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An unconditionally stable finite difference scheme for solving a 3D heat transport equation in a sub-microscale thin film

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Abstract

Heat transport at the microscale is of vital importance in microtechnology applications. The heat transport equation is different from the traditional heat diffusion equation since a second-order derivative of temperature with respect to time and a third-order mixed derivative of temperature with respect to space and time are introduced. In this study, we develop a finite difference scheme with two levels in time for the 3D heat transport equation in a sub-microscale thin film. It is shown by the discrete energy method that the scheme is unconditionally stable. The 3D implicit scheme is then solved by using a preconditioned Richardson iteration, so that only a tridiagonal linear system is solved for each iteration. The numerical procedure is employed to obtain the temperature rise in a gold sub-microscale thin film. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Finite difference; Stability; Heat transport equation; Thin film; Microscale

1. Introduction

Heat transport through thin films is of vital importance in microtechnology applications [9,10]. For instance, thin films of metals, of dielectrics such as SiO_2 , or Si semiconductors are important components of microelectronic devices. The reduction of the device size to microscale has the advantage of enhancing the switching speed of the device. On the other hand, size reduction increases the rate of heat generation which leads to a high thermal load on the microdevice. Heat transfer at the microscale is also important for the processing of materials with a pulsed-laser [12,13]. Examples in metal processing are laser micromachining, laser patterning, laser processing of diamond films from carbon ion implanted copper substrates, and laser surface hardening. Hence, studying the

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thermal behavior of thin films or of microobjects is essential for predicting the performance of a microelectronic device or for obtaining the desired microstructure [10]. The heat transport equations used to describe the thermal behavior of microstructures are expressed as [15]

$$-\nabla \cdot \vec{q} + Q = \rho C_p \frac{\partial T}{\partial t}, \quad (1)$$

$$\vec{q}(x, y, z, t + \tau_q) = -k \nabla T(x, y, z, t + \tau_T), \quad (2)$$

where $\vec{q} = (q_1, q_2, q_3)$ is heat flux, T is temperature, k is conductivity, C_p is specific heat, ρ is density, Q is a heat source, τ_q and τ_T are positive constants, which are the time lags of the heat flux and temperature gradient, respectively. In the classical theory of diffusion, the heat flux vector (\vec{q}) and the temperature gradient (∇T) across a material volume are assumed to occur at the same instant of time. They satisfy the Fourier's law of heat conduction:

$$\vec{q}(x, y, z, t) = -k \nabla T(x, y, z, t). \quad (3)$$

However, if the scale in one direction is at the sub-microscale, i.e., the order of $0.1 \mu\text{m}$ ($1 \mu\text{m} = 10^{-6} \text{m}$) then the heat flux and temperature gradient in this direction will occur at different times, as shown in Eq. (2) [15]. The significance of the heat transfer equations (1) and (2) as opposed to the classical heat transfer equations has been discussed in [15] (see pp. 127–128). In Fig. 5.9 (see p. 128 in [15]) the author shows that for $\tau_T = 90 \text{ps}$ and $\tau_q = 8.5 \text{ps}$ the predicted change in $\Delta T / \Delta T_{\max}$ over time gave an excellent fit to the data and was significantly different from that predicted by the classical heat transfer equations.

Using Taylor series expansion, the first-order approximation of Eq. (2) gives [15]

$$\vec{q} + \tau_q \frac{\partial \vec{q}}{\partial t} = -k \left[\nabla T + \tau_T \frac{\partial}{\partial t} [\nabla T] \right]. \quad (4)$$

Tzou et al. [14,15] considered Eqs. (1) and (4) in one dimension, and eliminated the heat flux \vec{q} to obtain a dimensionless heat transport equation as follows:

$$A \frac{\partial T}{\partial t} + D \frac{\partial^2 T}{\partial t^2} = \frac{\partial^2 T}{\partial x^2} + B \frac{\partial^3 T}{\partial x^2 \partial t} + G. \quad (5)$$

They studied the lagging behavior by solving the above heat transport equation (5) in a semi-infinite interval, $[0, +\infty)$. The solution was obtained by using the Laplace transform method and the Riemann-sum approximation for the inversion [1]. Recently, we have developed a two level finite difference scheme of the Crank–Nicholson type by introducing an intermediate function for solving Eq. (5) in a finite interval [2]. It is shown by the discrete energy method [11] that the scheme is unconditionally stable. Further, the scheme has been generalized to a 3D thin film case where the thickness is at sub-microscale [3].

In this article, we extend our research to a 3D case and consider the domain to be a sub-microscale thin film, i.e., $0 \leq x, y \leq L_1$ and $0 \leq z \leq L_2$, where L_1 and L_2 are of order of $0.1 \mu\text{m}$, as shown in Fig. 1. To this end, we first eliminate the heat flux \vec{q} in Eqs. (1) and (4) and obtain a single 3D heat transport equation for the temperature T . We then develop a two level finite difference scheme for the 3D heat transport equation in the sub-microscale thin film. Using the discrete energy method [11], we show that the scheme is unconditionally stable. To solve the 3D implicit scheme, a preconditioned Richardson iteration is developed based on the idea in our previous papers [4–7], so that only a tridiagonal linear systems is solved for each iteration. The method is then applied to

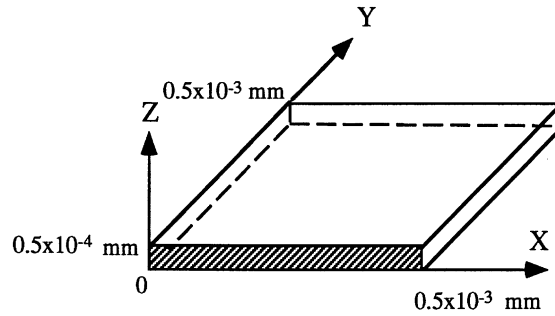


Fig. 1. Three dimensional configuration of a sub-microscale thin film.

obtain the temperature rise and the change of temperature on the surface of gold, where the length and width are assumed to $0.5 \mu\text{m}$ while the thickness is $0.05 \mu\text{m}$. It should be pointed out that predictions of temperature rise and temperature distribution in the thin film are essential to predict the thermal behavior in a nanophase structure.

