

AN UNCONDITIONALLY STABLE HYBRID FE-FD SCHEME FOR SOLVING A 3-D HEAT TRANSPORT EQUATION IN A CYLINDRICAL THIN FILM WITH SUB-MICROSCALE THICKNESS *

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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 transport 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 hybrid finite element-finite difference (FE-FD) scheme with two levels in time for the three dimensional heat transport equation in a cylindrical thin film with sub-microscale thickness. It is shown that the scheme is unconditionally stable. The scheme is then employed to obtain the temperature rise in a sub-microscale cylindrical gold film. The method can be applied to obtain the temperature rise in any thin films with sub-microscale thickness, where the geometry in the planar direction is arbitrary.

Key words: Finite element, 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 [11, 12]. Examples in metal processing are laser micro-machining, laser patterning, laser processing of diamond films from carbon ion implanted copper substrates, and laser surface hardening. Hence, studying the thermal behavior of thin films 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 [14]:

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

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

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

* Received May 15, 2001; final revised March 25, 2002.

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 $0.1\mu m$ ($1\mu m = 10^{-6}$ m) then the heat flux and temperature gradient in this direction will occur at different times, as shown in Eq. (2) [14]. The significance of the heat transfer equations (1) and (2) as opposed to the classical heat transfer equations has been discussed in [14] (see pp. 127-128). In Figure 5.9 (see p. 128 in [14]) the author shows that for $\tau_T = 90$ ps and $\tau_q = 8.5$ ps the predicted change in $\frac{\Delta T}{\Delta T_{\max}}$ 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 [14]

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

Tzou et al. [13, 14] considered Eqs. (1) and (4) in one dimension, and eliminated the heat flux \vec{q} to obtain a dimensionless heat transport equation as follows:

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

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 [3]. 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 [4]. The finite difference scheme has then been generalized to a rectangular thin film case where the thickness is at sub-microscale [5].

In this article, we consider the domain to be a cylindrical thin film with the radius in the xy -directions and the thickness to be of order of 1 mm and $0.1\mu m$, respectively, as shown in Figure 1. Since the finite element method is suitable for the cylindrical geometry, in this study we develop a two-level hybrid finite element-finite difference scheme for solving the three-dimensional heat transport equation in the sub-microscale thin film, by employing the finite element method to the xy -directions and the finite difference method to the z -direction. We show that the scheme is unconditionally stable. The method is then applied to obtain the temperature rise and the change of temperature on the surface of a cylindrical gold film, where the radius in the xy -directions is assumed to 1.0 mm and the thickness is $0.05\mu m$.

2. Hybrid Finite Element-Finite Difference

Since we consider a thin film with thickness of the order $0.1\mu m$ and the planar direction to be of the order of a millimeter, we may assume that there is thermal lagging in the thickness direction and no lagging in the planar direction. In essence, it presumes an orthotropic lagging response at short times, with τ_q and τ_T being nonzero in the thickness direction and zero in the planar direction perpendicular to the thickness direction. As such, the components of the heat flux in the x and y directions satisfy the traditional Fourier's law, while the component in the z direction satisfies Eq. (4). Hence, we obtain

$$q_1 = -k \frac{\partial T}{\partial x}, \quad (6)$$

$$q_2 = -k \frac{\partial T}{\partial y}, \quad (7)$$

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

Differentiating Eq. (8) with respect to z , and then substituting it with Eqs. (6) and (7) into Eq. (1), we obtain

$$\frac{\partial T}{\partial t} + A \frac{\partial^2 T}{\partial t^2} = B \nabla^2 T + \frac{\partial}{\partial t} \left\{ C \frac{\partial^2 T}{\partial x^2} + C \frac{\partial^2 T}{\partial y^2} + D \frac{\partial^2 T}{\partial z^2} \right\} + S, \tag{9}$$

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

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

The boundary conditions are assumed to be insulated, i.e.,

$$\frac{\partial T}{\partial \vec{n}} = 0, \tag{11}$$

where \vec{n} is the unit normal vector. 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 [14]. We also assume that the solution of the above initial and boundary value problem is smooth. Since the analytic solution for T is difficult to obtain if the shape of the film in the xy -directions is cylindrical or arbitrary, our motivation is to develop a hybrid finite element-finite difference scheme for solving the above initial and boundary value problem. Furthermore, unconditional stability is particularly important so that there are no restrictions on the mesh ratio, since the grid size in the z direction 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 and unconditional stability. To this end, we let

$$u = T + A \frac{\partial T}{\partial t}. \tag{12}$$

In theorem 1 (to be discussed in the next section), we can show that our scheme is unconditionally stable for two cases, 1) $AB - D \geq 0$ and 2) $AB - D < 0$. Since $AB - D = \frac{k}{\rho C_p} (\tau_q - \tau_T)$, $AB - D \geq 0$ implies that $\tau_q \geq \tau_T$ while $AB - D < 0$ implies that $\tau_q < \tau_T$. For case 1, we obtain $\frac{\partial T}{\partial t} = \frac{1}{A} (u - T)$ from Eq. (12). Substituting the $\frac{\partial T}{\partial t}$ expression into Eq. (9) gives (noted that

$$AB - C = 0)$$

$$\begin{aligned} \frac{\partial u}{\partial t} &= \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \left(\left(B - \frac{C}{A} \right) T + \frac{C}{A} u \right) + \frac{\partial^2}{\partial z^2} \left(\left(B - \frac{D}{A} \right) T + \frac{D}{A} u \right) + S \\ &= \frac{C}{A} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) u + \frac{\partial^2}{\partial z^2} \left(\left(B - \frac{D}{A} \right) T + \frac{D}{A} u \right) + S. \end{aligned} \tag{13}$$

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

$$\frac{\partial u}{\partial t} = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) B u + \frac{\partial^2}{\partial z^2} \left(B u + (D - AB) \frac{\partial T}{\partial t} \right) + S \tag{14}$$

