Temperature Field Dependent Variation Computational Method for Non-Fourier Heat Conduction in Thin Film Semiconductor

Dhanaraj Savary Nasan, T. Kishen Kumar Reddy

Abstract— In recent years, the Dual Phase Lag (DPL) heat conduction equation proved itself to be one of the best choices for predicting both observed micro scale and macro scale effects in the case of non-Fourier heat conduction in the micro/nano-scaled semiconductor devices and structures. In this publication, based on the Flow field Dependent Variation (FDV) methodology, we present a unique finite differenced Temperature field Dependent Variation Computational Method for characterizing and resolving the one dimensional DPL heat conduction equation for Silicon thin film resembling a micro-electronic structure subjected to a suddenly applied spatial temperature gradient at both the boundary ends. The uniqueness of this computational method is that at every time step, the matrix coefficients of finite differenced governing partial differential equation (PDE) based on FDV theory will change as the local adjacent spatial and temporal Temperature field changes and will correspondingly modify the governing PDE to solve the appropriate physics that are going on at each grid points. This work initiates the development of such local temperature based computational strategies for the numerical simulation of non-Fourier DPL heat conduction that will facilitate the optimized thermal stability and design of miniature transistors and circuits in the semiconductor industry

Index Terms— FDV theory; DPL model, non-Fourier; Heat waves, micro/nano heat transfer; Microelectronic devices, MOSFET.

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1 INTRODUCTION

To improve their function and speed, the modern electronic devices and circuits drastically reduce their sizes to micro/nano scale leading to a very high heat dissipation rates. As a result, the micro/nano heat conduction becomes an important issue for the accurate prediction of transient temperature and heat flux distributions in the optimized thermal design of such miniature devices like Metal Oxide Semiconductor Field Effect Transistors (MOSFETs) which has become the building blocks of the semiconductor industry. Further scaling down to nanoscale electronics will result in a very high numbers of transistors assembled on an IC chip area no greater than a few square centimeters.

In most commonly encountered practical engineering problems, the heat conduction is characterized and resolved by the classical heat flux constitutive model of the Fourier's type. However the parabolic Fourier model admits no delay between the instants of applied spatial temperature gradient and heat flux leading to infinite speed of heat propagation which physically inadmissible. When the temperature gradient is suddenly applied, the heat conduction is non-Fourier in nature i.e. hyperbolic heat waves with finite speed takes place in very short transient time required to reach the steady state. The electrons, phonons and photons are various energy carriers for heat transport at micro/nano levels. Among these energy carriers, phonons, the quanta of lattice vibrations, are the foremost heat carriers in semi-conductor like silicon at and above the room temperature.

As the length scale of the semiconductor devices and cir-

cuits reduces to the phonon's mean free path and the time scale are comparable to the thermal relaxation time for phonons collision, the classical heat flux constitutive model of the Fourier's type results in erroneous transient temperature distributions. Due miniaturization of semiconductor devices, the classical heat flux constitutive model of the Fourier's type is no longer [1], [2] an effective one for characterizing and resolving the micro/nano heat conduction in such electronic devices. On the other hand, the hyperbolic non-Fourier macro scale model records well the actual phenomena of finite heat propagation speed, it is the excellent choice for resolving the very rapid transient heat transfer process in micro/ nano electronic devices.

The non-Fourier effects which are based on the concept of hyperbolic wave nature can be found initially in the works on the Telegraph equation [3] by Maxwell. Tisza (1935) and Landau (1941) first encountered the problem of second sound arose in the studies of heat waves in liquid helium -II. Cattaneo (1948) first developed a mathematical theory [4] to correct the unacceptable nature of infinite speed of heat propagation in Fourier's diffusion theory. Later the problem that infinite speed of propagation is generated by diffusion was addressed independently by Morse and Feshbach (1953) and Vernotte (1958). Joseph and Preziosi (1989-90) based on the analogy of shear waves in liquids and the thermal waves, proposed a thermal model [5] analogous to the well known Jeffrey's model for stress and strain rate in liquids resulting in the heat flux constitutive model of Jeffrey's type. Ballistic Diffusive equation and the phonon Boltzmann equation or the molecular dynamics simulations can be applied to characterize and resolve [6] the heat conduction in nanoMOSFET. The numerical results indicate ballistic propagation as well as diffusive heat conduction. The draw backs [7] of micro/nano scale model based on phonon Boltzmann equation or the molecular dynamics simulations are the high computational complexity and long simu-

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lation time.

Tzou proposed a Dual Phase Lag model [8] , [9] which proved its capability to be the best choice for predicting both observed micro scale and macro scale effects in the case of non-Fourier heat conduction in the micro/nano-scaled semiconductor devices and structures . It permits to incorporate the micro/nano scale effects in the macro scale heat transport. This new heat flux constitutive model of the Tzou's type replacing the classical heat flux constitutive model of the Fourier's type to characterize and resolve the non-classical heat transport in ultra-fast laser heating of metals, hyperthermia treatment of tumor, and micro/nano scale structures have been confirmed. Ghazanfarian and Abbassi used the DPL model [10], [11] to simulate micro/nano scale heat conduction with temperature boundary conditions. Further application [2] of DPL model for a real 2D-MOSFET for temperature rise computation were carried out effectively. The DPL equation [8], [9] is presented below before proceeding to the FDV method. The one dimensional heat flux constitutive model of DPL's type is expressed as

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

Where τ_q and τ_T are phase lag of heat flux and phase lag of spatial temperature gradient respectively. The τ_q an τ_T are characteristics for a given material specimen.