2. Finite difference scheme

To develop a finite difference scheme, we first rewrite the heat transport equation (4) as follows:

$$q_1 + \tau_q \frac{\partial q_1}{\partial t} = -k \left[\frac{\partial T}{\partial x} + \tau_T \frac{\partial}{\partial t} \left(\frac{\partial T}{\partial x} \right) \right], \quad (6)$$

$$q_2 + \tau_q \frac{\partial q_2}{\partial t} = -k \left[\frac{\partial T}{\partial y} + \tau_T \frac{\partial}{\partial t} \left(\frac{\partial T}{\partial y} \right) \right], \quad (7)$$

$$q_3 + \tau_q \frac{\partial q_3}{\partial t} = -k \left[\frac{\partial T}{\partial z} + \tau_T \frac{\partial}{\partial t} \left(\frac{\partial T}{\partial z} \right) \right]. \quad (8)$$

Differentiating Eqs. (6)–(8) with respect to x , y , and z , respectively, and then substituting them into Eq. (1), we obtain

$$\frac{\partial T}{\partial t} + A \frac{\partial^2 T}{\partial t^2} = B \nabla^2 T + C \frac{\partial}{\partial t} \nabla^2 T + G, \quad (9)$$

where $A = \tau_q$, $B = k/\rho C_p$, $C = k\tau_T/\rho C_p$, and $G = (1/\rho C_p)(Q + \tau_q(\partial Q/\partial t))$. It should be pointed out that A , B and C are positive constants. The initial condition is assumed to be

$$T(x, y, z, 0) = T_0(x, y, z), \quad \frac{\partial T(x, y, z, 0)}{\partial t} = T_1(x, y, z). \quad (10)$$

For simplifying the proof for stability in Section 3, the boundary conditions are assumed to be

$$T(0, y, z, t) = T_2, \quad T(L_1, y, z, t) = T_3, \quad T(x, 0, z, t) = T_4, \quad (11)$$

$$T(x, L_1, z, t) = T_5, \quad T(x, y, 0, t) = T_6, \quad T(x, y, L_2, t) = T_7, \quad (12)$$

where T_2 to T_7 are assumed to be constants. We also assume that the solution of the above initial and boundary value problem is smooth. Since the exact solution is difficult to obtain in general, our motivation is to develop a finite difference scheme for solving the above initial and boundary value problem. It is noted that if Eq. (9) is discretized directly using a Crank–Nicholson type of finite difference and a second-order central difference in time, then the scheme is three levels in time. Furthermore, the scheme may not be unconditionally stable. Unconditional stability is particularly important so that there are no restrictions on the mesh ratio, since the grid size in the x , y , and z directions of the solution domain is very small compared with the time increment. In this study, our goal is to obtain a scheme with two levels in time, second-order accuracy and unconditional stability. To this end, we let

$$u = T + A \frac{\partial T}{\partial t}. \quad (13)$$

In Theorem 1 (to be discussed in Section 3), we can show that our scheme is unconditionally stable for two cases, (1) $AB - C \geq 0$, and (2) $AB - C < 0$. Since $AB - C = (k/\rho C_P)(\tau_q - \tau_T)$, $AB - C \geq 0$ implies that $\tau_q \geq \tau_T$ while $AB - C < 0$ implies that $\tau_q < \tau_T$. For case 1, we obtain $\partial T/\partial t = (1/A)(u - T)$ from Eq. (13). Substituting the $\partial T/\partial t$ expression into Eq. (9) gives

$$\frac{\partial u}{\partial t} = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \left(\left(B - \frac{C}{A} \right) T + \frac{C}{A} u \right) + G. \quad (14)$$

For case 2, we obtain $T = u - A(\partial T/\partial t)$. Substituting the T value into Eq. (9) gives

$$\frac{\partial u}{\partial t} = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \left(Bu + (C - AB) \frac{\partial T}{\partial t} \right) + G. \quad (15)$$

We let u_{ijk}^n denote $u(i\Delta x, j\Delta y, k\Delta z, n\Delta t)$, where Δx , Δy , Δz and Δt are the x , y , and z directional spatial and temporal mesh sizes, respectively, $0 \leq i, j, k = 0, 1, \dots, N$ and $N\Delta x = N\Delta y = L_1$, $N\Delta z = L_2$. We use the following difference operators:

$$\nabla_x u_{ijk}^n = \frac{u_{i+1,j,k}^n - u_{i,j,k}^n}{\Delta x}, \quad \nabla_{\bar{x}} u_{ijk}^n = \frac{u_{ijk}^n - u_{i-1,j,k}^n}{\Delta x},$$

$$\delta_x^2 u_{ijk}^n = \frac{1}{\Delta x^2} (u_{i+1,j,k}^n - 2u_{i,j,k}^n + u_{i-1,j,k}^n)$$

and so on. It can be seen that $\delta_x^2 u_{ijk}^n = \nabla_{\bar{x}} \cdot \nabla_x u_{ijk}^n$.

We now discretize Eqs. (14) and (15) using a Crank–Nicholson type of finite difference to obtain

$$\frac{u_{ijk}^{n+1} - u_{ijk}^n}{\Delta t} = \frac{C}{2A} (\delta_x^2 + \delta_y^2 + \delta_z^2) (u_{ijk}^{n+1} + u_{ijk}^n) + \frac{1}{2} \left(B - \frac{C}{A} \right) (\delta_x^2 + \delta_y^2 + \delta_z^2) (T_{ijk}^{n+1} + T_{ijk}^n) + G_{ijk}^{n+1/2} \quad (16)$$

if $AB - C \geq 0$, and

$$\frac{u_{ijk}^{n+1} - u_{ijk}^n}{\Delta t} = \frac{1}{2} B (\delta_x^2 + \delta_y^2 + \delta_z^2) (u_{ijk}^{n+1} + u_{ijk}^n) + \frac{1}{\Delta t} (C - AB) (\delta_x^2 + \delta_y^2 + \delta_z^2) (T_{ijk}^{n+1} - T_{ijk}^n) + G_{ijk}^{n+1/2} \quad (17)$$

if $AB - C < 0$. On the other hand, Eq. (13) is discretized using the trapezoidal method

$$A \frac{T_{ijk}^{n+1} - T_{ijk}^n}{\Delta t} = -\frac{1}{2}(T_{ijk}^{n+1} + T_{ijk}^n) + \frac{1}{2}(u_{ijk}^{n+1} + u_{ijk}^n). \quad (18)$$

