International Journal of Heat and Mass Transfer 64 (2013) 966–975

Contents lists available at SciVerse ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Accurate numerical method for solving dual-phase-lagging equation with temperature jump boundary condition in nano heat conduction

Weizhong Dai [a,*], Fei Han [a], Zhizhong Sun [b]

[a] College of Engineering and Science, Louisiana Tech University, Ruston, LA 71272, USA
[b] Department of Mathematics, Southeast University, Nanjing, PR China

ARTICLE INFO

Article history:
Received 28 January 2013
Received in revised form 25 April 2013
Accepted 2 May 2013
Available online 7 June 2013

Keywords:
Dual-phase-lagging model
Temperature jump boundary condition
Nano-scale
Finite difference scheme

ABSTRACT

Dual-phase-lagging (DPL) equation with temperature jump boundary condition shows promising for analyzing nano heat conduction. For solving it, development of higher-order accurate and unconditionally stable (no restriction on the mesh ratio) numerical schemes is important. Because the grid size may be very small at nano-scale, using a higher-order accurate scheme will allow us to choose a relative coarse grid and obtain a reasonable solution. For this purpose, in this article we present a higher-order accurate and unconditionally stable compact finite difference scheme based on the ratio of relaxation times ($0 \leqslant B \leqslant 1$ and $B > 1$). The method is illustrated by three numerical examples including a 2D case.

1. Introduction

For the problem of self-heating in micro-electronic devices or for situations involving very low temperature near absolute zero, heat source, such as laser, heat is found to propagate at a finite speed [1]. One of the best description of such heat transfer is the dual-phase-lagging (DPL) model which is non-Fourier heat conduction and was proposed by Tzou in 1995 as [2,3]:

$$q(t+\tau_q, x) = -k\nabla T(t+\tau_T, x), \tag{1}$$

where τ_q and τ_T stand for the heat flux q and temperature gradient ∇T phase lags, respectively, which are positive and intrinsic properties of the material.

Using Taylor series expansion of Eq. (1) with respect to time up to the first-order derivative yields:

$$q + \tau_q \frac{\partial q}{\partial t} = -k\frac{\partial T}{\partial x} - k\tau_T \frac{\partial^2 T}{\partial t \partial x}. \tag{2}$$

Coupled with the energy equation, $-\frac{\partial q}{\partial x} = c\frac{\partial T}{\partial t}$, where c is the heat capacity of the material, one may obtain the heat conduction equation under the DPL effect as follows:

$$\frac{\partial T}{\partial t} + \tau_q \frac{\partial^2 T}{\partial t^2} = \frac{k}{c}\left(\frac{\partial^2 T}{\partial x^2} + \tau_T \frac{\partial^3 T}{\partial t \partial x^2}\right). \tag{3}$$

This model considers only the effect of finite relaxation time by using the heat flux and temperature phase lags where the former is caused by micro structural interactions such as phonon scattering and the latter is interpreted as the relaxation time due to fast-transient effects of thermal inertia [3]. Well-posedness and solution structure as well as stability of the DPL heat conduction have been analyzed [4–9]. Analytical solutions and numerical methods for the DPL equation with Dirichlet or Neumann boundary condition have been well studied. In particular, Chen and Tzou [10,11] used the Laplace transform method to obtain the analytical solutions for the DPL equation with Dirichlet and Neumann boundary conditions, respectively. Lin et al. [12] employed the separation of variables method to obtain the analytical solutions of the DPL equation with homogeneous Dirichlet and Neumann boundary conditions. Smith et al. [13] also employed the separation of variables method to obtain the analytical solution for the DPL equation with the homogeneous Neumann boundary condition. Tang and Araki [14] derived an analytical solution by using the Green's function method and finite integral transform techniques for the DPL equation with a homogeneous Neumann boundary condition. Al-Nimr et al. [15] used the Laplace transform method to obtain the analytical solution for the DPL model with the Dirichlet boundary condition in a semi-infinite interval. Kulish and Novozhilov [16] presented an integral equation for the Cauchy problem of the DPL model. Lee et al. [17] gave the Green's function solution of the DPL model with a homogeneous Dirichlet boundary condition. Among those numerical solutions, Dai et al. [18–20] developed several finite difference schemes for solving the DPL model with the Dirichlet boundary condition. Zhang and Zhao [21] also presented a compact high accurate stable numerical solution for the DPL model with the Dirichlet boundary condition. Prakash et al. [22] solved the DPL equation

* Corresponding author. Tel.: +1 3182573301.
E-mail address: dai@coes.latech.edu (W. Dai).

