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ANALYTICAL AND NUMERICAL SOLUTIONS OF DIFFERENT TYPES OF EQUATIONS USED FOR MODELING HEAT CONDUCTION UNDER LASER PULSE HEATING

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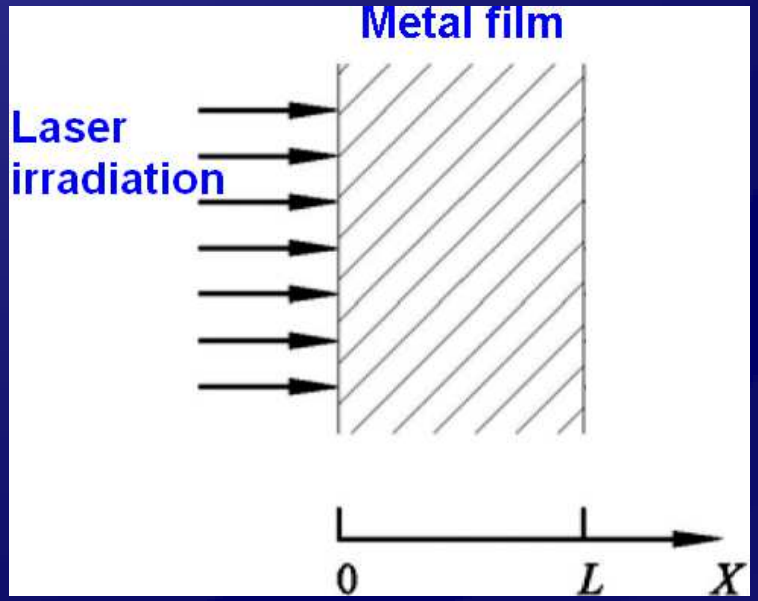
Introduction

In the paper, the problem of heat transfer proceeding in a thin film subjected to a short pulse laser heating is considered.

The mathematical model presented concerns a 1D problem.
For most short laser pulse interactions with thin films, the laser spot size is much larger than the film thickness.



Domain considered

The pulse duration is of the order of femtoseconds ($1\ \text{fs} = 10^{-15}\ \text{s}$).

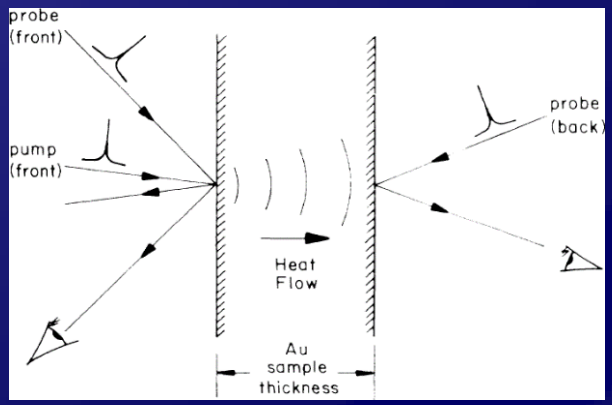
The thickness of the film is of the order of nanometers

$L \sim 100 - 200\ \text{nm}\ \ (1\ \text{nm} = 10^{-9}\ \text{m})$

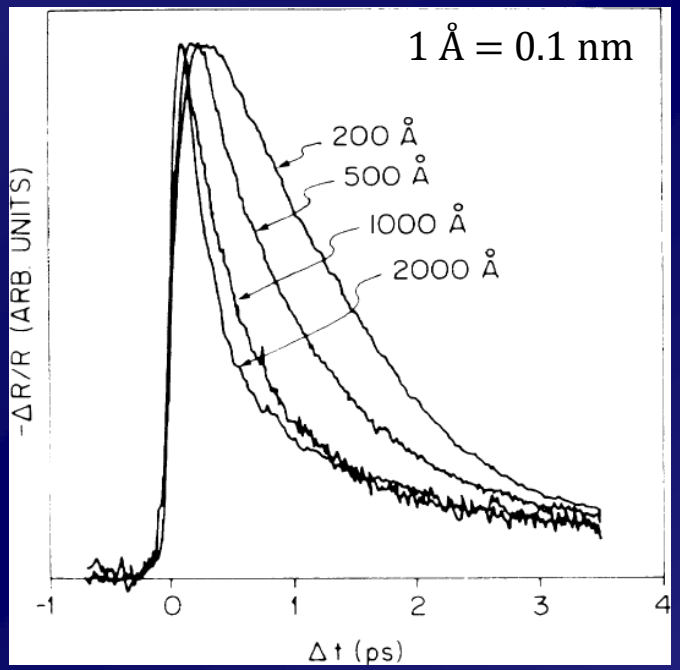
Experimental data

S.D. Brorson, J.G. Fujimoto, E.P. Ippen, *Femtosecond electronic heat-transport dynamics in thin gold films*, Phys. Rev. Lett. 59, 1987, pp. 1962-1965.

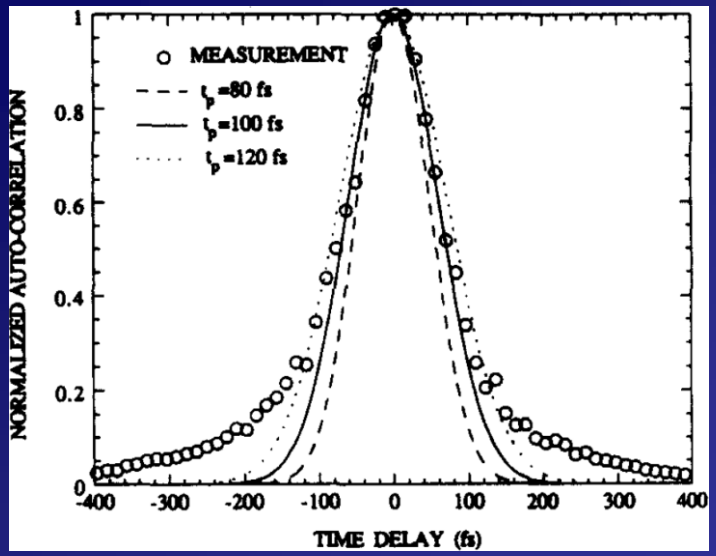
T.Q. Qiu, et al., *Femtosecond laser heating of multi-layer metals - II. Experiments*, International Journal of Heat and Mass Transfer 37, 17, 1994, pp. 2799–2808.



Schematic of the experimental setup



Front-surface data for Au films



Auto-correlation of laser pulses

Introduction

The dual phase lag model (DPLM) results from the generalization of the well known Fourier law. In particular, two lag times are introduced to this law.