Using Taylor's series expansion of (1) up to the first order derivative yields:

$$q(x,t) + \tau_q\ \frac{\partial q(x,\ t)}{\partial t} + O\ (\tau_q^{\ 2}\ ) = -k\frac{\partial[\ T(x,t) + \tau_T\frac{\partial T(x,\ t)}{\partial t} + O(\tau_T^{\ 2}\ )]}{\partial x}$$

$$q(x,t) + \tau_q\ \frac{\partial q(x,\ t)}{\partial t}\ = -\ k\ \frac{\partial T(x,t)}{\partial x} - k\tau_T\ \frac{\partial(\frac{\partial T(x,t)}{\partial x})}{\partial t} \tag{2}$$

The DPL heat conduction equation based on heat flux constitutive law (2) is expressed as

$$\frac{1}{\alpha}\frac{\partial T(x,t)}{\partial t} + (\frac{1}{a^2})\frac{\partial^2 T(x,t)}{\partial t^2}\ =\ \frac{\partial^2 T(x,t)}{\partial x^2} + \tau_T\frac{\partial^3 T(x,t)}{\partial x^2\partial t} \tag{3}$$

Depending upon the selection of the τ_q , τ_T and F_T in (2)-(3) DPL model yields to different [12], [13], [9] known heat conduction models as in Table 1:

Table 1
Different Heat conduction models

τ_q	τ	τ	0 or 1
τ_T	$\tau\ (k_1/k) = \mathbf{K}$	0	0 or 1
$F_T = \mathbf{K}/\tau$	$0 < F_T < 1$	$F_T = 0$	$F_T = 1$
Model	Jeffrey	Cattaneo-Vernotte	Fourier
Heat flux Eq.	q + τ ∂q/∂t = − k ∂T/∂x − τ k_1 ∂(∂T/∂x)/∂t	q + τ ∂q/∂t = − k ∂T/∂x	q = −k ∂T/∂x
Heat Cond.Eq.	1/α ∂T/∂t + (1/a^2) $\partial^2 T/\partial t^2$ = $\partial^2 T/\partial x^2$ + $\mathbf{K}$ $\partial^3 T/\partial x^2\partial t$	1/α ∂T/∂t + (1/a^2) $\partial^2 T/\partial t^2$ = $\partial^2 T/\partial x^2$	1/α ∂T/∂t = $\partial^2 T/\partial x^2$

This model incorporates the commonalities [9] among the phonon- electron interactions based models for metals and phonon scattering based models for semiconductors, dielectric crystals and insulators and thereby leading to a unified model for investigation of a variety of heat transfer problems. The generalized DPL model looks very promising for future research because it shows very good agreement with experiment across a wide range of both length and time scales in heat transfer situations. This paper presents a numerical simulation for very rapid transient heat conduction in a thin film of silicon by applying the DPL model. When compared to the other researchers for similar work of applying the DPL partial differential equation (3), the only difference of the present work is that we apply this partial differential equation not in its original form but in a modified form of incremental partial differential equation obtained by applying the FDV methodology to the original DPL equation (3). Brief note on FDV theory before we present the FDV based computational formulation in the next heading.

One of the tough challenges in Computational Fluid Dynamics (CFD) is how to deal with very rapid changes of the solution variables like pressure, temperature, velocity and density both in time and space, where we are faced with smallest time and length scales for very high gradient of such solution variables. Compounding these challenges are the computational difficulties in resolving real complex flows as they are mixtures of physical phenomena like transition from laminar to turbulent flow, interactions between viscous & inviscid flows, and incompressible & compressible flows. To tackle these challenges and resolve simultaneous all physical situations of fluid dynamics and classical heat transfer, Chung *et al.* [14], [15], [16], [17] have introduced FDV method just at dusk of the 20th century. Since its inception, many benchmark cases of fluid dynamics and classical heat transfer [18] have been solved by FDV method to prove its excellent solution accuracy and numerical stability. Here we apply FDV method to DPL equation (3) and resolve the heat transfer phenomena influenced by both non-Fourier and Fourier heat transport effects and mechanism in a single domain of a semiconductor material.

The energy equation component of the conservative Navier-Stokes System of equations (continuity equation, momentum equations and energy equation) for pure heat conduction in a constant density property static fluid i.e. zero flow velocity components is also [19] the well known unsteady heat conduction equation in solid. That is both energy equation constituent of Navier-Stokes System of equations for pure heat conduction in a static fluid and the unsteady heat conduction equation for solid is same if we substitute the density of the solid for the static fluid density. .Hence in the present work, for any analysis of unsteady heat conduction in solid (semiconductor) we opt the for equivalent energy equation component of Navier-Stokes System of equations for a pure heat conduction in static fluid whose constant density is same as that of the solid under consideration. For numerical simulation of very rapid transient heat conduction in a thin film of solid silicon, the need of energy equation component of the conservative Navier-Stokes System of equations arises from the fact that FDV computational formulation is derived from the specialized final form of Taylor series expansion up to and including second order time derivative of the conservative energy solution variables component of the Navier-Stokes Sys-

tem of equations with finite diffusion flux variables. The diffusion FDV parameters managing transient temperature field discontinuity i.e. heat waves are defined from the changes of temperature between the adjacent grids points at each time marching step. Thus the temperature based finite differenced FDV equation on applying to the computational domain grid points results into a system of linear, algebraic equations which can be solved using standard algorithm of matrix solver to compute transient temperature solution variables at all grid points in the domain.

The advantage of using original DPL equation (3) in the modified form of incremental partial differential is that at every time step, the matrix coefficients of the modified equation based on FDV theory will change as the local adjacent spatial and temporal temperature field changes and will correspondingly modify the governing PDE to solve the appropriate physics that are going on at each grid points. This is in contrast with other existing computational methods where normally such coefficients been expressed only in terms of conducting medium's thermo-physical properties and computational spatial & time increments remains same. Consequently in all such other computational methods in general, a pre-determined computational formulation dictates the computational heat transfer (CHT) solution for both non-Fourier and Fourier situations. On other hand, the FDV computational method provides the best *distinct* computational scheme for *every point* of the computational domain at a given instant of time when compared to the other CFD /CHT methods for heat transfer. This fact is established in this paper through the final presentation of the computational results which upholds the existence of heat waves in the thin Silicon film subjected impulsive boundary temperature conditions and demonstrates the propagation process of heat waves, the magnitude and profile of transient temperature in contrast with the classical Fourier heat conduction.