We now employ the finite element method to the xy -directions. To this end, from Eq. (13) we let

$$\iint_G \frac{\partial u}{\partial t} \varphi dx dy = \iint_G \left[\frac{C}{A} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) u + \frac{\partial^2}{\partial z^2} \left(\left(B - \frac{D}{A} \right) T + \frac{D}{A} u \right) + S \right] \varphi dx dy,$$

where $\varphi(x, y)$ is a function in the Sobolev space H^1 and G is the domain of the thin film in the xy -directions. Since we assume that $\frac{\partial T}{\partial \vec{n}} = 0$ on the boundary of G , the above equation

becomes, by the Green's formula,

$$\begin{aligned} \iint_G \frac{\partial u}{\partial t} \varphi dx dy &= -\frac{C}{A} \iint_G \left(\frac{\partial u}{\partial x} \frac{\partial \varphi}{\partial x} + \frac{\partial u}{\partial y} \frac{\partial \varphi}{\partial y} \right) dx dy \\ &+ \left(B - \frac{D}{A} \right) \iint_G \frac{\partial^2 T}{\partial z^2} \varphi dx dy + \frac{D}{A} \iint_G \frac{\partial^2 u}{\partial z^2} \varphi dx dy \\ &+ \iint_G S \varphi dx dy. \end{aligned} \tag{15}$$

We construct a finite element mesh in G , as shown in Figure 2, and write test functions for $T(x, y, z, t)$ and $u(x, y, z, t)$ as follows:

$$T_h(x, y, z, t) = \sum_{p=1}^N T_p(z, t) \varphi_p(x, y), \quad u_h(x, y, z, t) = \sum_{p=1}^N u_p(z, t) \varphi_p(x, y),$$

where $\varphi_p(x, y)$ is a basis function, N is the number of grid points in G , p is a nodal point. Also, we consider $S_h = \sum_{p=1}^N S_p \varphi_p(x, y)$ as an interpolant of Q . Replacing T, u, S and φ by T_h, u_h, S_h and φ_q in Eq. (15), respectively, we obtain

$$\begin{aligned} &\sum_{p=1}^N \frac{\partial u_p}{\partial t} \iint_G \varphi_p \varphi_q dx dy \\ &= -\frac{C}{A} \sum_{p=1}^N u_p \iint_G \left(\frac{\partial \varphi_p}{\partial x} \frac{\partial \varphi_q}{\partial x} + \frac{\partial \varphi_p}{\partial y} \frac{\partial \varphi_q}{\partial y} \right) dx dy \\ &+ \left(B - \frac{D}{A} \right) \sum_{p=1}^N \frac{\partial^2 T_p}{\partial z^2} \iint_G \varphi_p \varphi_q dx dy \\ &+ \frac{D}{A} \sum_{p=1}^N \frac{\partial^2 u_p}{\partial z^2} \iint_G \varphi_p \varphi_q dx dy \\ &+ \sum_{p=1}^N S_p \iint_G \varphi_p \varphi_q dx dy, \quad q = 1, 2, \dots, N. \end{aligned} \tag{16}$$

Introducing the vector notations $\vec{T}(z, t) = [T_1(z, t), \dots, T_N(z, t)]^T$, $\vec{u}(z, t) = (u_1, \dots, u_N)^T$, $\vec{S}(z, t) = (S_1, \dots, S_N)^T$ and the matrices $\mathbf{M}_{N \times N}$ and $\mathbf{K}_{N \times N}$ with the two respective entries,

$$\mathbf{M}_{qp} = \iint_G \varphi_p \varphi_q dx dy, \quad \mathbf{K}_{qp} = \iint_G \left(\frac{\partial \varphi_p}{\partial x} \frac{\partial \varphi_q}{\partial x} + \frac{\partial \varphi_p}{\partial y} \frac{\partial \varphi_q}{\partial y} \right) dx dy,$$

we can express the system in Eq. (16) into a matrix form as follows:

$$\mathbf{M} \frac{\partial \vec{u}}{\partial t} = -\frac{C}{A} \mathbf{K} \vec{u} + \left(B - \frac{D}{A} \right) \mathbf{M} \frac{\partial^2 \vec{T}}{\partial z^2} + \frac{D}{A} \mathbf{M} \frac{\partial^2 \vec{u}}{\partial z^2} + \mathbf{M} \vec{S}, \tag{17}$$

where \mathbf{M} is the capacitance matrix and \mathbf{K} is the conductance matrix. Both matrices are symmetric. Further, \mathbf{M} is positive definite and \mathbf{K} is semi-positive definite. Also, they are

sparse matrices. For simplification, we apply the lumped mass technique [1, 2] to obtain a diagonal matrix \mathbf{D}_M and then replace \mathbf{M} by \mathbf{D}_M in Eq. (17) to give

$$\mathbf{D}_M \frac{\partial \vec{u}}{\partial t} = -\frac{C}{A} \mathbf{K} \vec{u} + (B - \frac{D}{A}) \mathbf{D}_M \frac{\partial^2 \vec{T}}{\partial z^2} + \frac{D}{A} \mathbf{D}_M \frac{\partial^2 \vec{u}}{\partial z^2} + \mathbf{D}_M \vec{S}, \tag{18}$$

where each entry d_p at the diagonal of \mathbf{D}_M is $\frac{1}{3} \sum_{\Delta} S_{\Delta}$ (i.e., one-third of the sum of all elements with node p as one vertex). Similarly, we can obtain from Eq. (14) for case 2

$$\mathbf{D}_M \frac{\partial \vec{u}}{\partial t} = -B \mathbf{K} \vec{T} + B \mathbf{D}_M \frac{\partial^2 \vec{u}}{\partial z^2} + (D - AB) \mathbf{D}_M \frac{\partial^3 \vec{T}}{\partial z^2 \partial t} + \mathbf{D}_M \vec{S}. \tag{19}$$

Furthermore, we write Eq. (12) into a vector form

$$\vec{u} = \vec{T} + A \frac{\partial \vec{T}}{\partial t}. \tag{20}$$

We now discretize the above Eqs. (18)-(20) using the finite difference method. We let \vec{T}_m^n and \vec{u}_m^n denote $\vec{T}(m\Delta z, n\Delta t)$ and $\vec{u}(m\Delta z, n\Delta t)$, respectively, where Δz and Δt are the z -directional spatial and temporal mesh sizes, respectively, and $m = 0, 1, \dots, N_z$.