Generalized Fourier law [*] is defined in the form

$$\mathbf{q}\left(x,\, t+\tau_q\right) = -\lambda\, \nabla T(x, t+\tau_T) \tag{1}$$

where
$\mathbf{q}(x,\, t)$ is a heat flux vector,
λ is a thermal conductivity,
τ_q is a relaxation time (the mean time for electrons to change their energy states),
τ_T is a thermalization time (the mean time required for electrons and lattice to reach equilibrium),
$T,\, x,\, t$ denote the temperature, geometrical co-ordinates and time.

[*] Tzou D.Y., Macro- to Microscale Heat Transfer: The Lagging Behavior, John Wiley & Sons, Ltd., 2015.

Using the Taylor series expansions, the following first-order approximation of Eq. (1) can be taken into account

$$\mathbf{q}(x,t) + \tau_q \frac{\partial \mathbf{q}(x,t)}{\partial t} = -\lambda \left[\nabla T(x,t) + \tau_T \frac{\partial \nabla T(x,t)}{\partial t} \right]$$

Next, this formula is introduced to the well known macroscopic energy equation

$$c \frac{\partial T(x,t)}{\partial t} = -\nabla \cdot \mathbf{q}(x,t) + Q(x,t)$$

where

c is a volumetric specific heat,

Q is a capacity of internal heat sources.

Finally, the energy equation called the **dual phase lag equation** is defined as

$$c\left[\frac{\partial T(x,t)}{\partial t}+\tau_q\frac{\partial^2 T(x,t)}{\partial t^2}\right]=\nabla\cdot[\lambda\,\nabla T(x,t)]+\tau_T\frac{\partial\,\nabla\cdot[\lambda\,\nabla T(x,t)]}{\partial t}+Q(x,t)+\tau_q\frac{\partial Q(x,t)}{\partial t} \quad (2)$$

In 1-D Cartesian coordinates and for λ=const : $\nabla\cdot[\lambda\,\nabla T(x,t)]=\lambda\frac{\partial^2 T(x,t)}{\partial x^2}$

If $\tau_q=0,\tau_T=0$: the Fourier-type heat conduction
If $\tau_q>0,\tau_T=0$: the hyperbolic Cattaneo-Vernotte model
If $\tau_q>0,\tau_T>0$: the DPLM

The energy equation is the hyperbolic PDE containing a first and second order time derivative and higher order mixed derivative in both time and space.

Dual phase lag equation is supplemented by the appropriate boundary and initial conditions.

Initial-boundary conditions

The Eq. (2) is supplemented by the no-flux conditions

$$x \in \Gamma: \quad -\lambda \left[\mathbf{n} \cdot \nabla T(x,t) + \tau_T \frac{\partial \left[\mathbf{n} \cdot \nabla T(x,t) \right]}{\partial t} \right] = 0 \tag{3}$$

where $\mathbf{n} \cdot \nabla T(x,t)$ is a normal derivative.
One can see, that the Neumann-type boundary condition differs from the similar one in the classical heat conduction model.

The initial conditions for the problem considered are of the form

$$t = 0: \quad T(x,t) = T_0(x), \quad \frac{\partial T(x,t)}{\partial t}\Big|_{t=0} = T_1(x) \tag{4}$$

where $T_0(x)$ is the known temperature and $T_1(x)$ is the initial heating rate (for the task considered $T_1(x)$ is assumed to be equal to 0).

Introduction

The effects of the femtosecond laser pulse irradiation on the surface $x = 0$ causes that the energy is delivered into the metal and its absorption occurs.

The internal heat source $Q(x, t)$ generated inside of metal is related with the action of laser beam

$$Q(x,t) = \sqrt{\frac{\beta}{\pi}} \frac{1-R}{t_p \delta} I_0 \exp\left(-\frac{x}{\delta} - \beta\left(\frac{t-2t_p}{t_p}\right)^2\right)$$

where

I_0 is a laser intensity,

R is a reflectivity of irradiated surface,

δ is an optical penetration depth,

$\beta = 4 \ln 2$,

t_p is a characteristic time of laser pulse.

Analitytical solution

The solution of the 1D hypergeometric PDE (2)
with the initial conditions (4) and the no-flux boundary conditions (3)
can be found in the general form as [*]

$$T(x,t) = \int_0^t \int_0^L \Phi(\xi,\tau) G(x,\xi,t-\tau)\, d\xi d\tau$$

$$- \int_0^L T_0(\xi) \left[\frac{\partial}{\partial \tau} G(x,\xi,t-\tau) \right]_{\tau=0} d\xi + \int_0^L \left(T_1(\xi) + \frac{1}{\tau_q} T_0(\xi) \right) G(x,\xi,t) d\xi$$

where $G(x,\xi,t)$ is the Green function

and $\Phi(x,t) = \frac{1}{c\,\tau_q} \left(Q(x,t) + \tau_q \frac{\partial Q(x,t)}{\partial t} \right)$.

[*] Polyanin A.D., Nazaikinskii V.E., *Handbook of Linear Partial Differential Equations for Engineers and Scientists*, Second Edition, CRC Press, Boca Raton-London, 2016.

Analitytical solution

The Green function $G(x,\xi,t)$ is determined by solving the following homogenous equation

$$\frac{\partial^2 G(x,\xi,t)}{\partial t^2}+\frac{1}{\tau_q}\frac{\partial G(x,\xi,t)}{\partial t}=\frac{\lambda}{c\tau_q}\left(\frac{\partial^2 G(x,\xi,t)}{\partial x^2}+\tau_T\frac{\partial^3 G(x,\xi,t)}{\partial t\partial x^2}\right)$$

which satisfies the initial conditions $G(x,\xi,t)|_{t=0}=0,\quad \frac{\partial G(x,\xi,t)}{\partial t}|_{t=0}=\delta(x-\xi)$

and the homogenous boundary conditions $\frac{\partial G(x,\xi,t)}{\partial x}|_{x=0}=0,\quad \frac{\partial G(x,\xi,t)}{\partial x}|_{x=L}=0$

The Green's function can be expressed as

$$G(x,\xi,t)=\sum_{n=0}^{\infty}\frac{\varphi_n(x)\,\varphi_n(\xi)}{\|\varphi_n\|}\psi_n(t),\quad \|\varphi_n\|=\int_0^L\varphi_n^2(x)\,dx$$

where functions φ_n and ψ_n should be determined.

[*] Polyanin A.D., Nazaikinskii V.E., *Handbook of Linear Partial Differential Equations for Engineers and Scientists*, Second Edition, CRC Press, Boca Raton-London, 2016.