2 COMPUTATIONAL FORMULATION

By a Taylor's series expansion strategy [20], [21] and substituting the density of the thin silicon film for the static fluid density, the original DPL heat conduction equation can be redeveloped into an equation form resembling the *energy equation component* of conservative Navier-Stokes System of equations (continuity equation, momentum equations and energy equation) for pure heat conduction in a constant density property static fluid i.e. flow velocity components are zeros. The redeveloped DPL heat conduction equation is given respectively as:

$$\frac{\partial T(x,\ t+\tau_q)}{\partial t} = \alpha\,\frac{\partial^2[T(x,\ t+\tau_T)]}{\partial x^2} \tag{4a}$$

$$\frac{\partial[\rho c T(x,\ t+\tau_q)]}{\partial t} + \frac{\partial\left\{\frac{\partial[-kT(x,\ t+\tau_T)]}{\partial x}\right\}}{\partial x} = 0 \tag{4b}$$

The energy equation component of the Navier-Stokes System of Equations for pure heat conduction in a constant density (numerically equating to the density of silicon) property static fluid condition (velocity $v_1 = u = 0$) without source terms for 1-D can be expressed in conservative form [19], [17] as

$$\frac{\partial U}{\partial t} + \frac{\partial F_1}{\partial x_1} + \frac{\partial G_1}{\partial x_1} = 0 \tag{5}$$

Where $U = [\rho c T]$, $F_1 = [0]$ & $G_1 = [-kT_{,1}]$ (6)

$$\therefore \frac{\partial U}{\partial t} + \frac{\partial G_1}{\partial x_1} = 0 \tag{7a}$$

$$\frac{\partial[\rho c T]}{\partial t} + \frac{\partial[-kT_{,1}]}{\partial x_1} = 0 \tag{7b}$$

The comma in expression G_1 indicates partial derivative with respect to independent variable x_1 (= x). As discussed earlier that energy equation component of conservative Navier-Stokes System of equations for pure heat conduction in a constant density property static fluid is nothing but the well known unsteady heat conduction equation in solid (silicon). Hence (7b) is also the well known 1-D unsteady heat conduction equation in solid (silicon). On comparing (4b) & (7a), it shall be noted the form of the both equations are same. Therefore on equating the corresponding terms:

$$\rho c T(x,\ t+\tau_q) = U(x,\ t+\tau_q) = U_{\tau_q} \qquad \& \tag{8a}$$

$$\frac{\partial[-kT(x,\ t+\tau_T)]}{\partial x} = G(x,\ t+\tau_T) = G_{\tau_T} \tag{8b}$$

Thus we can transform the (3) into a form similar to (7a) [resulted from the (5)] through (4b). That is by Taylor's series expansion strategy as adopted in our earlier investigation [20], [21] the original two term L.H.S form DPL heat conduction equation (3) can be now redeveloped into such a single term L.H.S form (4a) which now resembles the energy equation component of the conservative Navier-Stokes System of equations whose specialized final form of Taylor series expansion up to and including second order time derivative yields to the final FDV computational formulation for DPL equation (4b).

Using Taylor's series expansion of (8) up to the first order derivative yields:

$$U_{\tau_q} = U(x,\ t+\tau_q) = U(x,\ t) + \tau_q\,\frac{\partial U(x,t)}{\partial t} \ \&$$

$$G_{\tau_T} = G(x,\ t+\tau_T) = G(x,\ t) + \tau_T\,\frac{\partial G(x,t)}{\partial t}$$

Also from (8a) & (8b), $\rho c T(x,\ t+\tau_q) = U(x,\ t+\tau_q)$

& $\frac{\partial[-kT(x,t+\tau_T)]}{\partial x} = G(x,\ t+\tau_T)$

Thus (4b) is expressed as

$$\frac{\partial U_{\tau_q}}{\partial t} + \frac{\partial G_{\tau_T}}{\partial x} = 0 \quad \textbf{or} \quad \frac{\partial U_{\tau_q}^n}{\partial t} + \frac{\partial G_{\tau_T}^n}{\partial x} = 0 \tag{9}$$

Applying the FDV methodology [17] to partial differential equation (9) whose original form is DPL heat conductionequation (3) and expanding $U_{\tau_q}^{n+1}$ in a special form of Taylor series about $U_{\tau_q}^n$ up to and the second - order time derivatives with inclusion the appropriate first order (s_3) & second order (s_4) FDV diffusion parameters for the first and second order derivatives of $U_{\tau_q}^n$ with respect to time respectively, yieldsto the present work's derived modified form of incremental differential equation for non-Fourier heat conduction in constant property static fluid or in solid (silicon) as presented below with $O(\Delta t^3)$:

$$\Delta U_{\tau_q}^{n+1} = -\,E_1^n\,\frac{\partial(\Delta U_{\tau_q}^{n+1})}{\partial x} - E_{11}^n\,\frac{\partial^2\left(\Delta U_{\tau_q}^{n+1}\right)}{\partial x^2} - Q^n \tag{10a}$$

$$\Delta U_{\tau_q}^{n+1} + E_1^n\,\frac{\partial(\Delta U_{\tau_q}^{n+1})}{\partial x} + E_{11}^n\,\frac{\partial^2\left(\Delta U_{\tau_q}^{n+1}\right)}{\partial x^2} = -\,Q^n \tag{10b}$$

Where

$$E_1^n = (\Delta t\, s_3\, b_1)^n \tag{11a}$$

$$E_{11}^n = \left(\Delta t\, s_3\, c_{11} - \frac{\Delta t^2}{2}\, s_4\, (b_1)^2\right)^n \tag{11b}$$

$$Q^n = \left(\Delta t\,\frac{\partial G_{\tau_T}^n}{\partial x} - \frac{\Delta t^2}{2}\, b_1^n\,\frac{\partial^2\left(G_{\tau_T}^n\right)}{\partial x^2}\right) \tag{11c}$$

In the FDV equattion (10b) for DPL heat conduction, for fur-

ther processing it for numerical simulation, the terms E_1^n and E_{11}^n are taken as constants during present numerical iteration time step , but updated for the next iteration time step.

Similarly the present work's derived FDV equation for three dimensional DPL heat conduction of non-Fourier's type in constant property static fluid or in solid (silicon) can expressed as below:

$$\Delta U_{\tau_q}^{n+1} + E_i^n \frac{\partial(\Delta U_{\tau_q}^{n+1})}{\partial x_i} + E_{ij}^n \frac{\partial^2\left(\Delta U_{\tau_q}^{n+1}\right)}{\partial x_i \partial x_j} = -Q^n \tag{12}$$

$$U_{\tau_q} = U\left[(x, y, z), (t + \tau_q)\right] \tag{13a}$$

$$G_{\tau_T i} = G\left(x_i, t + \tau_T\right) \tag{13b}$$

$$E_i^n = (\Delta t s_3 b_i)^n \tag{13c}$$

$$E_{ij}^n = \left(\Delta t s_3 c_{ij} - \frac{\Delta t^2}{2} s_4 b_i b_j\right)^n \tag{13d}$$

$$Q^n = \left(\Delta t \frac{\partial G_{\tau_T i}^n}{\partial x_i} - \frac{\Delta t^2}{2} b_i^n \frac{\partial^2\left(G_{\tau_T j}^n\right)}{\partial x_i \partial x_j}\right) \tag{13e}$$

$$b_i = \frac{\partial G_{\tau_T i}}{\partial U_{\tau_q}} \quad \& \quad c_{ij} = \frac{\partial G_{\tau_T i}}{\partial U_{\tau_q,j}} \tag{13f}$$

The finite difference method (FDM), finite element method (FEM) or finite volume method (FVM) can be used [17] to discretize numerically the present work's finally resulted governing FDV equations (10b) and (12) for 1D and 3D non-Fourier DPL heat conduction in constant property static fluid or in solid (silicon) respectively. Consequently the discretize method is set aside as the option of the computational heat transfer analysts / computational fluid dynamicists.