We now simplify Eq. (16) to obtain an equation for u_{ijk}^{n+1} . To this end, we solve for T_{ijk}^{n+1} from Eq. (18) to obtain

$$\left(A + \frac{\Delta t}{2}\right) T_{ijk}^{n+1} = \left(A - \frac{\Delta t}{2}\right) T_{ijk}^n + \frac{\Delta t}{2}(u_{ijk}^{n+1} + u_{ijk}^n)$$

and hence

$$\frac{1}{2} \left(A + \frac{\Delta t}{2}\right) (T_{ijk}^{n+1} + T_{ijk}^n) = AT_{ijk}^n + \frac{\Delta t}{4}(u_{ijk}^{n+1} + u_{ijk}^n).$$

Substituting $T_{ijk}^{n+1} + T_{ijk}^n$ into Eq. (16), we obtain

$$\begin{aligned} \left(A + \frac{\Delta t}{2}\right) \frac{u_{ijk}^{n+1} - u_{ijk}^n}{\Delta t} &= \frac{1}{2} \left(A + \frac{\Delta t}{2}\right) \frac{C}{A} (\delta_x^2 + \delta_y^2 + \delta_z^2) (u_{ijk}^{n+1} + u_{ijk}^n) \\ &\quad + \left(B - \frac{C}{A}\right) (\delta_x^2 + \delta_y^2 + \delta_z^2) \left[AT_{ijk}^n + \frac{\Delta t}{4}(u_{ijk}^{n+1} + u_{ijk}^n)\right] \\ &\quad + \left(A + \frac{\Delta t}{2}\right) G_{ijk}^{n+1/2} \\ &= \frac{1}{2} \left(C + \frac{\Delta t}{2}B\right) (\delta_x^2 + \delta_y^2 + \delta_z^2) (u_{ijk}^{n+1} + u_{ijk}^n) \\ &\quad + (AB - C) (\delta_x^2 + \delta_y^2 + \delta_z^2) T_{ijk}^n + \left(A + \frac{\Delta t}{2}\right) G_{ijk}^{n+1/2}. \end{aligned} \quad (19)$$

The same equation may be obtained by substituting T_{ijk}^{n+1} into Eq. (17). The initial and boundary conditions are:

$$T_{ijk}^0 = (T_0)_{ijk}, \quad u_{ijk}^0 = (T_0)_{ijk} + A(T_1)_{ijk}, \quad (20)$$

$$T_{0jk}^n = u_{0jk}^n = T_2, \quad T_{Njk}^n = u_{Njk}^n = T_3, \quad (21)$$

$$T_{i0k}^n = u_{i0k}^n = T_4, \quad T_{iNk}^n = u_{iNk}^n = T_5, \quad (22)$$

$$T_{ij0}^n = u_{ij0}^n = T_6, \quad T_{ijN}^n = u_{ijN}^n = T_7. \quad (23)$$

Hence, one may use Eq. (19) to obtain u_{ijk}^{n+1} and then use Eq. (18) to obtain T_{ijk}^{n+1} . Both equations are only two levels in time. Since we employ a Crank–Nicholson type of finite difference and the trapezoidal method, it can be seen that the truncation errors of Eqs. (16)–(18) at point $(i\Delta x, j\Delta y, k\Delta z, (n + \frac{1}{2})\Delta t)$ are second-order accurate.

3. Stability

We will employ the discrete energy method [11] to show the stability of the scheme, Eqs. (16) and (18), with initial and boundary conditions (20)–(23). To this end, we first introduce the definition of the inner product and norm between the mesh functions u_{ijk}^n and v_{ijk}^n . Let S_h be a set of $\{u^n = \{u_{ijk}^n\}$, with $u_{0jk}^n = u_{Njk}^n = u_{i0k}^n = u_{iNk}^n = u_{ij0}^n = u_{ijN}^n = 0\}$. For any $u^n, v^n \in S_h$, the inner product and norm are defined as follows:

$$(u^n, v^n) = \Delta x \Delta y \Delta z \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} \sum_{k=1}^{N-1} u_{ijk}^n v_{ijk}^n, \quad \|u^n\|^2 = (u^n, u^n),$$

$$\|\nabla_x u^n\|_1^2 = (\nabla_x u^n, \nabla_x u^n)_1 = \Delta x \Delta y \Delta z \sum_{i=0}^{N-1} \sum_{j=1}^{N-1} \sum_{k=1}^{N-1} (\nabla_x u_{ijk}^n)^2$$

and similarly for the y and z directions.

Lemma 1. For any $u^n, v^n \in S_h$,

$$(\nabla_x u^n, v^n) = -(u^n, \nabla_x v^n)$$

and

$$(\delta_x^2 u^n, v^n) = -(\nabla_x u^n, \nabla_x v^n)_1.$$

Similar results can be obtained for the y and z directions.

Proof. The above equations can be easily obtained by using the summation by parts (see [11]).

Theorem 1. Suppose that $\{u_{ijk}^n, T_{ijk}^n\}$ and $\{v_{ijk}^n, S_{ijk}^n\}$ are solutions of the scheme, Eqs. (16)–(18), with the same Dirichlet boundary conditions, and initial values $\{u_{ijk}^0, T_{ijk}^0\}$ and $\{v_{ijk}^0, S_{ijk}^0\}$, respectively. Let $\phi_{ijk}^n = u_{ijk}^n - v_{ijk}^n$, $\varepsilon_{ijk}^n = T_{ijk}^n - S_{ijk}^n$. Then $\{\phi_{ijk}^n, \varepsilon_{ijk}^n\}$ satisfy

$$\begin{aligned} \|\phi^n\|^2 + (AB - C)(\|\nabla_x \varepsilon^n\|_1^2 + \|\nabla_y \varepsilon^n\|_1^2 + \|\nabla_z \varepsilon^n\|_1^2) \\ \leq \|\phi^0\|^2 + (AB - C)(\|\nabla_x \varepsilon^0\|_1^2 + \|\nabla_y \varepsilon^0\|_1^2 + \|\nabla_z \varepsilon^0\|_1^2) \end{aligned} \quad (24)$$

if $AB - C \geq 0$ and

$$\begin{aligned} \|\phi^n\|^2 + (C - AB)(\|\nabla_x \varepsilon^n\|_1^2 + \|\nabla_y \varepsilon^n\|_1^2 + \|\nabla_z \varepsilon^n\|_1^2) \\ \leq \|\phi^0\|^2 + (C - AB)(\|\nabla_x \varepsilon^0\|_1^2 + \|\nabla_y \varepsilon^0\|_1^2 + \|\nabla_z \varepsilon^0\|_1^2) \end{aligned} \quad (25)$$

if $AB - C < 0$ for any n in $0 \leq n\Delta t \leq t_0$. Hence, this scheme is unconditionally stable with respect to the initial values.

