Journal of Computational Mathematics, Vol.21, No.5, 2003, 555–568.

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]:

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

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

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:

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

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]

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

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:

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

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 μm, 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 μm.

2. Hybrid Finite Element-Finite Difference

Since we consider a thin film with thickness of the order 0.1 μm 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

$$q_1 = -k\frac{\partial T}{\partial x}, \tag{6}$$

$$q_2 = -k\frac{\partial T}{\partial y}, \tag{7}$$

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