Eqs. (18)-(20) are discretized using a Crank-Nicholson type of finite difference

$$\begin{aligned} \mathbf{D}_M \frac{\vec{u}_m^{n+1} - \vec{u}_m^n}{\Delta t} &= -\frac{C}{2A} \mathbf{K} (\vec{u}_m^{n+1} + \vec{u}_m^n) \\ &+ \frac{1}{2} (B - \frac{D}{A}) \mathbf{D}_M \delta_z^2 (\vec{T}_m^{n+1} + \vec{T}_m^n) + \frac{D}{2A} \mathbf{D}_M \delta_z^2 (\vec{u}_m^{n+1} + \vec{u}_m^n) \\ &+ \mathbf{D}_M \vec{S}_m^{n+\frac{1}{2}}, \end{aligned} \tag{21}$$

$$\begin{aligned} \mathbf{D}_M \frac{\vec{u}_m^{n+1} - \vec{u}_m^n}{\Delta t} &= -\frac{B}{2} \mathbf{K} (\vec{u}_m^{n+1} + \vec{u}_m^n) \\ &+ \frac{B}{2} \mathbf{D}_M \delta_z^2 (\vec{u}_m^{n+1} + \vec{u}_m^n) + \frac{D - AB}{\Delta t} \mathbf{D}_M \delta_z^2 (\vec{T}_m^{n+1} - \vec{T}_m^n) \\ &+ \mathbf{D}_M \vec{S}_m^{n+\frac{1}{2}}, \end{aligned} \tag{22}$$

$$A \frac{\vec{T}_m^{n+1} - \vec{T}_m^n}{\Delta t} = -\frac{1}{2} (\vec{T}_m^{n+1} + \vec{T}_m^n) + \frac{1}{2} (\vec{u}_m^{n+1} + \vec{u}_m^n), \tag{23}$$

where $\delta_z^2 \vec{u}_m^{n+1} = \frac{1}{\Delta z^2} (\vec{u}_{m+1}^{n+1} - 2\vec{u}_m^{n+1} + \vec{u}_{m-1}^{n+1})$, and $m = 1, \dots, N_z - 1$. We now simplify Eq. (21) to obtain an equation for solving \vec{u}_m^{n+1} . To this end, we rewrite Eq. (23) as follows:

$$\frac{1}{2} (A + \frac{\Delta t}{2}) (\vec{T}_m^{n+1} + \vec{T}_m^n) = A \vec{T}_m^n + \frac{\Delta t}{4} (\vec{u}_m^{n+1} + \vec{u}_m^n). \tag{24}$$

Substituting $\vec{T}_m^{n+1} + \vec{T}_m^n$ into Eq. (21), we obtain

$$\begin{aligned}
 \left(A + \frac{\Delta t}{2}\right) \mathbf{D}_M \frac{\vec{u}_m^{n+1} - \vec{u}_m^n}{\Delta t} &= -\frac{1}{2} \left(A + \frac{\Delta t}{2}\right) \frac{C}{A} \mathbf{K} (\vec{u}_m^{n+1} + \vec{u}_m^n) \\
 &\quad + \left(B - \frac{D}{A}\right) \mathbf{D}_M \delta_z^2 \left[A \vec{T}_m^n + \frac{\Delta t}{4} (\vec{u}_m^{n+1} + \vec{u}_m^n)\right] \\
 &\quad + \frac{1}{2} \left(A + \frac{\Delta t}{2}\right) \frac{D}{A} \delta_z^2 \mathbf{D}_M (\vec{u}_m^{n+1} + \vec{u}_m^n) \\
 &\quad + \left(A + \frac{\Delta t}{2}\right) \mathbf{D}_M S_m^{n+\frac{1}{2}} \\
 &= -\frac{1}{2} \left(C + \frac{\Delta t C}{2A}\right) \mathbf{K} (\vec{u}_m^{n+1} + \vec{u}_m^n) \\
 &\quad + \frac{1}{2} \left(D + \frac{\Delta t}{2} B\right) \mathbf{D}_M \delta_z^2 (\vec{u}_m^{n+1} + \vec{u}_m^n) \\
 &\quad + (AB - D) \mathbf{D}_M \delta_z^2 \vec{T}_m^n + \left(A + \frac{\Delta t}{2}\right) \mathbf{D}_M S_{ijk}^{n+\frac{1}{2}}. \tag{25}
 \end{aligned}$$

We can obtain the same equation from Eqs. (22) and (23) for case 2. The initial and boundary conditions are discretized from Eqs. (10)-(12) as follows:

$$\vec{T}_m^0 = \left(\vec{T}_0\right)_m, \quad \vec{u}_m^0 = \left(\vec{T}_0\right)_m + A \left(\vec{T}_1\right)_m \tag{26}$$

and

$$\nabla_z \vec{T}_1^n = \nabla_z \vec{u}_1^n = \nabla_z \vec{T}_{N_z}^n = \nabla_z \vec{u}_{N_z}^n = \vec{0}, \tag{27}$$

where ∇_z is a backward difference operator, e.g., $\nabla_z \vec{u}_1^n = \frac{\vec{u}_1^n - \vec{u}_0^n}{\Delta z}$. Hence, one may use Eq. (25) to obtain \vec{u}_m^{n+1} and then use Eq. (23) to obtain \vec{T}_m^{n+1} .

3. Stability

To show the stability of the scheme, Eqs. (21)-(23), with initial and boundary conditions (26)-(27), we first introduce the definition of the inner product between the mesh functions \vec{u}_m^n and \vec{v}_m^n . Let \mathbf{G}_h be a set of $\{\vec{\mathbf{u}}^n = \{\vec{u}_m^n\}, \text{ with } \nabla_z \vec{u}_1^n = \nabla_z \vec{u}_{N_z}^n = \vec{0}\}$. For any $\vec{\mathbf{u}}^n, \vec{\mathbf{v}}^n \in \mathbf{G}_h$, since \mathbf{D}_M is symmetric and positive definite, and \mathbf{K} is symmetric and semi-positive definite, we can define the inner products as follows:

$$\begin{aligned}
 (\vec{\mathbf{u}}^n, \vec{\mathbf{v}}^n)_{\mathbf{D}} &= \Delta z \sum_{m=1}^{N_z-1} (\vec{u}_m^n)^T \mathbf{D}_M \vec{v}_m^n, & (\vec{\mathbf{u}}^n, \vec{\mathbf{v}}^n)_{\mathbf{K}} &= \Delta z \sum_{m=1}^{N_z-1} (\vec{u}_m^n)^T \mathbf{K} \vec{v}_m^n, \\
 (\vec{\mathbf{u}}^n, \vec{\mathbf{v}}^n)_{1, \mathbf{D}} &= \Delta z \sum_{m=1}^{N_z-1} (\nabla_z \vec{u}_m^n)^T \mathbf{D}_M \nabla_z \vec{v}_m^n,
 \end{aligned}$$

where $(\vec{u}_m^n)^T$ is the transpose of \vec{u}_m^n .

