shown. The computations have been done for time step  $\Delta t = 0.005$  and  $n = 200$  internal cells. A very good agreement between both solutions is visible. Additionally, one can see that the initial temperatures ( $t=0$ ) at the points  $x=G/4$  and  $x=G/2$  are different. It results from the harmonic form of condition (29).

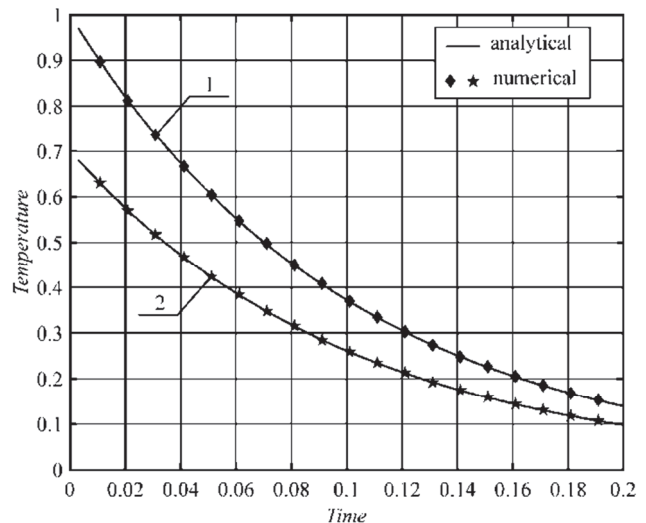


Fig. 1. Analytical and numerical solutions: 1 –  $x=G/4$ , 2 –  $x=G/2$

Let us define the error of numerical solution as follows

$$Err = \sqrt{\frac{1}{F(n+1)} \sum_{f=1}^F \sum_{j=0}^n (T_j^f - T_{aj}^f)^2} \quad (31)$$

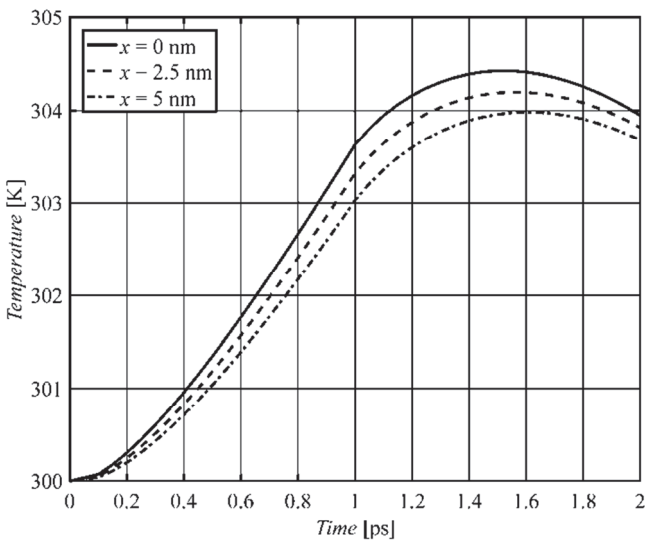
where  $F$  is the number of time steps, while  $T_{aj}^f$  are the local and temporary temperatures resulting from the analytical solution. The testing computations concerning the values of  $Err$  for different discretizations of time and space are collected in table 1.



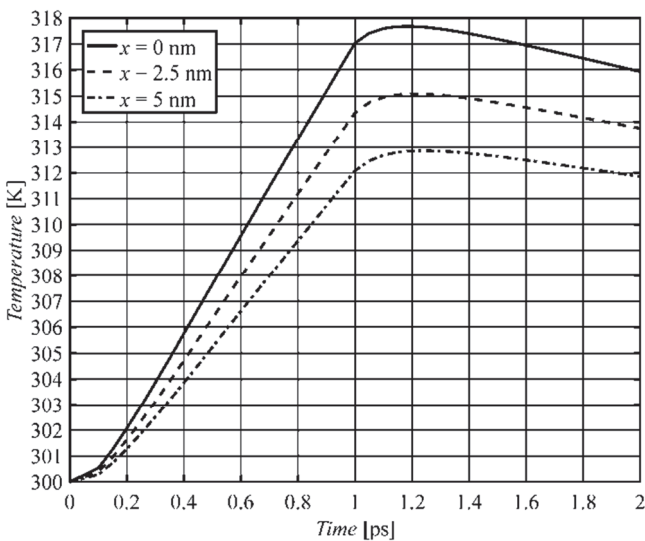
**Table 1.** Error for different time steps and number of internal cells.