Proof. We first rewrite Eq. (16) as follows:

$$\begin{aligned} A \frac{u_{ijk}^{n+1} - u_{ijk}^n}{\Delta t} &= \frac{1}{2} C (\delta_x^2 + \delta_y^2 + \delta_z^2) (u_{ijk}^{n+1} + u_{ijk}^n) \\ &\quad + \frac{1}{2} (AB - C) (\delta_x^2 + \delta_y^2 + \delta_z^2) (T_{ijk}^{n+1} + T_{ijk}^n) + AG_{ijk}^{n+1/2}. \end{aligned}$$

Since $\{u_{ijk}^n, T_{ijk}^n\}$ and $\{v_j^n, S_{ijk}^n\}$ are solutions of the scheme with the same boundary conditions and initial values $\{u_{ijk}^0, T_{ijk}^0\}$ and $\{v_{ijk}^0, S_{ijk}^0\}$, respectively, we let $\phi_{ijk}^n = u_{ijk}^n - v_{ijk}^n$, $\varepsilon_{ijk}^n = T_{ijk}^n - S_{ijk}^n$. Then, $\phi^n, \varepsilon^n \in S_h$, and satisfy (from the above equation and Eq. (18))

$$A \frac{\phi_{ijk}^{n+1} - \phi_{ijk}^n}{\Delta t} = \frac{1}{2} C (\delta_x^2 + \delta_y^2 + \delta_z^2) (\phi_{ijk}^{n+1} + \phi_{ijk}^n) + \frac{1}{2} (AB - C) [\delta_x^2 + \delta_y^2 + \delta_z^2] (\varepsilon_{ijk}^{n+1} + \varepsilon_{ijk}^n) \quad (26)$$

and

$$A \frac{\varepsilon_{ijk}^{n+1} - \varepsilon_{ijk}^n}{\Delta t} = -\frac{1}{2} (\varepsilon_{ijk}^{n+1} + \varepsilon_{ijk}^n) + \frac{1}{2} (\phi_{ijk}^{n+1} + \phi_{ijk}^n). \quad (27)$$

Multiplying Eq. (26) by $(\phi_{ijk}^{n+1} + \phi_{ijk}^n)$, then summing i, j, k from 1 to $N - 1$, one obtains

$$\begin{aligned} \frac{A}{\Delta t} (\|\phi^{n+1}\|^2 - \|\phi^n\|^2) &= \frac{1}{2} (AB - C) (\delta_x^2 (\varepsilon^{n+1} + \varepsilon^n), \phi^{n+1} + \phi^n) \\ &\quad + \frac{1}{2} (AB - C) (\delta_y^2 (\varepsilon^{n+1} + \varepsilon^n), \phi^{n+1} + \phi^n) \\ &\quad + \frac{1}{2} (AB - C) (\delta_z^2 (\varepsilon^{n+1} + \varepsilon^n), \phi^{n+1} + \phi^n) \\ &\quad + \frac{1}{2} C (\delta_x^2 (\phi^{n+1} + \phi^n), \phi^{n+1} + \phi^n) \\ &\quad + \frac{1}{2} C (\delta_y^2 (\phi^{n+1} + \phi^n), \phi^{n+1} + \phi^n) \\ &\quad + \frac{1}{2} C (\delta_z^2 (\phi^{n+1} + \phi^n), \phi^{n+1} + \phi^n). \end{aligned}$$

By Lemma 1, we have

$$\begin{aligned} \frac{A}{\Delta t} (\|\phi^{n+1}\|^2 - \|\phi^n\|^2) &= -\frac{1}{2} (AB - C) (\nabla_x (\varepsilon^{n+1} + \varepsilon^n), \nabla_x (\phi^{n+1} + \phi^n))_1 \\ &\quad - \frac{1}{2} (AB - C) (\nabla_y (\varepsilon^{n+1} + \varepsilon^n), \nabla_y (\phi^{n+1} + \phi^n))_1 \\ &\quad - \frac{1}{2} (AB - C) (\nabla_z (\varepsilon^{n+1} + \varepsilon^n), \nabla_z (\phi^{n+1} + \phi^n))_1 \\ &\quad - \frac{1}{2} C \|\nabla_x (\phi^{n+1} + \phi^n)\|_1^2 - \frac{1}{2} C \|\nabla_y (\phi^{n+1} + \phi^n)\|_1^2 \\ &\quad - \frac{1}{2} C \|\nabla_z (\phi^{n+1} + \phi^n)\|_1^2. \end{aligned} \quad (28)$$

Further, we multiply Eq. (27) by $\delta_x^2 (\varepsilon_{ijk}^{n+1} + \varepsilon_{ijk}^n)$, and sum i, j, k from 1 to $N - 1$ to obtain

$$\frac{A}{\Delta t} (\varepsilon^{n+1} - \varepsilon^n, \delta_x^2 (\varepsilon^{n+1} + \varepsilon^n)) = -\frac{1}{2} (\varepsilon^{n+1} + \varepsilon^n, \delta_x^2 (\varepsilon^{n+1} + \varepsilon^n)) + \frac{1}{2} (\phi^{n+1} + \phi^n, \delta_x^2 (\varepsilon^{n+1} + \varepsilon^n)).$$

By Lemma 1, we have

$$-\frac{A}{\Delta t}(\|\nabla_x \varepsilon^{n+1}\|_1^2 - \|\nabla_x \varepsilon^n\|_1^2) = \frac{1}{2}\|\nabla_x(\varepsilon^{n+1} + \varepsilon^n)\|_1^2 - \frac{1}{2}(\nabla_x(\varepsilon^{n+1} + \varepsilon^n), \nabla_x(\phi^{n+1} + \phi^n))_1. \quad (29)$$