Lemma 1. For any $\vec{\mathbf{u}}^n, \vec{\mathbf{v}}^n \in \mathbf{G}_h$,

$$(\delta_z^2 \vec{\mathbf{u}}^n, \vec{\mathbf{v}}^n)_{\mathbf{D}} = (\vec{\mathbf{v}}^n, \delta_z^2 \vec{\mathbf{u}}^n)_{\mathbf{D}} = -(\vec{\mathbf{u}}^n, \vec{\mathbf{v}}^n)_{1, \mathbf{D}}$$

Proof.

$$\begin{aligned}
(\delta_z^2 \vec{u}^n, \vec{v}^n)_{\mathbf{D}} &= \Delta z \sum_{m=1}^{N_z-1} (\delta_z^2 \vec{u}_m^n)^T \mathbf{D}_M \vec{v}_m^n \\
&= \frac{\Delta z}{\Delta z} \sum_{m=1}^{N_z-1} [(\nabla_z \vec{u}_{m+1}^n)^T - (\nabla_z \vec{u}_m^n)^T] \mathbf{D}_M \vec{v}_m^n \\
&= \frac{\Delta z}{\Delta z} \sum_{m=1}^{N_z-1} (\nabla_z \vec{u}_{m+1}^n)^T \mathbf{D}_M \vec{v}_m^n - \frac{\Delta z}{\Delta z} \sum_{m=1}^{N_z-1} (\nabla_z \vec{u}_m^n)^T \mathbf{D}_M \vec{v}_m^n \\
&= \frac{\Delta z}{\Delta z} \sum_{m=2}^{N_z} (\nabla_z \vec{u}_m^n)^T \mathbf{D}_M \vec{v}_{m-1}^n - \frac{\Delta z}{\Delta z} \sum_{m=1}^{N_z-1} (\nabla_z \vec{u}_m^n)^T \mathbf{D}_M \vec{v}_m^n \\
&= -\frac{\Delta z}{\Delta z} \sum_{m=2}^{N_z-1} (\nabla_z \vec{u}_m^n)^T \mathbf{D}_M (\vec{v}_m^n - \vec{v}_{m-1}^n) + (\nabla_z \vec{u}_{N_z}^n)^T \mathbf{D}_M \vec{v}_{N_z-1}^n \\
&\quad - (\nabla_z \vec{u}_1^n)^T \mathbf{D}_M \vec{v}_1^n \\
&= -\Delta z \sum_{m=2}^{N_z-1} (\nabla_z \vec{u}_m^n)^T \mathbf{D}_M \nabla_z \vec{v}_m^n + (\nabla_z \vec{u}_{N_z}^n)^T \mathbf{D}_M \vec{v}_{N_z-1}^n - (\nabla_z \vec{u}_1^n)^T \mathbf{D}_M \vec{v}_1^n.
\end{aligned}$$

Since $\nabla_z \vec{u}_1^n = \nabla_z \vec{u}_{N_z}^n = \vec{0}$, we obtain

$$\begin{aligned}
(\delta_z^2 \vec{u}^n, \vec{v}^n)_{\mathbf{D}} &= -\Delta z \sum_{m=1}^{N_z-1} (\nabla_z \vec{u}_m^n)^T \mathbf{D}_M \nabla_z \vec{v}_m^n \\
&= -(\vec{u}^n, \vec{v}^n)_{1, \mathbf{D}}.
\end{aligned}$$

Similarly, we have $(\vec{v}^n, \delta_z^2 \vec{u}^n)_{\mathbf{D}} = -(\vec{u}^n, \vec{v}^n)_{1, \mathbf{D}}$.

Theorem 1. Suppose that $\{\vec{u}_m^n, \vec{T}_m^n\}$ and $\{\vec{v}_m^n, \vec{W}_m^n\}$ are solutions of the scheme, Eqs. (21)-(23), with the same boundary conditions, and initial values $\{\vec{u}_m^0, \vec{T}_m^0\}$ and $\{\vec{v}_m^0, \vec{W}_m^0\}$, respectively. Let $\vec{\phi}_m^n = \vec{u}_m^n - \vec{v}_m^n$, $\vec{\varepsilon}_m^n = \vec{T}_m^n - \vec{W}_m^n$. Then $\{\vec{\phi}_m^n, \vec{\varepsilon}_m^n\}$ satisfy

$$(\vec{\phi}^n, \vec{\phi}^n)_{\mathbf{D}} + (AB - D) (\vec{\varepsilon}^n, \vec{\varepsilon}^n)_{1, \mathbf{D}} \leq (\vec{\phi}^0, \vec{\phi}^0)_{\mathbf{D}} + (AB - D) (\vec{\varepsilon}^0, \vec{\varepsilon}^0)_{1, \mathbf{D}} \quad (28)$$

if $AB - D \geq 0$ and

$$(\vec{\phi}^n, \vec{\phi}^n)_{\mathbf{D}} + (D - AB) (\vec{\varepsilon}^n, \vec{\varepsilon}^n)_{1, \mathbf{D}} \leq (\vec{\phi}^0, \vec{\phi}^0)_{\mathbf{D}} + (D - AB) (\vec{\varepsilon}^0, \vec{\varepsilon}^0)_{1, \mathbf{D}} \quad (29)$$

if $AB - D < 0$ 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. Since $\{\vec{u}_m^n, \vec{T}_m^n\}$ and $\{\vec{v}_m^n, \vec{W}_m^n\}$ are solutions of the scheme, Eqs. (21)-(23), with the same boundary conditions, and initial values $\{\vec{u}_m^0, \vec{T}_m^0\}$ and $\{\vec{v}_m^0, \vec{W}_m^0\}$, respectively. Let $\vec{\phi}_m^n = \vec{u}_m^n - \vec{v}_m^n$, $\vec{\varepsilon}_m^n = \vec{T}_m^n - \vec{W}_m^n$. Then, $\vec{\phi}^n, \vec{\varepsilon}^n \in \mathbf{G}_h$, and satisfy (from Eqs. (21) and (23))