Analitytical solution

The particular solution of Eq. (2) for $\Phi(x,t) = 0$ is the product of the functions

$$T(x,t) = \varphi(x)\psi(t) \qquad (*)$$

Introducing Eq. (*) into Eq. (2) (and omitting the term $\Phi(x,t)$) one obtains the equation

$$c\left(\varphi(x)\frac{d\psi(t)}{dt} + \tau_q\varphi(x)\frac{d^2\psi(t)}{dt^2}\right) = \lambda\left(\frac{d^2\varphi(x)}{dx^2}\psi(t) + \tau_T\frac{d^2\varphi(x)}{dx^2}\frac{d\psi(t)}{dt}\right)$$

Separating variables, we obtain

$$\frac{c}{\lambda}\frac{\tau_q\frac{d^2\psi(t)}{dt^2} + \frac{d\psi(t)}{dt}}{\psi(t) + \tau_T\frac{d\psi(t)}{dt}} = \frac{\frac{d^2\varphi(x)}{dx^2}}{\varphi(x)} = -\mu_n^2$$

where the two expressions have been set equal to the constant $-\mu_n^2$.

Analitytical solution

This yields two ODE's:

$$\frac{d^2\varphi(x)}{dx^2} + \mu_n^2\varphi(x) = 0, \qquad (*)$$

$$\tau_q \frac{d^2\psi(t)}{dt^2} + \left(1 + \mu_n^2 \frac{\lambda}{c\rho}\tau_T\right)\frac{d\psi(t)}{dt} + \mu_n^2 \frac{\lambda}{c\rho}\psi(t) = 0 \qquad (**)$$

The eigenfunctions and eigenvalues of the Sturm-Liouville problem (*) with the boundary conditions $\frac{d\varphi(x)}{dx}|_{x=0} = 0,\ \frac{d\varphi(x)}{dx}|_{x=L} = 0$ are the following

$$\varphi_n(x) = \cos(\mu_n x), \quad \mu_n = \frac{n\pi}{L}, \quad n = 0,1,\ldots$$

The functions ψ_n are determined by solving Eq. (**) with the initial conditions $\psi(0) = 0$ and $\mathrm{d}\psi(t)/dt|_{t=0} = 1$.

For $\tau_q < \tau_T$ the solution of the considered initial problem simplifies to the form

$$\psi_n(t) = \exp(-d_n t)\frac{\sinh(f_n t)}{f_n} \quad \text{where} \quad d_n = \frac{1}{2\tau_q}\left(1 + \mu_n^2 \frac{\lambda}{c}\tau_T\right) \quad f_n = \sqrt{d_n{}^2 - \mu_n^2 \frac{\lambda}{c}\frac{1}{\tau_q}}$$

Analitytical solution

The analytical solution of the initial-boundary value problem (2)-(4) under the assumption that $\tau_q < \tau_T$ is the following [*]

$$T(x,t) = \Phi\left(Z_0(t) + 2\sum_{n=1}^{\infty}\cos(\mu_n x)Z_n(t)\right) + T_0 \qquad (5)$$

where

$$Z_n(t) = \frac{1-(-1)^n\exp(-L/\delta)}{1+\delta^2(\mu_n)^2}\frac{\exp(-4\beta)}{4f_n}\left\{2\sqrt{\frac{\beta}{\pi}}\frac{\tau_q}{t_p}\left(\exp(-(d_n+f_n)t)-\exp(-(d_n-f_n)t)\right)\right.$$

$$+\left(1-\tau_q(d_n+f_n)\right)\exp\left((g_n^+)^2-(d_n+f_n)t\right)\left[\operatorname{erfc}(g_n^+)-\operatorname{erfc}\left(g_n^+-\frac{\sqrt{\beta}}{t_p}t\right)\right]$$

$$\left.-\left(1-\tau_q(d_n-f_n)\right)\exp\left((g_n^-)^2-(d_n-f_n)t\right)\left[\operatorname{erfc}(g_n^-)-\operatorname{erfc}\left(g_n^--\frac{\sqrt{\beta}}{t_p}t\right)\right]\right\}$$

$$\Phi = \frac{(1-R)I_0}{c\tau_q L} \qquad \mu_n = \frac{n\pi}{L} \qquad d_n = \frac{1}{2\tau_q}\left(1+\mu_n^2\frac{\lambda}{c}\tau_T\right) \qquad f_n = \sqrt{d_n^2-\mu_n^2\frac{\lambda}{c}\frac{1}{\tau_q}}$$

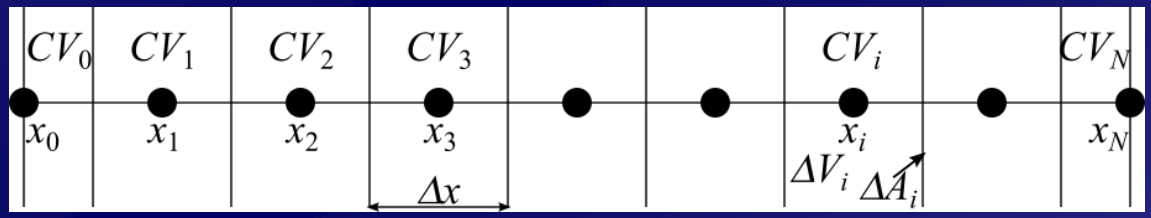
$$g_n^{\pm} = 2\sqrt{\beta}+\frac{t_p}{2\sqrt{\beta}}(d_n \pm f_n) \quad n=0,1,....$$

[*] M. Ciesielski, *Analytical solution of the dual phase lag equation decribing the laser heating of thin metal film*, Journal of Applied Mathematics and Computational Mechanics, 2017, 16, 1, 33-40.

Numerical solution

To find the approximate solution of the problem (2)-(4) the **Control Volume Method** (CVM) is used.

The first stage of the method application is the division of the domain considered into $N+1$ small cells (known as the control volumes CV) with the central nodes $0 = x_0 < x_1 < \ldots < x_i < \ldots < x_N = L$, $x_i = i\Delta x$, $\Delta x = L/N$. The values of the successive volumes ΔV_i and the values of surfaces ΔA_i limiting CV can be easily determined.



Mesh of control volumes

The aim of the CVM is to find the transient temperature field at the set of control volumes.

Numerical solution

The average temperatures in the all control volumes can be found on the basis of energy balances for the successive CV.

The energy balances corresponding to the heat exchange between the analyzed control volume and adjacent ones result from the integration of energy equation with respect to volume and time.