As exemplar, numerically discretizing the FDV equation (10b) by FDM is illustrated next. On approximating first order and second order spatial derivatives of (10b) at each grid point (i-1, i, i+1) by second order accurate central finite differences, we present the final derived finite-differenced FDV equation (14) for one dimensional non-Fourier DPL heat conduction in constant property static fluid or in solid(silicon)as below with O($\Delta x^2, \Delta t^3$) :

$$\left(\Delta U_{\tau_q}\right)_i^{n+1} + (E_1)_i^n\left[\frac{\left(\Delta U_{\tau_q}\right)_{i+1}^{n+1} - \left(\Delta U_{\tau_q}\right)_{i-1}^{n+1}}{2\Delta x}\right] +$$

$$(E_{11})_i^n\left[\frac{\left(\Delta U_{\tau_q}\right)_{i+1}^{n+1} - 2\left(\Delta U_{\tau_q}\right)_i^{n+1} + \left(\Delta U_{\tau_q}\right)_{i-1}^{n+1}}{\Delta x^2}\right] = -Q_i^n$$

$$\underbrace{\left[\frac{(E_{11})_i^n}{\Delta x^2} - \frac{(E_1)_i^n}{2\Delta x}\right]}_{A_i^n}\left(\Delta U_{\tau_q}\right)_{i-1}^{n+1} + \underbrace{\left[1 - \frac{2(E_{11})_i^n}{\Delta x^2}\right]}_{B_i^n}\left(\Delta U_{\tau_q}\right)_i^{n+1} +$$

$$\underbrace{\left[\frac{(E_1)_i^n}{2\Delta x} + \frac{(E_{11})_i^n}{\Delta x^2}\right]}_{C_i^n}\left(\Delta U_{\tau_q}\right)_{i+1}^{n+1} = -Q_i^n$$

$$A_i^n\left(\Delta U_{\tau_q}\right)_{i-1}^{n+1} + B_i^n\left(\Delta U_{\tau_q}\right)_i^{n+1} + C_i^n\left(\Delta U_{\tau_q}\right)_{i+1}^{n+1} = -Q_i^n \tag{14}$$

Where

$$(E_1)_i^n = (\Delta t s_3 b_i)^n \tag{15a}$$

$$(E_{11})_i^n = \left(\Delta t s_3 c_{11} - \frac{\Delta t^2}{2} s_4 (b_1)^2\right)_i^n \tag{15b}$$

$$\left(G_{\tau_T}\right)_i^n = -k\left[\frac{\left(T_{\tau_T}\right)_{i+1}^n - \left(T_{\tau_T}\right)_{i-1}^n}{2\Delta x}\right] \tag{15c}$$

$$(b_1)_i^n = \left(\frac{\partial G_{\tau_T}}{\partial U_{\tau_q}}\right)_i^n = \frac{\left(G_{\tau_T}\right)_i^n - \left(G_{\tau_T}\right)_i^{n-1}}{\left(U_{\tau_q}\right)_i^n - \left(U_{\tau_q}\right)_i^{n-1}} \tag{15d}$$

$$(c_{11})_i^n = \left(\frac{\partial G_{\tau_T}}{\partial U_{\tau_q'i}}\right)_i^n = \frac{\left(G_{\tau_T}\right)_i^n - \left(G_{\tau_T}\right)_i^{n-1}}{\left(\frac{\left(U_{\tau_q}\right)_{i+1} - \left(U_{\tau_q}\right)_{i-1}}{2\Delta x}\right)^n - \left(\frac{\left(U_{\tau_q}\right)_{i+1} - \left(U_{\tau_q}\right)_{i-1}}{2\Delta x}\right)^{n-1}} \tag{15e}$$

$$Q_i^n = \Delta t\left(\frac{\left(G_{\tau_T}\right)_{i+1} - \left(G_{\tau_T}\right)_{i-1}}{2\Delta x}\right)^n - \frac{\Delta t^2}{2} b_i^n\left(\frac{\left(G_{\tau_T}\right)_{i+1} - 2\left(G_{\tau_T}\right)_i + \left(G_{\tau_T}\right)_{i-1}}{\Delta x^2}\right)^n \tag{15f}$$

$$(s_3)_i^n = \left(s_{3 Spatiotemporal}\right)_i^n = \frac{\left(s_{3Spatial}\right)_i^n + \left(s_{3Temporal}\right)_i^n}{2} \tag{15g}$$

$$\left(s_{Spatial}\right)_i^n = \frac{\sqrt{max(T_{i-1}^n, T_{i+1}^n)^2 - min(T_{i-1}^n, T_{i+1}^n)^2}}{min(T_{i-1}^n, T_{i+1}^n)} \tag{15h}$$

$$\left(s_{Temporal}\right)_i^n = \frac{\sqrt{max(T_i^{n-1}, T_i^n)^2 - min(T_i^{n-1}, T_i^n)^2}}{min(T_i^{n-1}, T_i^n)} \tag{15i}$$

$$(s_3)_i^n = \begin{cases} min((s)_i^n, 1) & (s)_i^n > \omega \quad (\omega < 1) \\ 0 & (s)_i^n < \omega \quad T_{min} \neq 0 \end{cases} \tag{15j}$$

$$(s_4)_i^n = [f(s_3, \eta)]_i^n \text{ or } = \frac{1}{2}\{1 + [(s_3)_i^n]^\eta\} \tag{15k}$$

The value for ω in (15j) and the range for η in (15k) can be known from [17]. In (14) combined with (15a) to (15k) , because of the three time levels in this FDM, initial data must be known at two time levels i.e. n & n-1 time levels. These data can be known if the time derivative of temperature is specified at t=0. The finite-differenced FDV equation (14) on applying to the grid points in a one-dimensional computational domain combined with two initial & two boundary conditions, results into a system of linear, algebraic equations which can be solved using standard algorithm of matrix solver to compute compute $\left(\Delta U_{\tau_q}\right)_i^{n+1}$ variables at all grid points in the domain for time level n+1. Thomas algorithm of tri-diagonal matrix solver can be used if tri-diagonal system of linear, algebraic equations is generated at each time step. Whichever algorithm of matrix solver is used, it should include the provision of updating A_i^n, B_i^n, C_i^n & Q_i^n in (14) at subsequent time steps.