$\Delta t$ [s]	$n = 50$	$n = 100$	$n = 200$	$n = 1000$
0.0005	–	–	–	$4.797 \cdot 10^{-4}$
0.001	–	–	$3.988 \cdot 10^{-4}$	$1.026 \cdot 10^{-3}$
0.005	$2.810 \cdot 10^{-3}$	$4.218 \cdot 10^{-3}$	$4.608 \cdot 10^{-3}$	$4.744 \cdot 10^{-3}$
0.01	$7.276 \cdot 10^{-3}$	$8.019 \cdot 10^{-3}$	$8.227 \cdot 10^{-3}$	$8.306 \cdot 10^{-3}$
0.015	$1.004 \cdot 10^{-2}$	$1.055 \cdot 10^{-2}$	$1.070 \cdot 10^{-2}$	$1.076 \cdot 10^{-2}$

Selection of the appropriate time step for the presumed discretization of the domain is rather difficult. In a number of numerical simulations the time interval must be short (for example the action of the ultrashort laser pulse) and then the number of internal cells should be increased.



**Fig. 2.** Temperature history at the selected points ( $q_b=10^{12}$  W/m<sup>2</sup>)



**Fig. 3.** Temperature history at the selected points ( $q_b=5 \cdot 10^{12}$  W/m<sup>2</sup>)

Next, the more practical problems have been solved. The chromium layer with a thickness of 100 nm and thermophysical parameters collected in (Majchrzak et al., 2009c) has been considered. The surface  $x = 0$  is subjected to a heat flux equal to  $10^{12}$  W/m<sup>2</sup> and next  $5 \cdot 10^{12}$  W/m<sup>2</sup>, while the exposure time equals 1 ps. The surface  $x = G$  is insulated. For  $t = 0$ :  $T(x, 0) = 300$  K, heating rate  $v(x, 0) = 0$ . In figure 2 the temperature histories at the points 1 ( $x = 0$ ), 2 ( $x = 2.5$  nm), 3 ( $x = 5$  nm) for  $q_b = 10^{12}$  W/m<sup>2</sup>, while in figure 3 the similar solution for  $q_b = 5 \cdot 10^{12}$  W/m<sup>2</sup> are shown.

**5. CONCLUSIONS**

As would be expected the temporary temperatures corresponding to the second solution are higher, of course. In spite of the fact that the exposure time is exceeded the chromium layer further heats up. It results from the delay times included in the dual phase lag model. In the case of the Fourier-type models the beginning of temperature dropping (close to the boundary surface) takes place immediately after the timeout action of external heat source. This effect is particularly visible for the lower values of  $q_b$ .

At the stage of numerical computations the BEM using discretization in time has been applied. Transition from time  $t^{f-1}$  to  $t^f$  requires the solution of a system of two linear equations, next the internal temperatures are calculated separately. It is undoubtedly the advantage of the method. Unfortunately it is not easy to choose the proper time step. The authors also noticed that for  $x = G$  the boundary temperature slightly decreases below the initial temperature. It is incorrect from a physical point of view and results from the error of numerical method. Generally speaking the BEM using discretization in time is more effective in the case of parabolic equations. Comparing the finite difference method with the BEM using discretization in time it should be noted that these methods have their pros and cons. As mentioned, in the case of the BEM the system of equations is connected only with the boundary nodes, while the internal temperatures are calculated at the second stage of numerical algorithm. The BEM assures good approximation of the boundary conditions. On the other hand, however, the FDM is simpler from the theoretical and numerical points of view. Additionally, the proper choice of time step is very simple and limited only by the stability condition (for explicit scheme, of course). The essentially



better seems to be the generalized boundary element method developed by Majchrzak (2010) and Majchrzak and Turchan (2015) in the scope of bioheat transfer. The authors intend to use the GBEM for the solution of the tasks similar to the problem discussed in this paper.

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## MODEL NUMERYCZNY NAGRZEWANIA ULTRACIENKIEJ WARSTWY METALOWEJ Z WYKORZYSTANIEM KOMBINOWANEJ METODY ELEMENTÓW BRZEGOWYCH

Streszczenie

Temat pracy jest związany z mikroskalowym przepływem ciepła zachodzącym w ultracienkich warstwach metalowych. W szczególności rozpatruje się nagrzewanie warstwy poddanej działaniu zewnętrznego strumienia ciepła o zadanej wydajności. Procesy cieplne zachodzące w rozpatrywanym obszarze opisano wykorzystując równanie z dwoma czasami opóźnienia uzupełnione odpowiednimi warunkami brzegowo-początkowymi. Na etapie obliczeń numerycznych wykorzystano tzw. kombinowany wariant metody elementów brzegowych. Jak dotąd, metoda ta nie była używana do przybliżonego rozwiązywania hiperbolicznych równań różniczkowych cząstkowych opisujących przepływ ciepła w mikroskali. W końcowej części pracy pokazano wyniki obliczeń numerycznych.

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