Integration of Eq. (2) over the control volume CV_i leads to

$$c \int_{CV_i} \left(\frac{\partial T(x,t)}{\partial t} + \tau_q \frac{\partial^2 T(x,t)}{\partial t^2} \right) d\Omega \qquad (6)$$

$$= \lambda \int_{CV_i} \left(\frac{\partial^2 T(x,t)}{\partial x^2} + \tau_T \frac{\partial}{\partial t} \frac{\partial^2 T(x,t)}{\partial x^2} \right) d\Omega + \int_{CV_i} \left(Q(x,t) + \tau_q \frac{\partial Q(x,t)}{\partial t} \right) d\Omega$$

Numerical solution

The integral occurring on the left-hand side of Eq. (6) can be approximated in the form

$$c\int_{CV_i}\left(\frac{\partial T(x,t)}{\partial t}+\tau_q\frac{\partial^2 T(x,t)}{\partial t^2}\right)d\Omega \cong c\left(\frac{dT_i}{dt}+\tau_q\frac{d^2T_i}{dt^2}\right)\Delta V_i \qquad (7)$$

where $T_i \equiv T(x_i,t)$.

In a similar way the numerical approximation of the source term in Eq. (6) can be found

$$\int_{CV_i}\left(Q(x,t)+\tau_q\frac{\partial Q(x,t)}{\partial t}\right)d\Omega \cong \left(Q_i+\tau_q\frac{dQ_i}{dt}\right)\Delta V_i \qquad (8)$$

where $Q_i \equiv Q_i(t)$ is the average value of the heat source in the volume CV_i.

- $Q_i \cong Q(x_i,t)$ - the simplest way, but inexact approximation,
- $Q_i \cong \frac{1}{\Delta V_i}\int_{CV_i} Q(x,t)d\Omega$ - can be calculated analytically or using numerical integration methods.

Numerical solution

Applying the divergence theorem to the term determining heat conduction (right hand side of Eq. (6)) between the volume CV_i bounded by the surfaces ΔA_i and its neighbourhoods one obtains (taking into account the boundary conditions)

$$\lambda \int_{CV_i} \left(\frac{\partial^2 T(x,t)}{\partial x^2} + \tau_T \frac{\partial}{\partial t} \frac{\partial^2 T(x,t)}{\partial x^2} \right) d\Omega = \lambda \, \mathbf{n} \cdot \int_{A_i} \left(\frac{\partial T(x,t)}{\partial x} + \tau_T \frac{\partial}{\partial t} \frac{\partial T(x,t)}{\partial x} \right) dA$$

$$\cong \lambda \, \Delta A_i \begin{cases} \dfrac{T_1 - T_0}{\Delta x} + \tau_T \dfrac{d}{dt} \dfrac{T_1 - T_0}{\Delta x} & \text{for } i = 0 \\ \left(\dfrac{T_{i+1} - T_i}{\Delta x} + \tau_T \dfrac{d}{dt} \dfrac{T_{i+1} - T_i}{\Delta x} \right) + \left(\dfrac{T_{i-1} - T_i}{\Delta x} + \tau_T \dfrac{d}{dt} \dfrac{T_{i-1} - T_i}{\Delta x} \right) & \text{for } i = 1, \ldots, N-1 \\ \dfrac{T_{N-1} - T_N}{\Delta x} + \tau_T \dfrac{d}{dt} \dfrac{T_{N-1} - T_N}{\Delta x} & \text{for } i = N \end{cases} \qquad (9)$$

$$= \Delta A_i \, \theta_i$$

where $\theta_i = \left(\dfrac{T_{i+1} - T_i}{R} + \tau_T \dfrac{d}{dt} \dfrac{T_{i+1} - T_i}{R} \right) \Bigg|^{\text{if } i<N} + \left(\dfrac{T_{i-1} - T_i}{R} + \tau_T \dfrac{d}{dt} \dfrac{T_{i-1} - T_i}{R} \right) \Bigg|^{\text{if } i>0}$

while $R = \Delta x / \lambda$ is the thermal resistance.

Putting Eqs. (7)-(9) into Eq. (6), one obtains

$$c\left(\frac{dT_i}{dt}+\tau_q\frac{d^2T_i}{dt^2}\right)\Delta V_i=\theta_i\,\Delta A_i+\left(Q_i+\tau_q\frac{dQ_i}{dt}\right)\Delta V_i$$

or

$$c\left(\frac{dT_i}{dt}+\tau_q\frac{d^2T_i}{dt^2}\right)=\theta_i\,\Phi_i+Q_i+\tau_q\frac{dQ_i}{dt} \qquad (10)$$

where

$$\Phi_i=\frac{1}{\Delta x},\ \text{for } i=1,\ldots,N-1, \qquad \Phi_0=\Phi_N=\frac{2}{\Delta x}$$

Numerical solution

The second stage of CVM is the integration of Eq. (10) with respect to time. So, the time grid: $0 = t^0 < t^1 < \ldots < t^f < \ldots < t^F$, $t^f = f\,\Delta t$ is introduced.

The Crank-Nicolson method involves a combination of implicit and explicit schemes. The energy balance for the transition $t^f \rightarrow t^{f+1}$, $f = 2,\ldots,F$ written in the convention of the α-scheme takes the form

$$c\left(\frac{T_i^{f+1} - T_i^f}{\Delta t} + \tau_q \frac{T_i^{f+1} - 2T_i^f + T_i^{f-1}}{(\Delta t)^2}\right) \qquad (11)$$

$$= \alpha\,\theta_i^{f+1}\Phi_i + (1-\alpha)\,\theta_i^f\Phi_i + Q_i^{f+1} + \tau_q \frac{Q_i^{f+1} - Q_i^f}{\Delta t}$$

where $\alpha \in [0,1]$ is the weighting factor
($\alpha = 0$ leads to the 'explicit' scheme, and $\alpha = 1$ to the fully 'implicit' scheme).

Numerical solution

After the transformations, the following system of equations is obtained

$$\left(c\frac{1+\mu_q}{\Delta t}+\alpha\frac{1+\mu_T}{R}\Phi_i\Big|^{\text{if } i<N}+\alpha\frac{1+\mu_T}{R}\Phi_i\Big|^{\text{if } i>0}\right)T_i^{f+1} \tag{12}$$

$$-\alpha\frac{1+\mu_T}{R}\Phi_i T_{i+1}^{f+1}\Big|^{\text{if } i<N}-\alpha\frac{1+\mu_T}{R}\Phi_i T_{i-1}^{f+1}\Big|^{\text{if } i>0} \qquad \text{for } i=0,\ldots,N$$

$$=c\frac{(1+2\mu_q)T_i^f-\mu_q T_i^{f-1}}{\Delta t}+\left(s_{i-1}^f\Big|^{\text{if } i>0}+s_{i+1}^f\Big|^{\text{if } i<N}\right)\Phi_i+(1+\mu_q)Q_i^{f+1}-\mu_q Q_i^f$$

where $\mu_q=\tau_q/\Delta t$, $\mu_T=\tau_T/\Delta t$ and

$$s_{i-1}^f=\frac{\alpha\mu_T-(1-\alpha)(1+\mu_T)}{R}\left(T_i^f-T_{i-1}^f\right)+\frac{(1-\alpha)\mu_T}{R}\left(T_i^{f-1}-T_{i-1}^{f-1}\right)$$

$$s_{i+1}^f=\frac{\alpha\mu_T-(1-\alpha)(1+\mu_T)}{R}\left(T_i^f-T_{i+1}^f\right)+\frac{(1-\alpha)\mu_T}{R}\left(T_i^{f-1}-T_{i+1}^{f-1}\right)$$

From the initial conditions (4) results $T_i^0=T_i^1=T_0$.