To obtain the primitive temperature solution variables, we must decode the computed element $\left(\Delta U_{\tau_q}\right)_i^{n+1}$ as follows

$$\left(U_{\tau_q}\right)_i^{n+1} - \left(U_{\tau_q}\right)_i^n = \left(\Delta U_{\tau_q}\right)_i^{n+1}$$

From (8),

$$\left[\rho c T(x, t + \tau_q)\right]_i^{n+1} - \left[\rho c T(x, t + \tau_q)\right]_i^n = \left(\Delta U_{\tau_q}\right)_i^{n+1}$$

$$\left[T(x, t + \tau_q)\right]_i^{n+1} = \frac{\left(\Delta U_{\tau_q}\right)_i^{n+1}}{\rho c} + \left[T(x, t + \tau_q)\right]_i^n \tag{16}$$

Using Taylor's series expansion of T(x, t +τ_q) up to the first order derivative yields [20] with truncation error O (τ_q^2)

$$T(x, t + \tau_q) = T(x, t) + \tau_q \frac{\partial T(x,t)}{\partial t} \tag{17}$$

Applying (17) in (16)

$$\left[T(x, t + \tau_q \frac{\partial T(x,t)}{\partial t}\right]_i^{n+1} = \frac{\left(\Delta U_{\tau_q}\right)_i^{n+1}}{\rho c} + \left[T(x, t) + \tau_q \frac{\partial T(x,t)}{\partial t}\right]_i^n \tag{18a}$$

$$[T(x, t)]_i^{n+1} + \left[\tau_q \frac{\partial T(x,t)}{\partial t}\right]_i^{n+1} = \frac{\left(\Delta U_{\tau_q}\right)_i^{n+1}}{\rho c} + [T(x, t)]_i^n + \left[\tau_q \frac{\partial T(x,t)}{\partial t}\right]_i^n \tag{18b}$$

In the (18b), approximating the first order time derivative at

(n+1)[th] and (n)[th] time level by the temporal first order backward finite differences, we have

$$[T(x,t)]_i^{n+1} + \tau_q \left[\frac{[T(x,t)]_i^{n+1} - [T(x,t)]_i^{n}}{\Delta t} \right] = \frac{(\Delta U_{\tau_q})_i^{n+1}}{\rho c} + [T(x,t)]_i^{n}$$

$$+ \tau_q \left[\frac{[T(x,t)]_i^{n} - [T(x,t)]_i^{n-1}}{\Delta t} \right]$$

On re-arranging the terms in the above equation,

$$[T(x,t)]_i^{n+1} = \frac{1}{\left(1 + \frac{\tau_q}{\Delta t}\right)} \left[\frac{(\Delta U_{\tau_q})_i^{n+1}}{\rho c} + \right.$$

$$\left. \left(1 + \frac{2\tau_q}{\Delta t}\right)[T(x,t)]_i^{n} - \left(\frac{\tau_q}{\Delta t}\right)[T(x,t)]_i^{n-1} \right] \quad (19a)$$

Dropping (x, t) for clarity, we have

$$\boxed{T_i^{n+1} = \frac{1}{\left(1 + \frac{\tau_q}{\Delta t}\right)} \left[\frac{(\Delta U_{\tau_q})_i^{n+1}}{\rho c} + \left(1 + \frac{2\tau_q}{\Delta t}\right)T_i^{n} - \left(\frac{\tau_q}{\Delta t}\right)T_i^{n-1} \right]}$$

$$(19b)$$

Thus from (19b) based on FDV method, primitive temperature solution of a one dimensional non-Fourier DPL heat conduction is computed that is repeated for each time step as the heat wave proceeds through the static fluid with constant mass density or the solid medium (silicon) with a constant speed . Further we can also derive finite differenced FDV equation for three non-Fourier DPL heat conduction problems in static fluid with constant mass density or in medium (silicon) by approximating the first order and the second order spatial derivatives of (12) at each grid point by second order central differences schemes or any other differences schemes of higher-order accuracy. The resulting finite-differenced FDV equations at various grid points are then solved by using standard algorithm of matrix solver to compute $\Delta U_{\tau_q}^{n+1}[=[\Delta U(x,y,z,t+\tau_q)]^{n+1}]$ variables at all grid points (x, y, z) in the 3D-domain. Further on decoding the computed element $[\Delta U(x,y,z,t+\tau_q)]^{n+1}$, we can obtain the primitive temperature solution variables $[T(x,y,z,t)]^{n+1}$ at all grid points (x, y, z) in the 3D-domain non-Fourier DPL heat conduction.

3 RESULTS AND DISCUSSION

As a computational example, we consider one dimensional non-Fourier DPL heat transport effects in a solid medium like semiconductor material. Silicon been the most common materials in semiconductor devices, we opt this material as medium for which numerical simulation of non-Fourier DPL heat conduction is carried by FDV method. The elementary thermo-physical properties like density, specific heat and thermal conductivity of the silicon are taken from any material property table respectively as 2328 kg / m³, 700 J/kg-K and 155 W/m-K. We assume these thermo-physical properties are constant. Heat Conduction Model Number $F_T = \frac{K}{\tau}$ was introduced by Tamma and Zhou [12], [13] to improve the understanding relationships between the various heat flux constitutive models. From the Table.1, when we apply this number to the DPL heat flux constitutive model, we obtain F_T

$= \frac{\tau_T}{\tau_q}$. Working out to determine [22] τ_q and τ_T values for semiconductor material the silicon [9], [23] for a phonon frequency 2X10^{13} s^{-1} and temperature range of 300K -320K and substituting the values, we obtain $F_T = 0.45$.