In a similar manner, we obtain for the y and z directions

$$-\frac{A}{\Delta t}(\|\nabla_y \varepsilon^{n+1}\|_1^2 - \|\nabla_y \varepsilon^n\|_1^2) = \frac{1}{2}\|\nabla_y(\varepsilon^{n+1} + \varepsilon^n)\|_1^2 - \frac{1}{2}(\nabla_y(\varepsilon^{n+1} + \varepsilon^n), \nabla_y(\phi^{n+1} + \phi^n))_1 \quad (30)$$

and

$$-\frac{A}{\Delta t}(\|\nabla_z \varepsilon^{n+1}\|_1^2 - \|\nabla_z \varepsilon^n\|_1^2) = \frac{1}{2}\|\nabla_z(\varepsilon^{n+1} + \varepsilon^n)\|_1^2 - \frac{1}{2}(\nabla_z(\varepsilon^{n+1} + \varepsilon^n), \nabla_z(\phi^{n+1} + \phi^n))_1. \quad (31)$$

If Eqs. (29)–(31) are multiplied by $-(AB - C)$, respectively, and added to Eq. (28), we obtain

$$\begin{aligned} & \frac{A}{\Delta t}(\|\phi^{n+1}\|^2 - \|\phi^n\|^2) + \frac{A(AB - C)}{\Delta t}(\|\nabla_x \varepsilon^{n+1}\|_1^2 - \|\nabla_x \varepsilon^n\|_1^2) \\ & + \frac{A(AB - C)}{\Delta t}(\|\nabla_y \varepsilon^{n+1}\|_1^2 - \|\nabla_y \varepsilon^n\|_1^2) + \frac{A(AB - C)}{\Delta t}(\|\nabla_z \varepsilon^{n+1}\|_1^2 - \|\nabla_z \varepsilon^n\|_1^2) \\ & + \frac{1}{2}C\|\nabla_x(\phi^{n+1} + \phi^n)\|_1^2 + \frac{1}{2}C\|\nabla_y(\phi^{n+1} + \phi^n)\|_1^2 + \frac{1}{2}C\|\nabla_z(\phi^{n+1} + \phi^n)\|_1^2 \\ & + \frac{1}{2}(AB - C)\|\nabla_x(\varepsilon^{n+1} + \varepsilon^n)\|_1^2 + \frac{1}{2}(AB - C)\|\nabla_y(\varepsilon^{n+1} + \varepsilon^n)\|_1^2 \\ & + \frac{1}{2}(AB - C)\|\nabla_z(\varepsilon^{n+1} + \varepsilon^n)\|_1^2 = 0. \end{aligned}$$

Since $AB - C \geq 0$, one may drop the last six terms on the left-hand side from the above equation and obtain

$$\begin{aligned} & \frac{A}{\Delta t}(\|\phi^{n+1}\|^2 - \|\phi^n\|^2) + \frac{A(AB - C)}{\Delta t}(\|\nabla_x \varepsilon^{n+1}\|_1^2 - \|\nabla_x \varepsilon^n\|_1^2) \\ & + \frac{A(AB - C)}{\Delta t}(\|\nabla_y \varepsilon^{n+1}\|_1^2 - \|\nabla_y \varepsilon^n\|_1^2) + \frac{A(AB - C)}{\Delta t}(\|\nabla_z \varepsilon^{n+1}\|_1^2 - \|\nabla_z \varepsilon^n\|_1^2) \leq 0. \end{aligned}$$

Hence,

$$\begin{aligned} & \|\phi^{n+1}\|^2 + (AB - C)(\|\nabla_x \varepsilon^{n+1}\|_1^2 + \|\nabla_y \varepsilon^{n+1}\|_1^2 + \|\nabla_z \varepsilon^{n+1}\|_1^2) \\ & \leq \|\phi^n\|^2 + (AB - C)(\|\nabla_x \varepsilon^n\|_1^2 + \|\nabla_y \varepsilon^n\|_1^2 + \|\nabla_z \varepsilon^n\|_1^2). \end{aligned} \quad (32)$$

Summing n from 0 to n , we obtain Eq. (24)

$$\begin{aligned} & \|\phi^n\|^2 + (AB - C)(\|\nabla_x \varepsilon^n\|_1^2 + \|\nabla_y \varepsilon^n\|_1^2 + \|\nabla_z \varepsilon^n\|_1^2) \\ & \leq \|\phi^0\|^2 + (AB - C)(\|\nabla_x \varepsilon^0\|_1^2 + \|\nabla_y \varepsilon^0\|_1^2 + \|\nabla_z \varepsilon^0\|_1^2). \end{aligned}$$

For the case of $AB - C < 0$, one may use a similar argument. We first obtain from Eqs. (17) and (18)

$$\frac{\phi_{ijk}^{n+1} - \phi_{ijk}^n}{\Delta t} = \frac{1}{2}B(\delta_x^2 + \delta_y^2 + \delta_z^2)[\phi_{ijk}^{n+1} + \phi_{ijk}^n] + (C - AB)\frac{1}{\Delta t}(\delta_x^2 + \delta_y^2 + \delta_z^2)[\varepsilon_{ijk}^{n+1} - \varepsilon_{ijk}^n] \quad (33)$$

and

$$A\frac{\varepsilon_{ijk}^{n+1} - \varepsilon_{ijk}^n}{\Delta t} = -\frac{1}{2}(\varepsilon_{ijk}^{n+1} + \varepsilon_{ijk}^n) + \frac{1}{2}(\phi_{ijk}^{n+1} + \phi_{ijk}^n). \quad (34)$$