Example of computations

The 1D domain (plate) with dimensions $L = 100 \cdot 10^{-9}$ m is considered.

Thermophysical parameters of thin film (gold):

$\lambda = 317$ W/(mK),

$c = 2.4897 \cdot 10^{6}$ J/(m^{3}K),

$\tau_q = 8.5 \cdot 10^{-12}$ s,

$\tau_T = 90 \cdot 10^{-12}$ s.

The parameters of the laser pulse:

$I_0 = 13.7$ W/m^2,

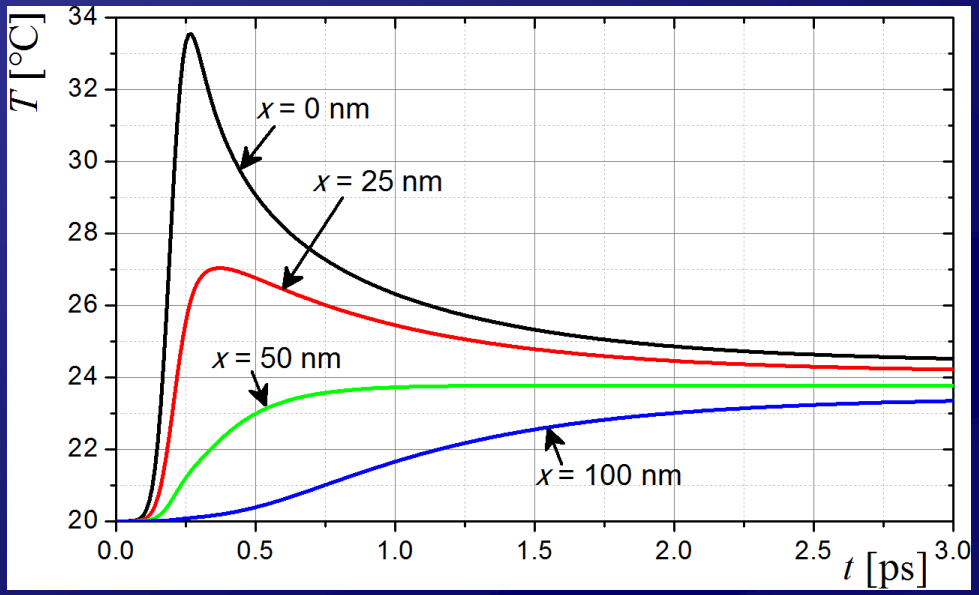
$R = 0.93$,

$\delta = 15.3 \cdot 10^{-9}$ m,

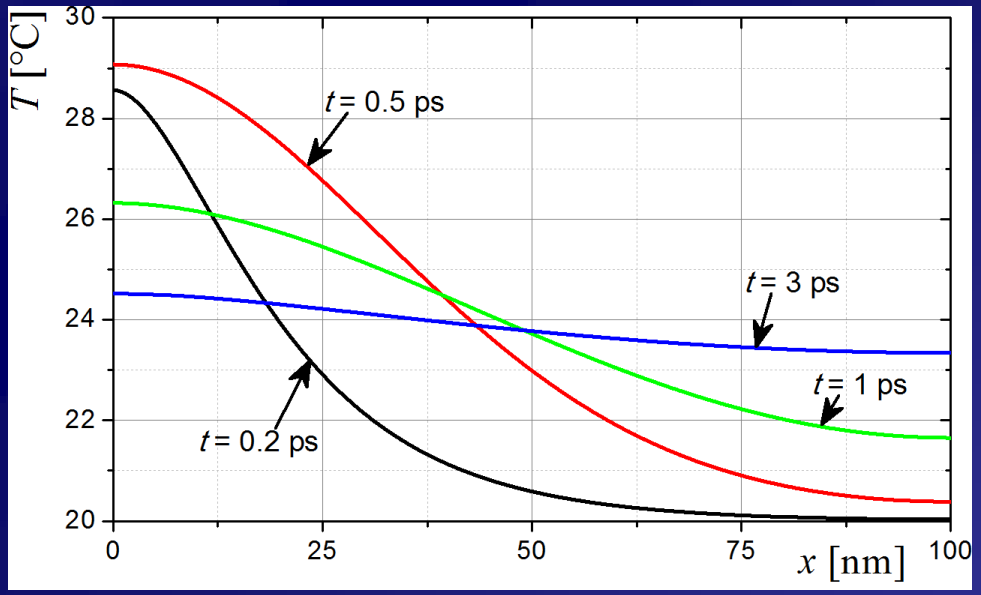
$t_p = 100 \cdot 10^{-15}$ s.

The initial temperature of the metal: $T_0 = 20$ ^{o}C.

The analytical solution of the DPL equation



The temperature histories
at the selected points from the domain:
$x = \{0, 25, 50, 100\ \text{nm}\}$



The temperature profiles
for the times:
$t = \{0.2, 0.5, 1, 3\ \text{ps}\}$

Results of computations

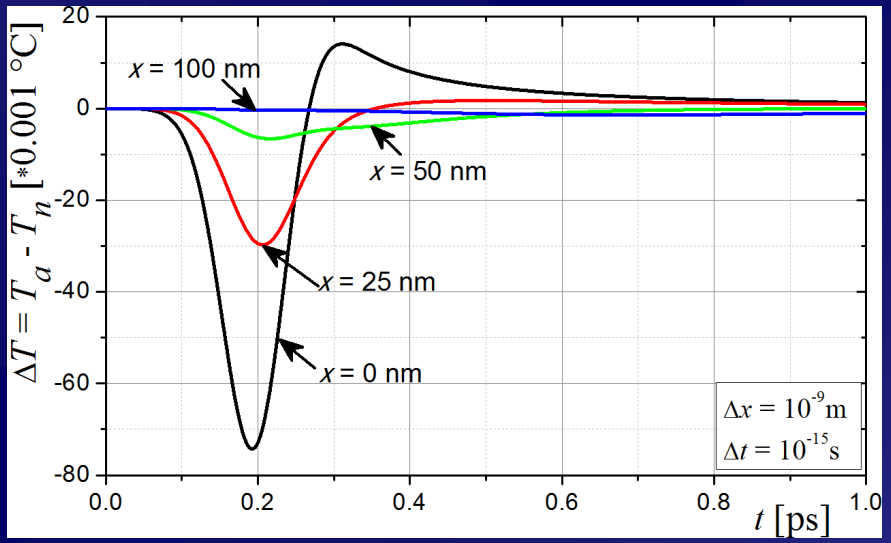
The errors of the numerical solutions (the Crank-Nicolson method)