One dimensional constant thermo-physical property silicon thin film of thickness l of the order of μm is considered for analysis and is discretized into total fifty grids points i.e. forty eighty intermediate grid points in x-direction. The criteria for obtaining a stable numerical solution for hyperbolic characterized non-Fourier DPL heat conduction in the silicon thin film in general is to keep [19], [24], [25], [26] the Courant number, $C = a\frac{\Delta t}{\Delta x}$, less than or at most to unity. In this work, we tested various Courant numbers from 0.40 to 1.00 and opted for C= 0.80 as it allows a stable numerical solutions and as well it is advantageous to moderately minimize the number of computational iterations for convergence of the solution. As a result based on C= 0.80, the time step for stable numerical solution, was determined as, $\Delta t = C \Delta x/a = C (l/49)/\sqrt{\alpha/\tau} = 0.8(3.41\text{X}10^{-6}/49)/\sqrt{0.95\text{X}10^{-4}/1.28\text{X}10^{-9}} = 2.049\text{X}10^{-10}$ s i.e. the order of time step for computational iteration is 10^{-10} s

The various thermal boundary conditions [27] affecting the temperature distributions of non-Fourier heat conduction in electronic package are specified temperature, constant heat flux, convective heat transfer and periodic heat flux/short pulsed laser heating. The major objective of the present work is to carry out under specified temperature boundary conditions, a numerical simulation of non-Fourier DPL heat conduction in silicon, the most common material for micro / nano electronic devices. The one dimensional bench mark miniature structure analyzed in this paper as mentioned earlier is a thin film of silicon of order $1\mu m$ which is subjected to specified impulsive temperature at both boundary ends. This structure could *resemble a real electronic micro structure*, whose lateral dimensions are typically larger than its thickness.

At t=0, the thin silicon film is at temperature T_0. At the time t >0, both the end surfaces of the thin silicon film at x=0 and x=l are impulsively increased to a temperature T_w. The sudden application of spatial temperature gradient at both ends sets up a non-Fourier transient temperature distributions of DPL character ($F_T = 0.45$) in the silicon film. With time progressing, final steady state distributions is given by a single value temperature T_w which get into all linear points of the fluid. Thus the solution of the finite-differenced FDV equation (14) characterizing this numerical problem of one dimensional ($F_T = 0.45$) non-Fourier DPL heat transfer in the silicon can be performed with the initial & boundary conditions and dimensional-less variables:

$$(x, t) = T_0 = 300 \ K \quad \text{and} \quad \frac{\partial [T(x, 0)]}{\partial t} = 0 \qquad t = 0$$

(20)

$$T (0, t) = T (l, t) = T_w = 320 \ K \qquad t > 0 \qquad (21)$$

$$T^* = \frac{T(x,t) - T_0}{T_w - T_0} \ ; \quad x^* = \frac{x}{l} \ ; \quad t^* = \frac{t}{l^2/\alpha} \qquad (22)$$

We can compute the T^* by two means, first by solving (14) & (19b) to obtain T(x, t) which on substituting in (22) gives T^*. Secondly by substituting (22) in (14) and solving the (14) re-

sults in dimensionless $\left(\Delta \mathbf{U}_{\tau_q}^*\right)_i^{n+1}$ which on decoding through the steps similar to (16) to (19b) results in T*.

As discussed earlier, because of the three time levels in this FDV method, initial data must be known at two time levels i.e. n-1 & n time levels. These data can be determined if the time derivative of temperature is specified at t=0. That is for the first time step Δt, based on zero value of second order central finite difference expression of time derivative of temperature as given in (20) we obtain an initial condition as

$$\frac{\partial\,[\,T(x,\,0)\,]}{\partial t}=0 \therefore \frac{T(x,\,0)^{n+1}-T(x,\,0)^{n-1}}{2\Delta t} \approx 0$$
$$\rightarrow T(x,0)^{n-1}= T(x,0)^{n+1}\rightarrow T_i^{n-1}=T_i^{n+1} \qquad (23)$$

The finite differenced expression for 1-D DPL heat conduction equation (3) can be written as:

$$-\frac{\tau_T\lambda}{\Delta t}T_{i-1}^{n+1} + (1 +\frac{\Delta t}{\tau_q} +\frac{2\tau_T\lambda}{\Delta t})\,T_i^{n+1} -\frac{\tau_T\lambda}{\Delta t}T_{i+1}^{n+1} =$$
$$-T_i^{n-1}+ (\lambda-\frac{\tau_T\lambda}{\Delta t})T_{i-1}^n + (2 +\frac{\Delta t}{\tau_q} -2\lambda+\frac{2\tau_T\lambda}{\Delta t})\,T_i^n\ +(\lambda-\frac{\tau_T\lambda}{\Delta t})T_{i+1}^n \quad (24)$$

Substituting the initial condition (23) in (24), we obtain the finite differenced expression for first time step Δt as:

$$-\frac{\tau_T\lambda}{\Delta t}T_{i-1}^{n+1} + (2 +\frac{\Delta t}{\tau_q} +\frac{2\tau_T\lambda}{\Delta t})\,T_i^{n+1}\ -\frac{\tau_T\lambda}{\Delta t}T_{i+1}^{n+1} = (\lambda-\frac{\tau_T\lambda}{\Delta t})T_{i-1}^n +$$
$$(2 +\frac{\Delta t}{\tau_q}- 2\lambda+\frac{2\tau_T\lambda}{\Delta t})\,T_i^n\ + (\lambda-\frac{\tau_T\lambda}{\Delta t})T_{i+1}^n \qquad (25)$$

In the R.H.S of (25), the temperature values at all the grid points of 1-D domain are known from the initial (20) conditions i.e. T_0 . In the L.H.S of (25), for i= first and last intermediate grid points , i-1 = left boundary grid point and i+1 = right boundary grid point of 1-D domain respectively are at the temperature T_w as at both boundaries, the temperature is impulsively increased from T_0 to T_w for t > 0. On applying the (25) to the all intermediate grid points , we obtain a tri-diagonal system of linear, algebraic equations whose solution by means of Thomas' Algorithm results in the values of the unknown temperature at all the intermediate grid points of 1-D domain at time t=Δt.