Multiplying Eq. (33) by $(\phi_{ijk}^{n+1} + \phi_{ijk}^n)$ and multiplying Eq. (34) by $\delta_x^2(\varepsilon_{ijk}^{n+1} - \varepsilon_{ijk}^n)$, $\delta_y^2(\varepsilon_{ijk}^{n+1} - \varepsilon_{ijk}^n)$ and $\delta_z^2(\varepsilon_{ijk}^{n+1} - \varepsilon_{ijk}^n)$, respectively, then summing i, j, k from 1 to $N - 1$, we obtain, by Lemma 1,

$$\begin{aligned} \frac{1}{\Delta t}(\|\phi^{n+1}\|^2 - \|\phi^n\|^2) &= -\frac{1}{\Delta t}(C - AB)(\nabla_x(\varepsilon^{n+1} - \varepsilon^n), \nabla_x(\phi^{n+1} + \phi^n))_1 \\ &\quad - \frac{1}{\Delta t}(C - AB)(\nabla_y(\varepsilon^{n+1} - \varepsilon^n), \nabla_y(\phi^{n+1} + \phi^n))_1 \\ &\quad - \frac{1}{\Delta t}(C - AB)(\nabla_z(\varepsilon^{n+1} - \varepsilon^n), \nabla_z(\phi^{n+1} + \phi^n))_1 \\ &\quad - \frac{1}{2}B\|\nabla_x(\phi^{n+1} + \phi^n)\|_1^2 - \frac{1}{2}B\|\nabla_y(\phi^{n+1} + \phi^n)\|_1^2 \\ &\quad - \frac{1}{2}B\|\nabla_z(\phi^{n+1} + \phi^n)\|_1^2 \end{aligned} \quad (35)$$

and

$$-\frac{A}{\Delta t}\|\nabla_x(\varepsilon^{n+1} - \varepsilon^n)\|_1^2 = \frac{1}{2}(\|\nabla_x \varepsilon^{n+1}\|_1^2 - \|\nabla_x \varepsilon^n\|_1^2) - \frac{1}{2}(\nabla_x(\varepsilon^{n+1} - \varepsilon^n), \nabla_x(\phi^{n+1} + \phi^n))_1, \quad (36)$$

$$-\frac{A}{\Delta t}\|\nabla_y(\varepsilon^{n+1} - \varepsilon^n)\|_1^2 = \frac{1}{2}(\|\nabla_y \varepsilon^{n+1}\|_1^2 - \|\nabla_y \varepsilon^n\|_1^2) - \frac{1}{2}(\nabla_y(\varepsilon^{n+1} - \varepsilon^n), \nabla_y(\phi^{n+1} + \phi^n))_1, \quad (37)$$

$$-\frac{A}{\Delta t}\|\nabla_z(\varepsilon^{n+1} - \varepsilon^n)\|_1^2 = \frac{1}{2}(\|\nabla_z \varepsilon^{n+1}\|_1^2 - \|\nabla_z \varepsilon^n\|_1^2) - \frac{1}{2}(\nabla_z(\varepsilon^{n+1} - \varepsilon^n), \nabla_z(\phi^{n+1} + \phi^n))_1. \quad (38)$$

If Eqs. (36)–(38) are multiplied by $(-2/\Delta t)(C - AB)$, respectively, and added to Eq. (35), one obtains

$$\begin{aligned} &\frac{1}{\Delta t}(\|\phi^{n+1}\|^2 - \|\phi^n\|^2) + \frac{C - AB}{\Delta t}(\|\nabla_x \varepsilon^{n+1}\|_1^2 - \|\nabla_x \varepsilon^n\|_1^2) \\ &\quad + \frac{C - AB}{\Delta t}(\|\nabla_y \varepsilon^{n+1}\|_1^2 - \|\nabla_y \varepsilon^n\|_1^2) + \frac{C - AB}{\Delta t}(\|\nabla_z \varepsilon^{n+1}\|_1^2 - \|\nabla_z \varepsilon^n\|_1^2) \\ &\quad + \frac{1}{2}B\|\nabla_x(\phi^{n+1} + \phi^n)\|_1^2 + \frac{1}{2}B\|\nabla_y(\phi^{n+1} + \phi^n)\|_1^2 + \frac{1}{2}B\|\nabla_z(\phi^{n+1} + \phi^n)\|_1^2 \end{aligned}$$

$$\begin{aligned}
& + \frac{2}{\Delta t^2} A(C - AB) \|\nabla_x(\varepsilon^{n+1} + \varepsilon^n)\|_1^2 + \frac{2}{\Delta t^2} A(C - AB) \|\nabla_y(\varepsilon^{n+1} + \varepsilon^n)\|_1^2 \\
& + \frac{2}{\Delta t^2} A(C - AB) \|\nabla_z(\varepsilon^{n+1} + \varepsilon^n)\|_1^2 = 0.
\end{aligned} \tag{39}$$

Since $AB - C < 0$, Eq. (39) can be simplified as follows:

$$\begin{aligned}
& \frac{1}{\Delta t} (\|\phi^{n+1}\|^2 - \|\phi^n\|^2) + \frac{(C - AB)}{\Delta t} (\|\nabla_x \varepsilon^{n+1}\|_1^2 - \|\nabla_x \varepsilon^n\|_1^2) \\
& + \frac{C - AB}{\Delta t} (\|\nabla_y \varepsilon^{n+1}\|_1^2 - \|\nabla_y \varepsilon^n\|_1^2) + \frac{C - AB}{\Delta t} (\|\nabla_z \varepsilon^{n+1}\|_1^2 - \|\nabla_z \varepsilon^n\|_1^2) \leq 0.
\end{aligned}$$

Hence, we obtain Eq. (25)

$$\begin{aligned}
& \|\phi^n\|^2 + (C - AB) (\|\nabla_x \varepsilon^n\|_1^2 + \|\nabla_y \varepsilon^n\|_1^2 + \|\nabla_z \varepsilon^n\|_1^2) \\
& \leq \|\phi^0\|^2 + (C - AB) (\|\nabla_x \varepsilon^0\|_1^2 + \|\nabla_y \varepsilon^0\|_1^2 + \|\nabla_z \varepsilon^0\|_1^2). \quad \square
\end{aligned}$$

4. Preconditioned Richardson iteration

Since Eq. (19) is a 3D implicit scheme, it involves very heavy computation. To simplify the computation, we first rewrite Eq. (19) as follows:

$$\begin{aligned}
(u_{ijk}^{n+1} - u_{ijk}^n) &= \frac{\Delta t}{2} \left(A + \frac{\Delta t}{2} \right)^{-1} \left(C + \frac{\Delta t}{2} B \right) (\delta_x^2 + \delta_y^2 + \delta_z^2) (u_{ijk}^{n+1} + u_{ijk}^n) \\
&+ \Delta t \left(A + \frac{\Delta t}{2} \right)^{-1} (AB - C) (\delta_x^2 + \delta_y^2 + \delta_z^2) T_{ijk}^n + \Delta t G_{ijk}^{n+(1/2)}
\end{aligned} \tag{40}$$