$$\begin{aligned}
A \mathbf{D}_M \frac{\vec{\phi}_m^{n+1} - \vec{\phi}_m^n}{\Delta t} &= -\frac{C}{2} \mathbf{K} (\vec{\phi}_m^{n+1} + \vec{\phi}_m^n) + \frac{1}{2} (AB - D) \mathbf{D}_M \delta_z^2 (\vec{\varepsilon}_m^{n+1} + \vec{\varepsilon}_m^n) \\
&\quad + \frac{D}{2} \mathbf{D}_M \delta_z^2 (\vec{\phi}_m^{n+1} + \vec{\phi}_m^n), \quad (30)
\end{aligned}$$

$$A \frac{\vec{\varepsilon}_m^{n+1} - \vec{\varepsilon}_m^n}{\Delta t} = -\frac{1}{2} (\vec{\varepsilon}_m^{n+1} + \vec{\varepsilon}_m^n) + \frac{1}{2} (\vec{\phi}_m^{n+1} + \vec{\phi}_m^n). \quad (31)$$

Multiplying Eq. (30) by $(\vec{\phi}_m^{n+1} + \vec{\phi}_m^n)$, then summing m from 1 to $N_z - 1$, one obtains

$$\begin{aligned} \frac{A}{\Delta t} \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \vec{\phi}^{n+1} - \vec{\phi}^n \right)_{\mathbf{D}} &= \frac{1}{2} (AB - D) \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \delta_z^2 (\vec{\varepsilon}^{n+1} + \vec{\varepsilon}^n) \right)_{\mathbf{D}} \\ &\quad + \frac{1}{2} D \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \delta_z^2 (\vec{\phi}^{n+1} + \vec{\phi}^n) \right)_{\mathbf{D}} \\ &\quad - \frac{1}{2} C \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \vec{\phi}^{n+1} + \vec{\phi}^n \right)_{\mathbf{K}}. \end{aligned}$$

By lemma 1 and $\left(\vec{\phi}^{n+1}, \vec{\phi}^n \right)_{\mathbf{D}} = \left(\vec{\phi}^n, \vec{\phi}^{n+1} \right)_{\mathbf{D}}$, we have

$$\begin{aligned} \frac{A}{\Delta t} \left(\left(\vec{\phi}^{n+1}, \vec{\phi}^{n+1} \right)_{\mathbf{D}} - \left(\vec{\phi}^n, \vec{\phi}^n \right)_{\mathbf{D}} \right) &= -\frac{1}{2} (AB - D) \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \vec{\varepsilon}^{n+1} + \vec{\varepsilon}^n \right)_{1, \mathbf{D}} \\ &\quad - \frac{1}{2} D \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \vec{\phi}^{n+1} + \vec{\phi}^n \right)_{1, \mathbf{D}} \\ &\quad - \frac{1}{2} C \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \vec{\phi}^{n+1} + \vec{\phi}^n \right)_{\mathbf{K}}. \end{aligned} \tag{32}$$

Further, we multiply Eq. (31) by $\mathbf{D}_M \delta_z^2 (\vec{\varepsilon}_m^{n+1} + \vec{\varepsilon}_m^n)$, respectively, and sum m from 1 to $N_z - 1$ to obtain

$$\begin{aligned} \frac{A}{\Delta t} \left(\vec{\varepsilon}^{n+1} - \vec{\varepsilon}^n, \delta_z^2 (\vec{\varepsilon}^{n+1} + \vec{\varepsilon}^n) \right)_{\mathbf{D}} &= -\frac{1}{2} \left(\vec{\varepsilon}^{n+1} + \vec{\varepsilon}^n, \delta_z^2 (\vec{\varepsilon}^{n+1} + \vec{\varepsilon}^n) \right)_{\mathbf{D}} \\ &\quad + \frac{1}{2} \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \delta_z^2 (\vec{\varepsilon}^{n+1} + \vec{\varepsilon}^n) \right)_{\mathbf{D}}. \end{aligned} \tag{33}$$

By lemma 1 and $(\vec{\varepsilon}^{n+1}, \vec{\varepsilon}^n)_{1, \mathbf{D}} = (\vec{\varepsilon}^n, \vec{\varepsilon}^{n+1})_{1, \mathbf{D}}$, Eq. (33) becomes

$$\begin{aligned} -\frac{A}{\Delta t} \left[(\vec{\varepsilon}^{n+1}, \vec{\varepsilon}^{n+1})_{1, \mathbf{D}} - (\vec{\varepsilon}^n, \vec{\varepsilon}^n)_{1, \mathbf{D}} \right] &= \frac{1}{2} \left(\vec{\varepsilon}^{n+1} + \vec{\varepsilon}^n, \vec{\varepsilon}^{n+1} + \vec{\varepsilon}^n \right)_{1, \mathbf{D}} \\ &\quad - \frac{1}{2} \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \vec{\varepsilon}^{n+1} + \vec{\varepsilon}^n \right)_{1, \mathbf{D}}. \end{aligned} \tag{34}$$

If Eq. (34) are multiplied by $-(AB - D)$, and added to Eq. (32), we obtain

$$\begin{aligned} &\frac{A}{\Delta t} \left(\left(\vec{\phi}^{n+1}, \vec{\phi}^{n+1} \right)_{\mathbf{D}} - \left(\vec{\phi}^n, \vec{\phi}^n \right)_{\mathbf{D}} \right) + \frac{A(AB - D)}{\Delta t} \left[(\vec{\varepsilon}^{n+1}, \vec{\varepsilon}^{n+1})_{1, \mathbf{D}} - (\vec{\varepsilon}^n, \vec{\varepsilon}^n)_{1, \mathbf{D}} \right] \\ &\quad + \frac{1}{2} D \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \vec{\phi}^{n+1} + \vec{\phi}^n \right)_{1, \mathbf{D}} + \frac{1}{2} C \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \vec{\phi}^{n+1} + \vec{\phi}^n \right)_{\mathbf{K}} \\ &\quad + \frac{1}{2} (AB - D) \left(\vec{\varepsilon}^{n+1} + \vec{\varepsilon}^n, \vec{\varepsilon}^{n+1} + \vec{\varepsilon}^n \right)_{1, \mathbf{D}} \\ &= 0. \end{aligned} \tag{35}$$