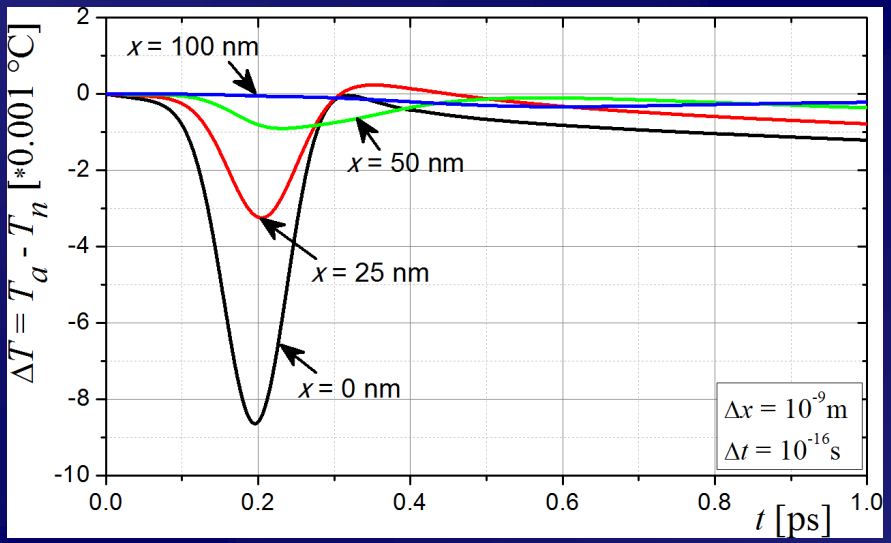
$$\Delta T(x,t) = T_{analytical}(x,t) - T_{numerical}(x,t)$$

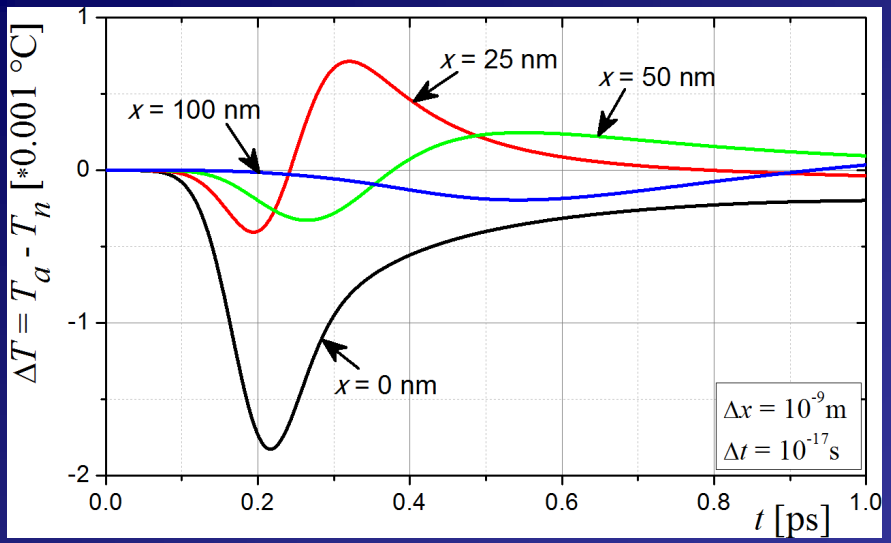
The numerical calculations were performed for different time mesh sizes: $\Delta t = \{10^{-15}, 10^{-16}, 10^{-17}\ \text{s}\}$ and

$\Delta x = 10^{-9}$ m ($N = 100$)

$\alpha = 0.5$







Results of computations

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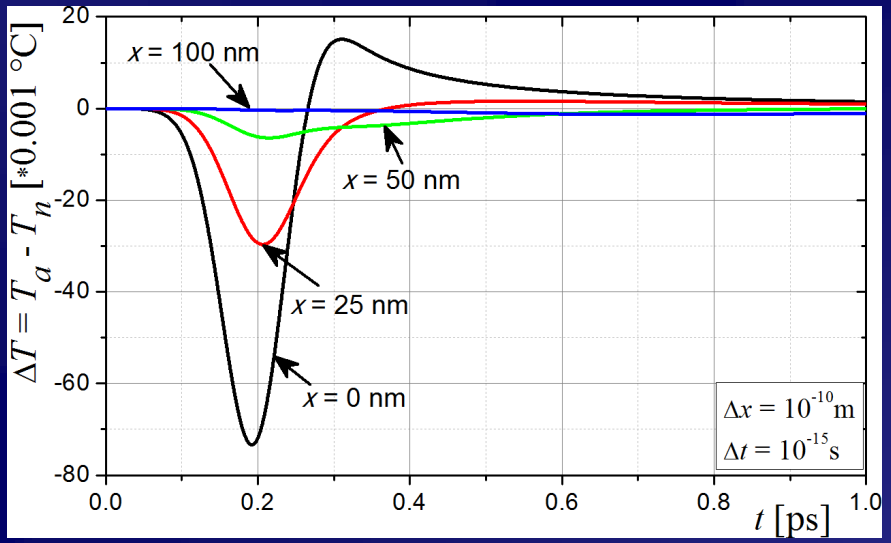
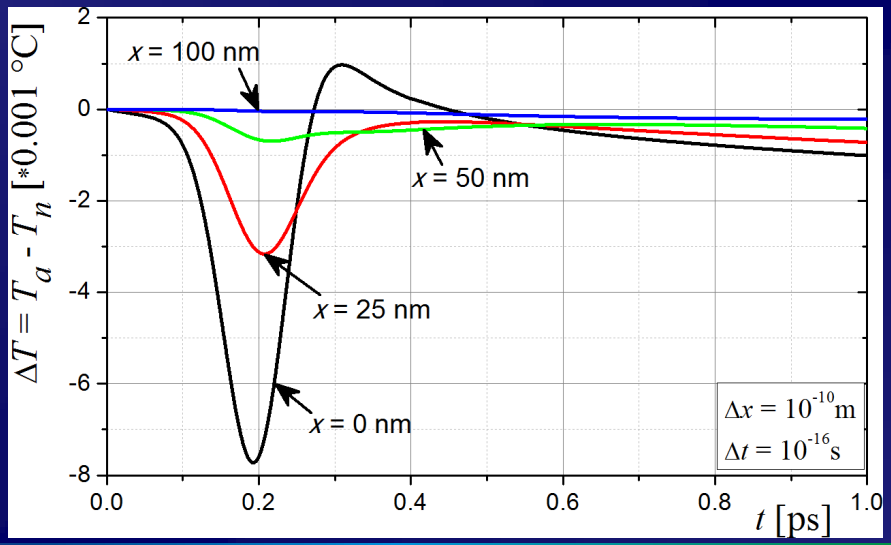
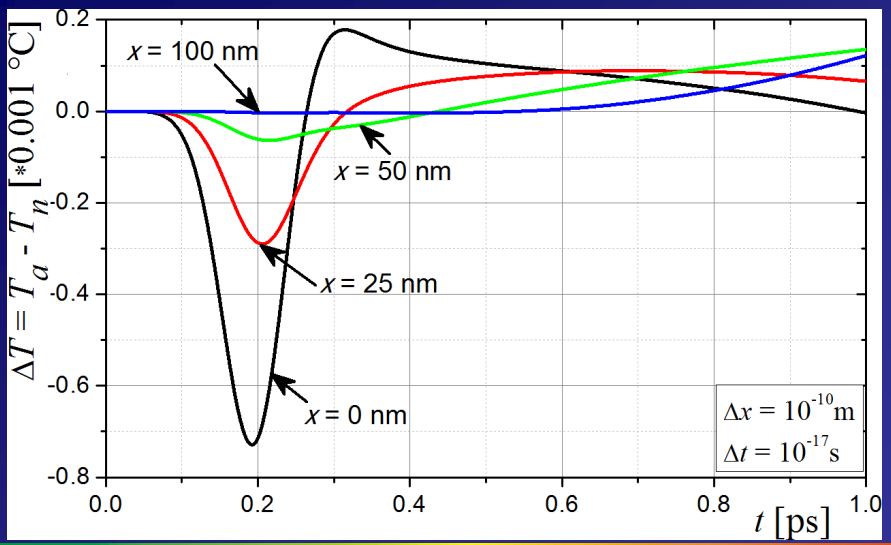
$\Delta x = 10^{-10}$ m ($N = 1000$)