We then simplify the linear system (40) into a tridiagonal linear system by simplifying the coefficients related to the x and y based on the idea in [4–7] and develop a preconditioned Richardson iteration as follows:

$$\begin{aligned}
L_{\text{pre}}(u_{ijk}^{n+1})^{(m+1)} &= L_{\text{pre}}(u_{ijk}^{n+1})^{(m)} - \omega \left\{ [(u_{ijk}^{n+1})^{(m)} - u_{ijk}^n] \right. \\
&- \frac{\Delta t}{2} \left(A + \frac{\Delta t}{2} \right)^{-1} \left(C + \frac{\Delta t}{2} B \right) (\delta_x^2 + \delta_y^2 + \delta_z^2) [(u_{ijk}^{n+1})^{(m)} + u_{ijk}^n] \\
&- \Delta t \left(A + \frac{\Delta t}{2} \right)^{-1} (AB - C) (\delta_x^2 + \delta_y^2 + \delta_z^2) T_{ijk}^n \\
&\left. - \Delta t G_{ijk}^{n+(1/2)} \right\}, \quad m = 0, 1, 2, \dots,
\end{aligned} \tag{41}$$

where the preconditioner is chosen to be

$$L_{\text{pre}} = 1 + \left(A + \frac{\Delta t}{2}\right)^{-1} \left(C + \frac{\Delta t}{2}B\right) \left(\frac{2\Delta t}{\Delta x^2} + \frac{2\Delta t}{\Delta y^2} - \frac{\Delta t}{2}\delta_z^2\right). \quad (42)$$

Here, ω is a relaxation parameter, $0 \leq \omega \leq 1$. L_{pre} in Eq. (42) is obtained from Eq. (41) by dropping out the coefficients of u_{i-1jk}^{n+1} , u_{i+1jk}^{n+1} , u_{ij-1k}^{n+1} and u_{ij+1k}^{n+1} , selecting the coefficients of u_{ijk}^{n+1} and doubling those related to x and y . It can be seen that the method in Eq. (41) is convergent. In fact, let

$$(\mathbf{A}_x \bar{\mathbf{u}}^{n+1})_{ijk} = -\frac{\Delta t}{2} \left(A + \frac{\Delta t}{2}\right)^{-1} \left(C + \frac{\Delta t}{2}B\right) \delta_x^2 u_{ijk}^{n+1},$$

$$(\mathbf{A}_y \bar{\mathbf{u}}^{n+1})_{ijk} = -\frac{\Delta t}{2} \left(A + \frac{\Delta t}{2}\right)^{-1} \left(C + \frac{\Delta t}{2}B\right) \delta_y^2 u_{ijk}^{n+1},$$

$$(\mathbf{A}_z \bar{\mathbf{u}}^{n+1})_{ijk} = -\frac{\Delta t}{2} \left(A + \frac{\Delta t}{2}\right)^{-1} \left(C + \frac{\Delta t}{2}B\right) \delta_z^2 u_{ijk}^{n+1},$$

where \mathbf{A}_x , \mathbf{A}_y and \mathbf{A}_z are matrices, and $\bar{\mathbf{u}}^{n+1}$ is a vector consisting of u_{ijk}^{n+1} , $i, j, k = 1, \dots, N-1$. Then the system (41) can be written in a vector form:

$$\mathbf{L}_{\text{pre}}(\bar{\mathbf{u}}^{n+1})^{(m+1)} = \mathbf{L}_{\text{pre}}(\bar{\mathbf{u}}^{n+1})^{(m)} - \omega\{(\bar{\mathbf{u}}^{n+1})^{(m)} + (\mathbf{A}_x + \mathbf{A}_y + \mathbf{A}_z)(\bar{\mathbf{u}}^{n+1})^{(m)} - \bar{\mathbf{f}}\}, \quad (43)$$

where the preconditioner is chosen as follows:

$$\mathbf{L}_{\text{pre}} = \left[1 + \left(A + \frac{\Delta t}{2}\right)^{-1} \left(C + \frac{\Delta t}{2}B\right) \left(\frac{2\Delta t}{\Delta x^2} + \frac{2\Delta t}{\Delta y^2}\right)\right] \mathbf{I} + \mathbf{A}_z$$

and

$$\begin{aligned} (\bar{\mathbf{f}})_{ijk} = & \left\{1 + \frac{\Delta t}{2} \left(A + \frac{\Delta t}{2}\right)^{-1} \left(C + \frac{\Delta t}{2}B\right) (\delta_x^2 + \delta_y^2 + \delta_z^2)\right\} u_{ijk}^n \\ & + \Delta t \left(A + \frac{\Delta t}{2}\right)^{-1} (AB - C) (\delta_x^2 + \delta_y^2 + \delta_z^2) T_{ijk}^n + \Delta t G_{ijk}^{n+(1/2)}. \end{aligned}$$

It should be pointed out that \mathbf{L}_{pre} is a tridiagonal matrix and hence only a tridiagonal linear system is solved for each iteration. Therefore, the computation is simple. It is well known from numerical linear algebra that the iteration process converges if the iteration operator

$$\mathbf{R} \equiv \mathbf{I} - \omega \mathbf{L}_{\text{pre}}^{-1} [\mathbf{I} + \mathbf{A}_x + \mathbf{A}_y + \mathbf{A}_z] \quad (44)$$

has a spectral radius $\rho(\mathbf{R}) < 1$. It can be shown that the eigenvalues of $\mathbf{L}_{\text{pre}}^{-1} [\mathbf{I} + \mathbf{A}_x + \mathbf{A}_y + \mathbf{A}_z]$ have the form

$$\lambda_{ijk} = \frac{1 + r_x \sin^2(i\pi\Delta x/2) + r_y \sin^2(j\pi\Delta y/2) + r_z \sin^2(k\pi\Delta z/2)}{1 + r_x + r_y + r_z \sin^2(k\pi\Delta z/2)},$$

where $r_x = 2(\Delta t/\Delta x^2)(A + (\Delta t/2))^{-1}(C + (\Delta t/2)B)$, $r_y = 2(\Delta t/\Delta y^2)(A + (\Delta t/2))^{-1}(C + (\Delta t/2)B)$, and $r_z = 2(\Delta t/\Delta z^2)(A + (\Delta t/2))^{-1}(C + (\Delta t/2)B)$. It is obvious that $0 < \lambda_{ijk} \leq 1$. If one chooses a relaxation parameter $\omega = 1$, then from Eq. (44) the spectral radius $\rho(\mathbf{R})$ will be less than 1. Hence, we conclude that the iteration method (43) is convergent when $\omega = 1$.