Since $AB - D \geq 0$, \mathbf{D}_M is symmetric and positive definite, and \mathbf{K} is symmetric and semi-positive definite, one may drop the last three terms on the left hand side from the above equation and obtain

$$\begin{aligned} &\frac{A}{\Delta t} \left(\left(\vec{\phi}^{n+1}, \vec{\phi}^{n+1} \right)_{\mathbf{D}} - \left(\vec{\phi}^n, \vec{\phi}^n \right)_{\mathbf{D}} \right) + \frac{A(AB - D)}{\Delta t} \left[(\vec{\varepsilon}^{n+1}, \vec{\varepsilon}^{n+1})_{1, \mathbf{D}} - (\vec{\varepsilon}^n, \vec{\varepsilon}^n)_{1, \mathbf{D}} \right] \\ &\leq 0. \end{aligned}$$

Hence,

$$\left(\vec{\phi}^{n+1}, \vec{\phi}^{n+1} \right)_{\mathbf{D}} + (AB - D) \left(\vec{\varepsilon}^{n+1}, \vec{\varepsilon}^{n+1} \right)_{1, \mathbf{D}} \leq \left(\vec{\phi}^n, \vec{\phi}^n \right)_{\mathbf{D}} + (AB - D) \left(\vec{\varepsilon}^n, \vec{\varepsilon}^n \right)_{1, \mathbf{D}}. \tag{36}$$

Summing n from 0 to n , we obtain Eq. (28)

$$\left(\vec{\phi}^n, \vec{\phi}^n\right)_{\mathbf{D}} + (AB - D) (\vec{\varepsilon}^n, \vec{\varepsilon}^n)_{1, \mathbf{D}} \leq \left(\vec{\phi}^0, \vec{\phi}^0\right)_{\mathbf{D}} + (AB - D) (\vec{\varepsilon}^0, \vec{\varepsilon}^0)_{1, \mathbf{D}}.$$

For the case of $AB - D < 0$, one may use a similar argument. We first obtain from Eq. (22) and Eq. (23)

$$\begin{aligned} \mathbf{D}_M \frac{\vec{\phi}_m^{n+1} - \vec{\phi}_m^n}{\Delta t} &= -\frac{1}{2} B \mathbf{K} (\vec{\phi}_m^{n+1} + \vec{\phi}_m^n) + \frac{B}{2} \mathbf{D}_M \delta_z^2 (\vec{\phi}_m^{n+1} + \vec{\phi}_m^n) \\ &\quad + \frac{D - AB}{\Delta t} \mathbf{D}_M \delta_z^2 (\vec{\varepsilon}_m^{n+1} - \vec{\varepsilon}_m^n) \end{aligned} \tag{37}$$

and

$$A \frac{\vec{\varepsilon}_m^{n+1} - \vec{\varepsilon}_m^n}{\Delta t} = -\frac{1}{2} (\vec{\varepsilon}_m^{n+1} + \vec{\varepsilon}_m^n) + \frac{1}{2} (\vec{\phi}_m^{n+1} + \vec{\phi}_m^n). \tag{38}$$

Multiplying Eq. (37) by $(\vec{\phi}_m^{n+1} + \vec{\phi}_m^n)^T$ and multiplying Eq. (38) by $\mathbf{D}_M \delta_z^2 (\vec{\varepsilon}_m^{n+1} - \vec{\varepsilon}_m^n)$, respectively, then summing m from 1 to $N_z - 1$, we obtain, by lemma 1,

$$\begin{aligned} \frac{1}{\Delta t} \left(\left(\vec{\phi}^{n+1}, \vec{\phi}^{n+1}\right)_{\mathbf{D}} - \left(\vec{\phi}^n, \vec{\phi}^n\right)_{\mathbf{D}} \right) &= -\frac{1}{\Delta t} (D - AB) \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \vec{\varepsilon}^{n+1} - \vec{\varepsilon}^n\right)_{1, \mathbf{D}} \\ &\quad - \frac{1}{2} B \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \vec{\phi}^{n+1} + \vec{\phi}^n\right)_{\mathbf{K}} \\ &\quad - \frac{1}{2} B \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \vec{\phi}^{n+1} + \vec{\phi}^n\right)_{1, \mathbf{D}} \end{aligned} \tag{39}$$

and

$$\begin{aligned} -\frac{A}{\Delta t} (\vec{\varepsilon}^{n+1} - \vec{\varepsilon}^n, \vec{\varepsilon}^{n+1} - \vec{\varepsilon}^n)_{1, \mathbf{D}} &= \frac{1}{2} \left((\vec{\varepsilon}^{n+1}, \vec{\varepsilon}^{n+1})_{1, \mathbf{D}} - (\vec{\varepsilon}^n, \vec{\varepsilon}^n)_{1, \mathbf{D}} \right) \\ &\quad - \frac{1}{2} \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \vec{\varepsilon}^{n+1} - \vec{\varepsilon}^n\right)_{1, \mathbf{D}}. \end{aligned} \tag{40}$$

If Eq. (40) is multiplied by $-\frac{2}{\Delta t} (D - AB)$, and added to Eq. (39), one obtains

$$\begin{aligned} &\frac{1}{\Delta t} \left(\left(\vec{\phi}^{n+1}, \vec{\phi}^{n+1}\right)_{\mathbf{D}} - \left(\vec{\phi}^n, \vec{\phi}^n\right)_{\mathbf{D}} \right) \\ &\quad + \frac{D - AB}{\Delta t} \left((\vec{\varepsilon}^{n+1}, \vec{\varepsilon}^{n+1})_{1, \mathbf{D}} - (\vec{\varepsilon}^n, \vec{\varepsilon}^n)_{1, \mathbf{D}} \right) \\ &\quad + \frac{1}{2} B \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \vec{\phi}^{n+1} + \vec{\phi}^n\right)_{\mathbf{K}} + \frac{1}{2} B \left(\vec{\phi}^{n+1} + \vec{\phi}^n, \vec{\phi}^{n+1} + \vec{\phi}^n\right)_{1, \mathbf{D}} \\ &\quad + \frac{2}{\Delta t^2} A (D - AB) (\vec{\varepsilon}^{n+1} - \vec{\varepsilon}^n, \vec{\varepsilon}^{n+1} - \vec{\varepsilon}^n)_{1, \mathbf{D}} \\ &= 0. \end{aligned} \tag{41}$$