As a result of (20), (21) and (25), we have known initial temperature data at two time levels i.e. n-1 (t=0) & n (t=Δt) time levels. Based on these initial temperature data at (n-1) & n time levels and (21), we now proceed to apply the present work's derived FDV equation (14) along with (15a) to (15k) to all the intermediate grid points of 1-D domain for t= 2Δt. This leads to a tri-diagonal system of linear, algebraic equations with unknowns $\Delta \mathbf{U}_{\tau_q}$ at time level (n+1) for all the intermediate points of 1-D domain. Using Thomas' Algorithm as standard for the treatment of the generated tri-diagonal systems of equations, we compute the values of $\left(\Delta \mathbf{U}_{\tau_q}\right)_i^{n+1}$ at all intermediate grids. Finally the primitive transient temperature solution variables T_i^{n+1} at various intermediate grid points for (n+1) time level is obtained by substituting the computed element $\left(\Delta \mathbf{U}_{\tau_q}\right)_i^{n+1}$ in (19b). By this computational methodology, the computation of primitive temperature solution for one dimensional non-Fourier DPL heat conduction (F_T = 0.45) is repeated for each time step as the heat wave proceeds through the constant property silicon thin film with constant speed 'a'.

Thomas' algorithm of matrix solver should include the provision of updating A_i^n, B_i^n, C_i^n & Q_i^n in (14) at subsequent time steps. The computational iteration through increasing time is continued till a final steady-state temperature distributions are reached throughout the grid points of the 1-D domain based on a pre-selected convergence criteria.

From the starting time t=0, final results of spatial dimensionless temperature distributions based on (22) at different instants of dimensionless time predicted by the FDV computational model are presented in Fig.1 (a)-(d). The FDV computational model upholds the existence of heat waves in the thin silicon film subjected to a specified impulsive temperature at both boundary ends and demonstrates the propagation process of heat waves, the magnitude and profile of transient temperature. This brings FDV computational model in par with other existing computational models for non-Fourier DPL heat conduction simulation. As the temperature at the thin silicon film end boundaries are spontaneously raised, the left and the right curves moves towards the mid zone of the film i.e. the spatial dimensionless position x* =0.50 as the time marches . At latter times, as the heat reaches near mid zone of the film, there is rise in the temperature of such zone. This can be clearly seen in Fig.1 (b)-(c).That is the temperature is propagated through the film with a finite speed contrasting the Fourier's law of infinite speed which is physically inadmissible. This finite speed of temperature transfer indicates that mode of heat transfer is by heat waves for the initial nano / micro time. As the time further marches, the inverted dome at the middle zone rises toward T* = 1.0 line and the overall approximate 'U' shaped temperature profile curve flatten and approach the steady state mode of heat conduction. Numerically as shown in Fig.1 (c), at dimensional less t* = 0.7497 denoting t = 0.0922 μs the numerical solution is on the verge of converging and correspondingly steady state temperature distribution conditions are initiated to start temperature filling the whole silicon film with dimensionless temperature T* →1.0 i.e. absolute temperature T(x, 0.0922) →T$_w$ (=320 K). Furthermore it was noted during the numerical iteration that beyond t* = 0.7497, the change in the dimensional less temperature T*for each iteration is very small and it shall be noted in Fig.1 (d) that at t* = 0.9996 denoting t = 0.1230 μs the numerical solution is lastly converged based on a pre-selected convergence criteria, the final steady state temperature distribution conditions are reached with temperature filling the whole silicon film at T(x, t ≥ 0.1230) =T$_w$ (=320 K).
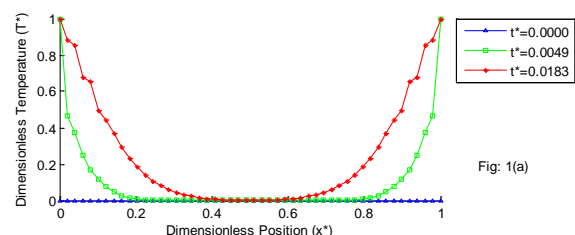
Contour plots of the calculated 1st and 2nd order spatial,

Fig: 1(a)

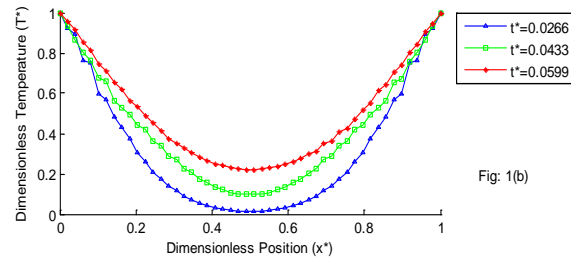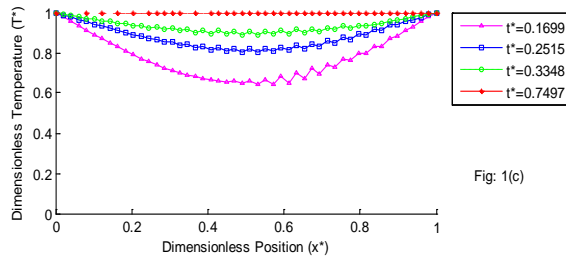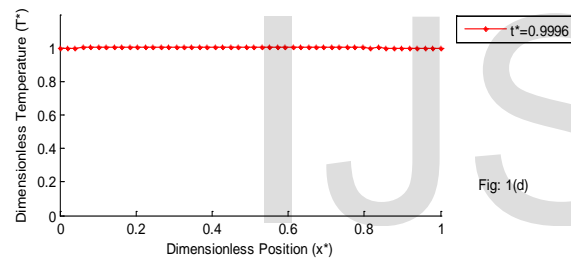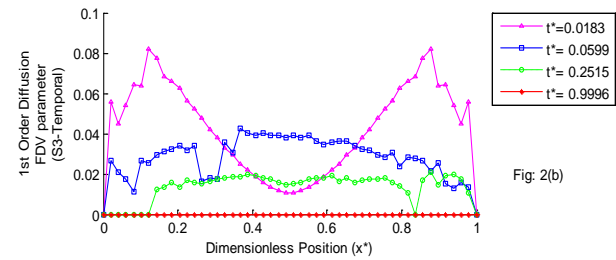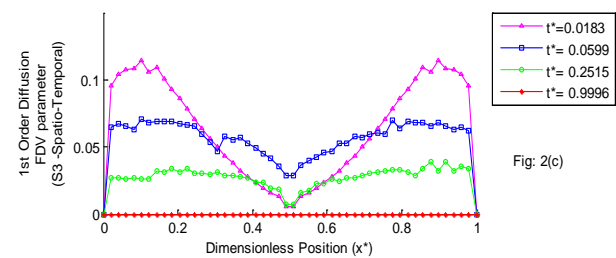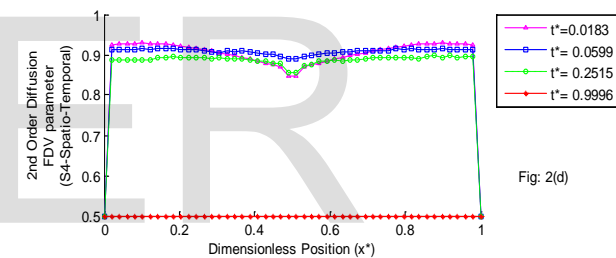**Fig. 1**.Non-Fourier DPL heat conduction solutions from the starting time t =0 for F_T = 0.45 predicted by FDV computational method at different instants of time (a) t*=0.0000, 0.0049, 0.0183 (b) t*=0.0266, 0.0433, 0.0599 (c) t*=0.1699, 0.2515, 0.3348, 0.7497 (d) 0.9996