$\alpha = 0.5$







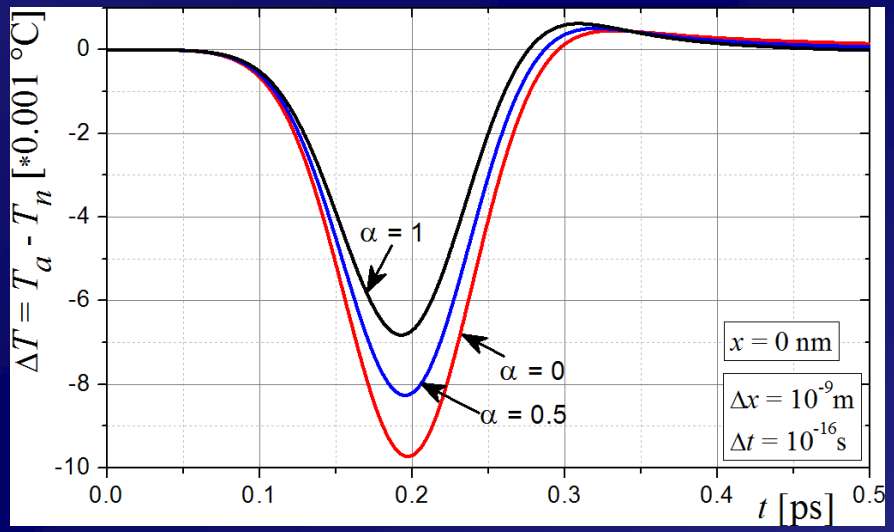
Results of computations

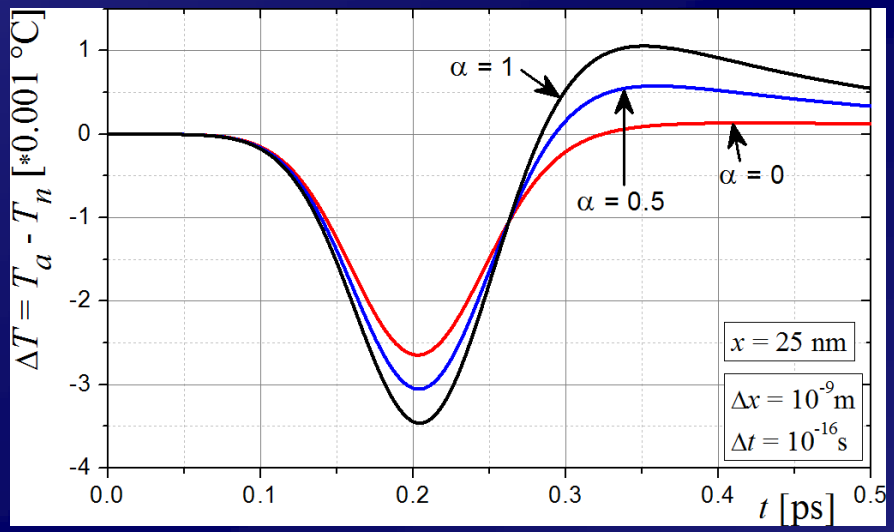
The errors of the numerical solutions (the Crank-Nicolson method)

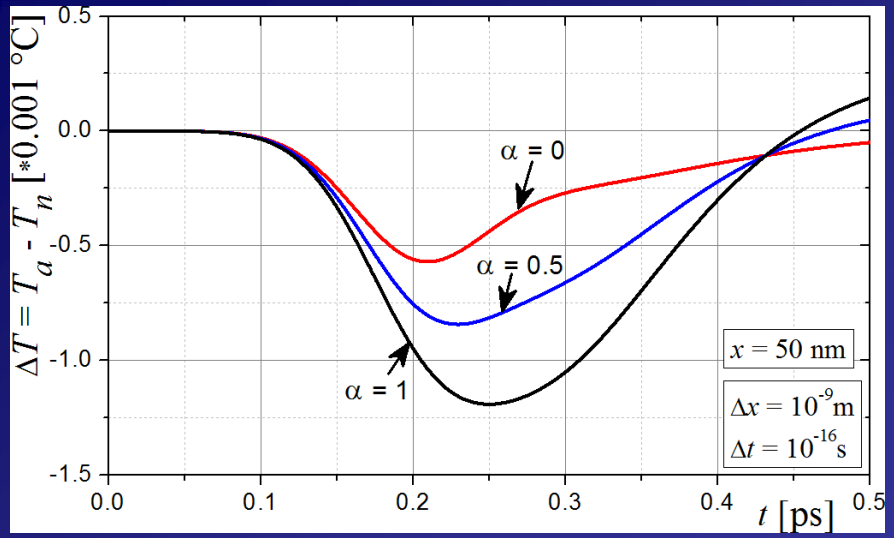
$$\Delta T(x,t) = T_{analytical}(x,t) - T_{numerical}(x,t)$$

The numerical calculations were performed for $\Delta t = 10^{-16}$ s, $\Delta x = 10^{-9}$ m at the points $x = (0, 25, 50$ nm).