Since $AB - D < 0$, Eq. (41) can be simplified as follows:

$$\begin{aligned} &\frac{1}{\Delta t} \left(\left(\vec{\phi}^{n+1}, \vec{\phi}^{n+1}\right)_{\mathbf{D}} - \left(\vec{\phi}^n, \vec{\phi}^n\right)_{\mathbf{D}} \right) + \frac{D - AB}{\Delta t} \left((\vec{\varepsilon}^{n+1}, \vec{\varepsilon}^{n+1})_{1, \mathbf{D}} - (\vec{\varepsilon}^n, \vec{\varepsilon}^n)_{1, \mathbf{D}} \right) \\ &\leq 0. \end{aligned} \tag{42}$$

Therefore, we obtain Eq. (29)

$$\left(\vec{\phi}^n, \vec{\phi}^n\right)_{\mathbf{D}} + (D - AB) (\vec{\varepsilon}^n, \vec{\varepsilon}^n)_{1, \mathbf{D}} \leq \left(\vec{\phi}^0, \vec{\phi}^0\right)_{\mathbf{D}} + (D - AB) (\vec{\varepsilon}^0, \vec{\varepsilon}^0)_{1, \mathbf{D}}$$

and hence we conclude the theorem.

Since Eq. (25) is a three-dimensional implicit scheme, it involves heavy computations. To simplify the computation, we develop a preconditioned Richardson iteration based on the idea of our previous paper as follows [6]:

$$\begin{aligned}
L_{pre} (\vec{u}_m^{n+1})^{(i+1)} &= L_{pre} (\vec{u}_m^{n+1})^{(i)} - \omega \{ \mathbf{D}_M [(\vec{u}_m^{n+1})^{(i)} - \vec{u}_m^n] \\
&\quad + \frac{\Delta t}{2} (A + \frac{\Delta t}{2})^{-1} (C + \frac{\Delta t}{2} B) \mathbf{K} [(\vec{u}_m^{n+1})^{(i)} + \vec{u}_m^n] \\
&\quad - \frac{\Delta t}{2} (A + \frac{\Delta t}{2})^{-1} (D + \frac{\Delta t}{2} B) \mathbf{D}_M \delta_z^2 [(\vec{u}_m^{n+1})^{(i)} + \vec{u}_m^n] \\
&\quad - \Delta t (A + \frac{\Delta t}{2})^{-1} (AB - D) \mathbf{D}_M \delta_z^2 \vec{T}_m^n \\
&\quad - \Delta t \mathbf{D}_M \vec{S}_m^{n+\frac{1}{2}} \}, \quad i = 0, 1, 2, \dots,
\end{aligned} \tag{43}$$

where the preconditioner is

$$L_{pre} = \mathbf{D}_M + \frac{\Delta t}{2} (A + \frac{\Delta t}{2})^{-1} [(C + \frac{\Delta t}{2} B) \mathbf{D}_K - (D + \frac{\Delta t}{2} B) \mathbf{D}_M \delta_z^2]. \tag{44}$$

Here, ω is a relaxation parameter, $0 \leq \omega \leq 1$, \mathbf{D}_K is a diagonal matrix where each diagonal entry of \mathbf{D}_K is chosen to be the sum of elements in absolute value in the corresponding row of \mathbf{K} . It can be seen that the iteration method (43)-(44) converges. A similar argument can be seen in [6].

It should be pointed out that only a block tridiagonal linear system is solved for each iteration in Eq. (43). Further, the Thomas' algorithm [7] can be employed since only inverse of diagonal matrices are involved. Hence, the computation is simple.

4. Numerical Example

To demonstrate the applicability of the numerical procedure we investigate the temperature rise in a sub-microscale cylindrical gold film. The thickness for the gold film is $0.05 \mu m$, while the radius in the planar direction is $0.5 \mu m$, as shown in Figure 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 $\tau_T = 90 \text{ ps}$ [14, 8].

The heat source was chosen to be [14]

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

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

The initial conditions were chosen as follows:

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

where $T_\infty = 300 \text{ K}$. The boundary conditions were assumed to be insulated.

To apply our numerical method, we chose a finite element mesh with the same 97 nodes in the xy -directions, as shown in Figure 2, and chose 50 grid points in the z -direction for the gold film. The basis function was chosen to be the linear function. The time increment was chosen to be 0.005 ps . To use the preconditioned Richardson iteration, Eqs. (43)-(44), we chose $\omega = 1.0$ and the convergent solution $\{T_{pm}^{n+1}\}$ was obtained if the convergence criterion $\max_{p,m} |(u_{pm}^{n+1})^{(i+1)} - (u_{pm}^{n+1})^{(i)}| < 10^{-5}$ was satisfied.

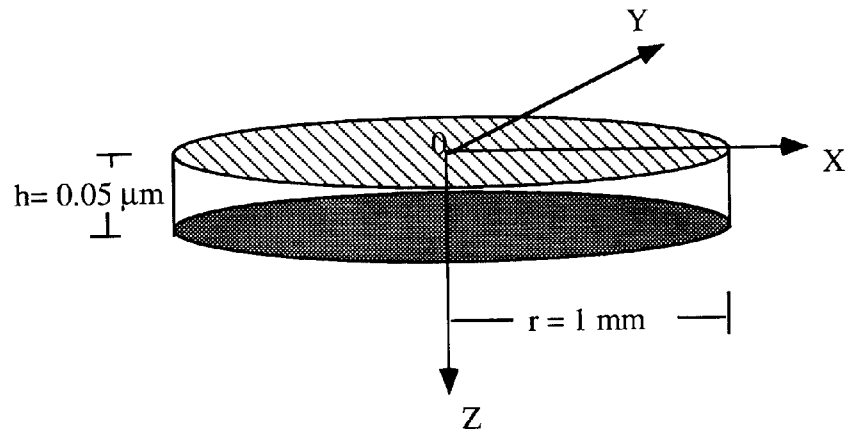


Figure 1. Three-dimensional configuration of a sub-microscale cylindrical thin film with sub-microscale thickness