0017-9310/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.ijheatmasstransfer.2013.05.005

Nomenclature

B	ratio τ_T/τ_q of relaxation times
c	heat capacity
h	grid size
k	thermal conductivity
K_n	Knudsen number
N	number of grid points
n	time level
q	heat flux
T	temperature
T_w	wall temperature
t	time
T_i^n	numerical solution of $T(ih, n\Delta t)$
u	an intermediate function
u_i^n	numerical solution of $u(ih, n\Delta t)$
Δt	time step
x	Cartesian coordinate
α	coefficient related to temperature-jumped boundary condition
∇	gradient
∇_x	first-order forward finite difference operator in x
δ_t	second-order central difference operator in t
δ_x^2	second-order central difference operator in x
τ_T, τ_q	relaxation time

with various Dirichlet and Neumann boundary conditions using the finite element method. Ho et al. [23] used the lattice Boltzmann method to obtain numerical solutions for the DPL model with homogeneous Neumann boundary in multilayered structure. Kunadian et al. [24] presented a finite difference solution for the DPL equation with the Dirichlet and Neumann boundary conditions in a semi-infinite interval. Liu and Cheng [25] applied the Laplace transform method together with the control volume method to obtain a numerical solution of the DPL model with the Dirichlet boundary condition in layered films. Shen and Zhang [26] gave a numerical solution for the DPL model with the Dirichlet boundary condition obtained using a high-order TVD scheme with Roe's superbee limiter function. Chou and Yang [27,28] employed the space–time conservation element and solution element (CESE) method to solve the DPL model in finite medium with pulse surface heating. In recent years, utilization of the DPL model to simulate heat transfer in nano-structures has been considered by researchers [1,29–31]. In particular, one-dimensional problem of heat conduction for the Knudsen numbers greater than 0.1 corresponding to micro/nano-structures was implemented by Basirat et al. [31] using the DPL model. It has been found that the DPL model with no-temperature-jump on boundaries neglects the effects of boundary phonon scattering. As a result, the obtained results lead to unsatisfying results especially near boundaries [1]. It was suggested that a temperature jump boundary condition should be introduced to couple with the DPL model for nano-scale heat conduction [1]:

$$T - T_w = \alpha K_n \left(\frac{\partial T}{\partial \mathbf{n}}\right)_w, \tag{4}$$

where T_w is the wall jumped temperature, $\mathbf{n}$ is the unit outward normal vector on the boundary, K_n is the Knudsen number, and α is a coefficient which may be tuned. Heat transfer regimes for a thin slab was analyzed in [1] by choosing different values for relaxation time ratios between 0.0 and 0.1, and for Knudsen numbers from 0.1 to 10 to find how accurate the prediction of the DPL model responses in the heat conduction of nano-structures. Result shows that the DPL model coupled with the temperature jump boundary condition is promising.

In this article, we present a higher-order accurate and unconditionally stable compact finite difference scheme for solving the DPL equation with the temperature jump boundary condition. Because at nano-scale the grid size may be very small, higher-order accuracy and unconditional stability are particularly important. Using a higher-order accurate scheme will allow us to choose a relative coarse grid and obtain a reasonable solution. On the other hand, unconditional stability will give no restriction on the mesh ratio. The obtained scheme is illustrated by three numerical examples.

2. Governing equations

We first normalize Eq. (3) by introducing non-dimensional parameters [1] as follows:

$$\theta = \frac{T - T_0}{T_w - T_0}, \quad t^* = \frac{t}{\tau_q}, \quad B = \frac{\tau_T}{\tau_q}, \quad \eta = \frac{x}{L}, \quad K_n = \frac{\lambda}{L}, \tag{5}$$

where λ and L are the mean molecular mean free path and characteristic length, respectively. As a result, Eq. (3) can be rewritten as:

$$\frac{\partial \theta}{\partial t^*} + \frac{\partial^2 \theta}{\partial t^{*2}} = \frac{K_n^2}{3}\left(\frac{\partial^2 \theta}{\partial \eta^2} + B\frac{\partial^3 \theta}{\partial t^* \partial \eta^2}\right) \tag{6}$$

and the boundary condition, Eq. (4), becomes

$$\theta - \theta_w = \alpha K_n \left(\frac{\partial \theta}{\partial \mathbf{n}}\right)_w, \tag{7}$$

where θ_w is the wall jumped temperature. It should be pointed out that if $K_n \approx 1.0$ or is greater than 1.0, the mean molecular mean free path is almost same order as or greater than the characteristic length, which is typically the case at nano-scale. For simple notation, we rewrite the above equations and consider the nano heat conduction equation as follows:

$$\frac{\partial T}{\partial t} + \frac{\partial^2 T}{\partial t^2} = \frac{K_n^2}{3}\left(\frac{\partial^2 T}{\partial x^2} + B\frac{\partial^3 T}{\partial t \partial x^2}\right), \quad 0 < x < 1, \ t > 0 \tag{8}$$

with the temperature jump boundary condition

$$T(0,t) - T_w(0,t) = \alpha K_n \frac{\partial T(0,t)}{\partial x}, \tag{9a}$$

$$T(1,t) - T_w(1,t) = -\alpha K_n \frac{\partial T(1,t)}{\partial x} \tag{9b}$$

and an appropriate initial condition.

3. Higher-order compact finite difference scheme

To develop an accurate finite difference scheme, we first design an uniform mesh on [0,1], where grid points are $x_i = ih$, $i = 0, 1, \ldots, N$, and $h = \frac{1}{N}$. We denote $t_n = n\Delta t$, where Δt is the time step and n is the time level. It is noted that when discretizing the term $\frac{\partial^2 T}{\partial t^2}$, one needs to use three time levels of finite difference to approximate it. This may cause some difficulty to analyze the stability sometimes. To avoid this troublesome, one often introduces an intermediate function so that the obtained finite difference scheme is two-level in time. As seen in the derivations below, we consider two different cases, depending on either $0 \leqslant B \leqslant 1$ or $B > 1$. The purpose of this consideration is to guarantee that the