In Figures, the influence of parameter $\alpha = \{0, 0.5, 1\}$ on numerical errors is presented.

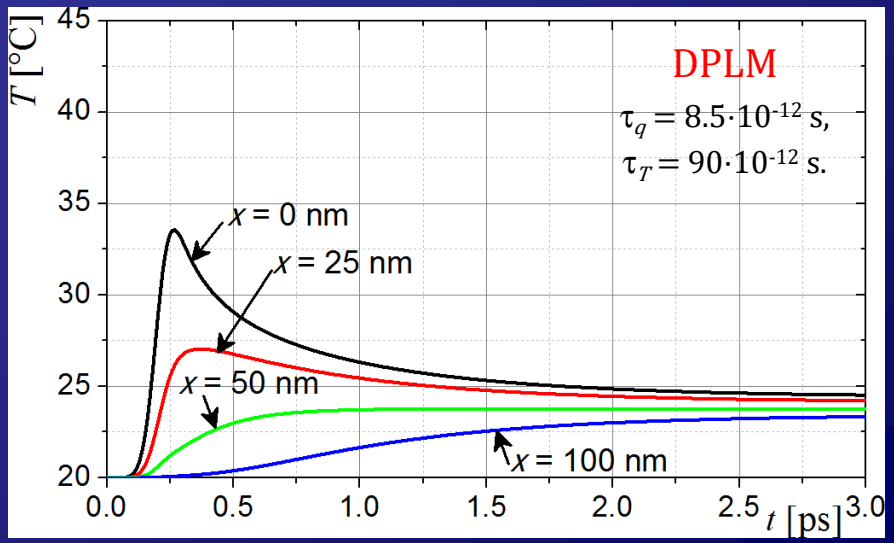


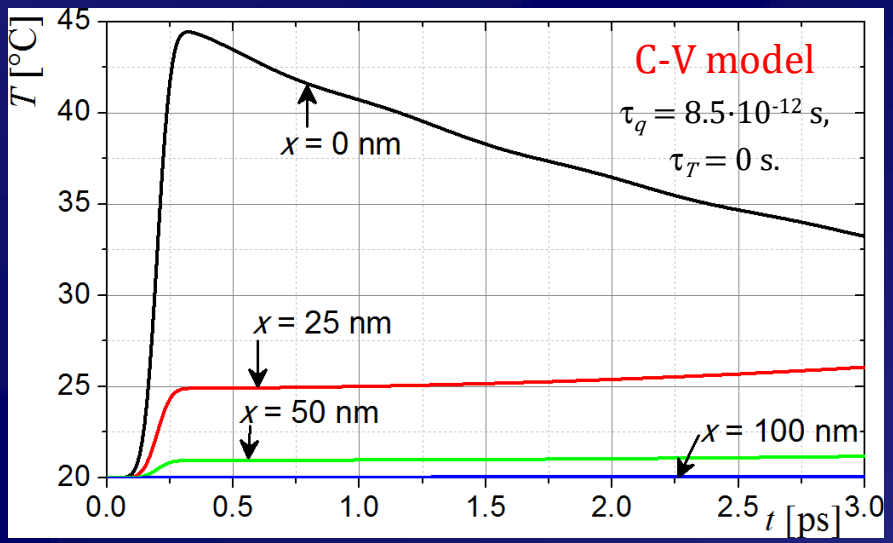


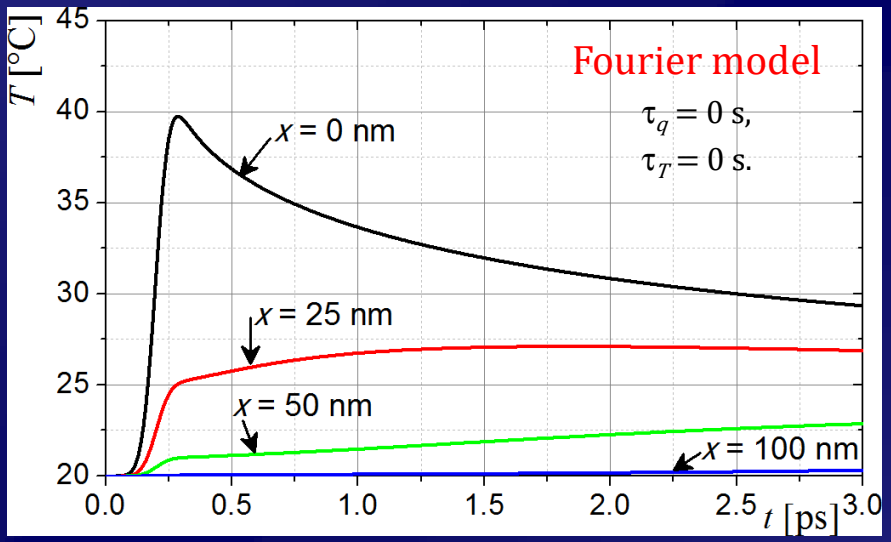


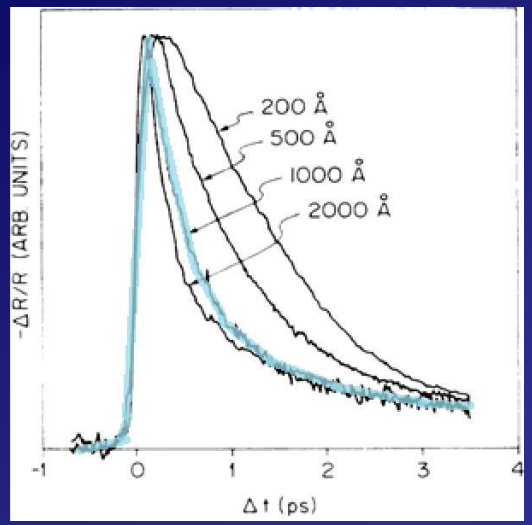
Results of computations

The influence of different values of parameters τ_q, τ_T on the solutions









Conclusions

Heat transfer processes can be described using the Fourier and non-Fourier heat conduction models, but the dual phase lag model seems to be adequate for mathematical description of microscale heat transfer.

One of the main subjects of the paper is the comparison of the results obtained using the analytical and numerical methods. In the case of the numerical solution, the control volume method and Crank-Nicolson scheme have been used.

The results of numerical computations confirm the effectiveness of the presented algorithm.

The 1D solution of the problem discussed is, as a rule, sufficiently exact, but the author has developed the computer programs realizing the computations for geometrically more complex domains.