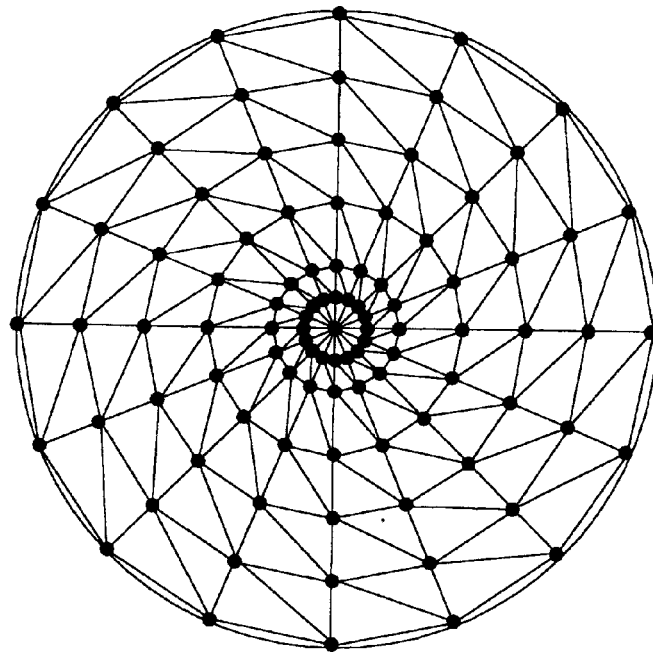
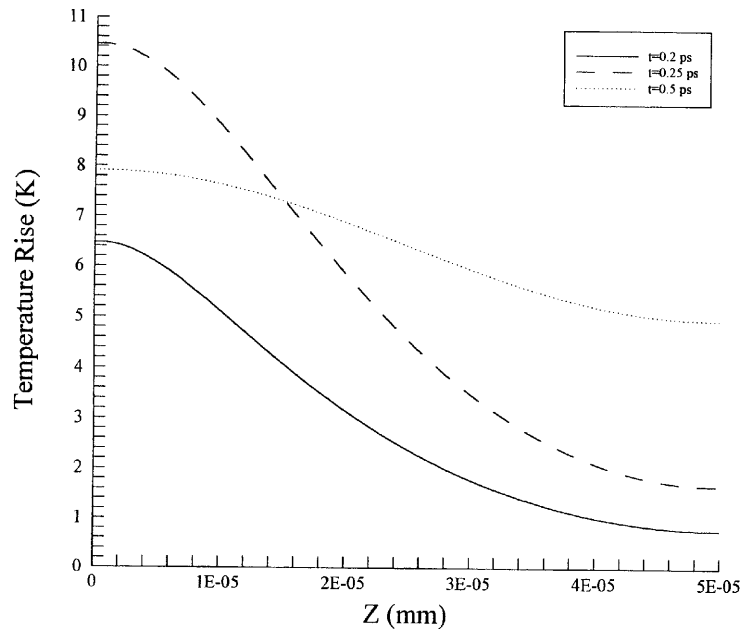
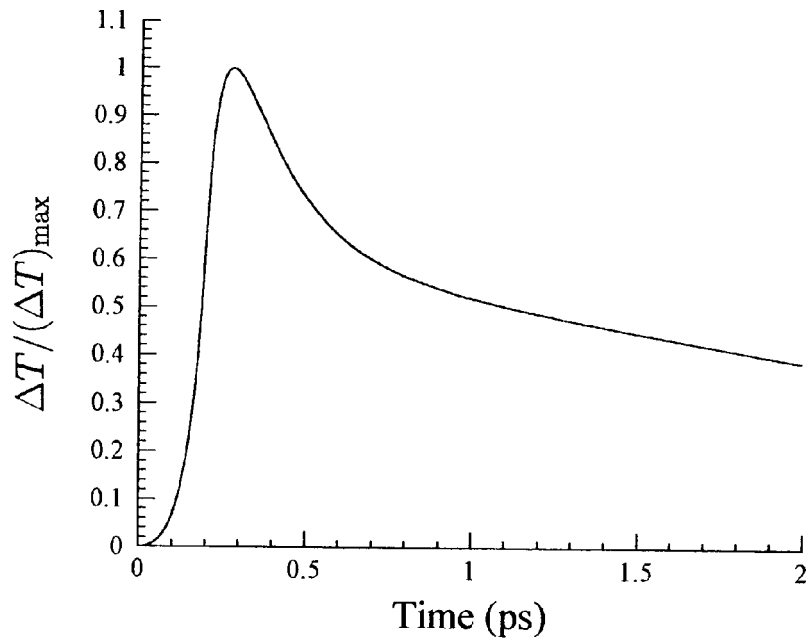
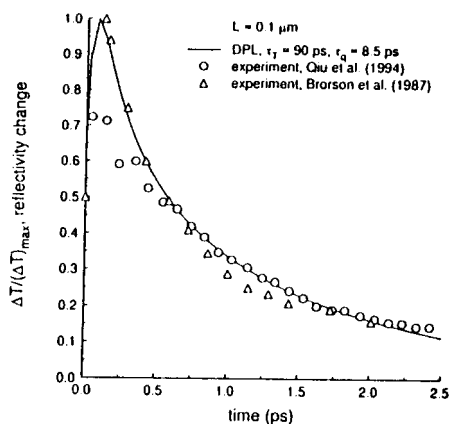


Figure 2. A finite element mesh in the xy -directions

Figure 3. Temperature profiles along the z -axis

(a)



(b)

Figure 4. Temperature change on the surface of the gold film.

The maximum temperature rise ($T_{Max} = 10.80K$) was obtained. (b) is obtained in [14].

Figure 3 gives the temperature rise along the z -axis for different times ($t = 0.2 ps$, $0.25 ps$, and $0.5 ps$). It can be seen from the figure that the heat is transferred from the top to the bottom.

Figure 4 shows the change in temperature ($\frac{\Delta T}{(\Delta T)_{Max}}$) on the surface of the gold film. The maximum temperature rise of T (i.e., $(\Delta T)_{Max}$) on the surface of the gold film is about $10.80 K$. 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 [14] for one dimensional case (see p. 125 in [14]) except that the temperature rises start at $t = 0$. This is because in [14] it appears that the initial time was set equal to $2t_p$ in Eq. (46).

Furthermore, the preconditioned Richardson iteration is fast since the solution converges at most after 2 iterations for each time step. The cpu time $t = 0.5 ps$ on a SUN workstation is about 3.5 minutes.

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