5. Numerical example

To demonstrate the applicability of the numerical procedure we investigate the temperature rise in a sub-microscale gold film. The thickness for the gold film is $0.5 \mu\text{m}$, while the length and width are $0.5 \mu\text{m}$, as shown in Fig. 1. The properties of gold are $C_p = 129 \text{ kJ/kg/K}$, $k = 317 \text{ W/m/K}$, $\rho = 19300 \text{ kg/m}^3$, $\tau_q = 8.5 \text{ ps}$ ($1 \text{ ps} = 10^{-12} \text{ s}$) and $\tau_T = 90 \text{ ps}$ [15,8].

The heat source was chosen to be [15]

$$Q(x, y, z, t) = 0.94J \left[\frac{1-R}{t_p \delta} \right] e^{-(z/\delta) - a|t-2t_p|/t_p} \quad (45)$$

where $J = 13.7(\text{J/m}^2)$, $t_p = 100 \text{ fs}$ ($1 \text{ fs} = 10^{-15} \text{ s}$), $\delta = 15.3 \text{ nm}$ ($1 \text{ nm} = 10^{-9} \text{ m}$), and $R = 0.93$.

The initial conditions were chosen as follows:

$$T(x, y, z, 0) = T_\infty, \quad \frac{\partial T}{\partial t}(x, y, z, 0) = 0, \quad (46)$$

where $T_\infty = 300 \text{ K}$.

The boundary conditions were assumed to be insulated. Such boundary conditions arise from the case that the thin film is subjected to a short-pulse laser irradiation. Hence, one may assume no heat losses from the film surfaces in the short-time response [15].

We chose a variety of meshes of $20 \times 20 \times 20$, $20 \times 20 \times 50$ and $20 \times 20 \times 100$ with a time increment of 0.005 ps . To use the preconditioned Richardson iteration (41), we chose $\omega = 1.0$ and the convergent solution $\{T_{ijk}^{n+1}\}$ was obtained if the convergence criterion

$$\max_{i,j,k} |(u_{ijk}^{n+1})^{(m+1)} - (u_{ijk}^{n+1})^{(m)}| < 10^{-7}$$

was satisfied.

Fig. 2 gives the temperature rise along the vertical line $x = 0.25 \mu\text{m}$ and $y = 0.25 \mu\text{m}$ for different times ($t = 0.2, 0.25$, and 0.5 ps) for the mesh $20 \times 20 \times 20$. It can be seen from the figure that the heat is transferred from the top to the bottom.

Fig. 3 shows the change in temperature $(\Delta T_1/(\Delta T_1)\text{Max})$ on the surface of the gold film using three different meshes. The maximum temperature rise of T_1 (i.e., $(\Delta T_1)\text{Max}$) on the surface of the gold film is about 10.25 K obtained using a mesh $20 \times 20 \times 20$. From this figure, it is seen that the temperature rises to a maximum at about 0.275 ps and then goes down. This figure is similar to that obtained in [15] for one dimension case (see p. 125 in [15]) except that the temperature rises start at $t = 0$. This is because in [15] it appears that the initial time was set equal to $2t_p$ in Eq. (45).

Furthermore, the preconditioned Richardson iteration is fast since the solution converges at most after a couple of iterations for each time step. The cpu time for a mesh of $20 \times 20 \times 50$ and $t = 0.5 \text{ ps}$ on a SUN workstation is about 6.5 min .

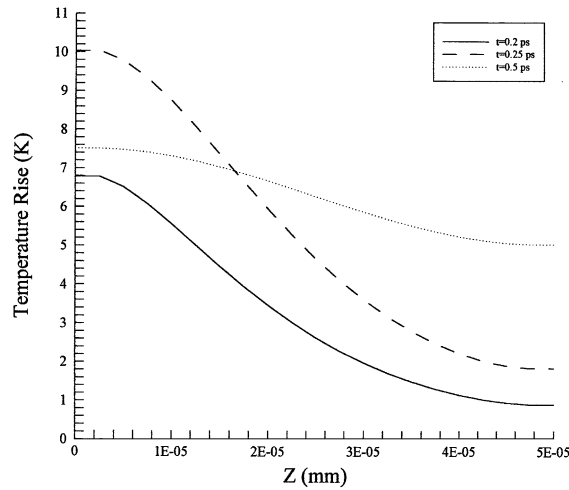


Fig. 2. Temperature profiles along the vertical line, $x = 0.25 \mu\text{m}$ and $y = 0.25 \mu\text{m}$. The mesh is $20 \times 20 \times 20$ with a time increment of 0.005 ps.

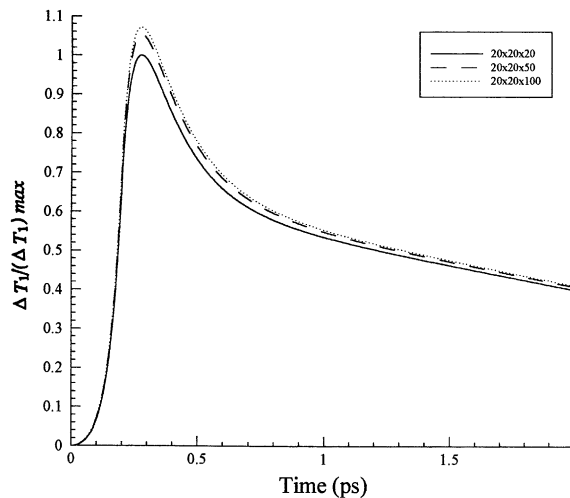


Fig. 3. Temperature change on the surface of the gold layer. The maximum temperature rise ($T_1 \text{ Max} = 10.25 \text{ K}$) was obtained using a grid of $20 \times 20 \times 20$.

6. Conclusion

In this study, we develop a finite difference scheme of the Crank–Nicholson type by introducing an intermediate function (Eq. 13) to the heat transport equation, Eq. (9). The scheme is two levels in time. It is shown by the discrete energy method that this scheme is unconditionally stable with respect to the initial values. To solve the 3D implicit finite difference scheme, a preconditioned Richardson iteration is developed so that only a tridiagonal linear system is solved for each iteration.

The numerical procedure is employed to obtain the temperature rise in a gold submicroscale thin film.

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