Fig.2. Diffusion FDV parameters contours for different instants of times t*= 0.0183, 0.0599, 0.2515 & 0.9996 (a) 1st order-Spatial s_3 (b) 1st order-Temporal s_3 (c) 1st order-Spatio-temporal s_3 (d) 2nd order-Spatio-temporal s_4

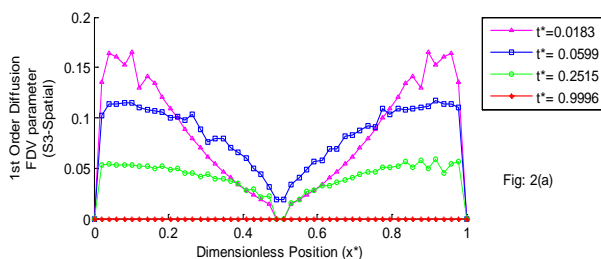temporal and spatio-temporal diffusion FDV parameters are shown in Fig.2 (a)-(d) for t* = 0.0183 , 0.0599, 0.2515 and 0.9996 which are the some of the dimensionless time values taken from Figs .1(a) , 1(b), 1(c) and 1(d) respectively. It can be observed that contour distributions of the 1st order spatial diffusion FDV parameters as shown in Fig.2 (a) resembles the contour of transient temperature field distributions illustrating the non-Fourier / non-classical DPL heat conduction in Fig. 1. (a) – (d) . Further on coalescing 1st order spatial diffusion FDV parameters with the 1st order temporal diffusion FDV parameters as in Fig. 2 (b), we obtain the overall and effective 1st order

spatio-temporal diffusion FDV parameters as shown in the Fig. 2.(c). It can be observed that these 1st order spatio-temporal diffusion FDV parameters 's$_3$' resembles more close-ly the contour of of transient temperature field distributions illustrating the non-Fourier / non-classical DPL heat con-duction in Fig.1 (a)-(d).Such intrinsic characteristics of 1st order convection & diffusion FDV parameters resembling the flow field contour distributions were found in the earlier research [14], [15], [17], [18] on applying FDV method to fluid dynam-ics and *classical* heat transfer problems. In the present work also true to its built-in nature, the character of the 1st order FDV parameters to resemble the field (temperature) contour distributions reappeared on applying FDV method to non-Fourier / *non- classical* DPL heat transfer problems. This demonstrates the extension capabilities of FDV method to characterize and resolve non-Fourier / *non- classical* heat con-duction. The contour plot of 2nd order FDV parameters s$_4$, ex-ponentially proportional to the 1st order FDV parameters s$_3$ is also shown in Fig.2 (d).

Final results of spatial dimensionless transient temperature distributions based on (22) at different instants of dimension-less time predicted by the *finite difference method* (FDM) were also carried out in the present work for the thin silicon film (F$_T$ = 0.45) with the same initial & boundary conditions as that for FDV method and is as shown in the Fig.3 (a)-(d). The dis-crete dimensionless times t* in the figure are the same as that opted in the Fig.1 (a)-(d)which depicts the non-Fourier DPL heat conduction solution by FDV method. In this method, the absolute transient temperatures 'T' are computed by the 1-D DPL heat conduction's finite differenced expression given by (24). Based on the initial temperature data at (n-1) & n time levels, we proceed to apply *Finite difference* equation (24) to all the intermediate grid points of 1-D domain for t= 2Δt. This leads to a tri-diagonal system of linear, algebraic equations with unknowns 'T' at time level (n+1) for all the intermediate points of 1-D domain. Using Thomas' Algorithm as standard for the treatment of the generated tri-diagonal systems of equations, we compute the values of 'T' at all intermediate grids. With 'T' values based on (22), the dimensionless tem-perature T* can be computed. On comparing the computation-al results of FDM in the Fig.3 (a)-(d) with that of FDV method in the Fig.1 (a)-(d) for same discrete dimensionless times t* , we observe the respective contour of the transient temperature fields resemble to each other approximately but not exact to each other for the non-Fourier DPL heat conduction. This dif-ference in the numerical values creep due to the fact that in FDV algorithm for every time step, coefficients $(A_i^n, B_i^n \& C_i^n)$ of (14) will change as the local temperature field changes and will modify the governing FDV (14) to solve the appropriate physics of hyperbolic, parabolic or mixed nature that are go-ing on at each grid point. This is in contrast with FDM where normally such coefficients [coefficients in the L.H.S of (24)] are
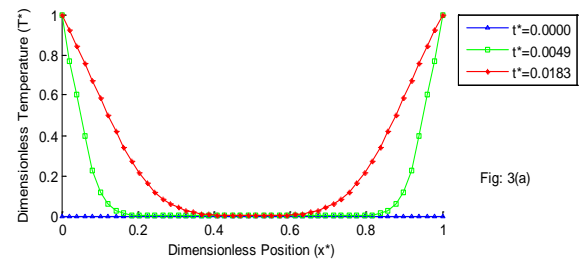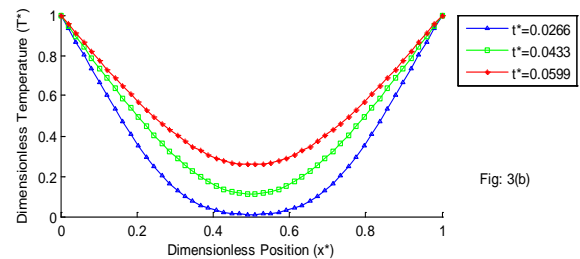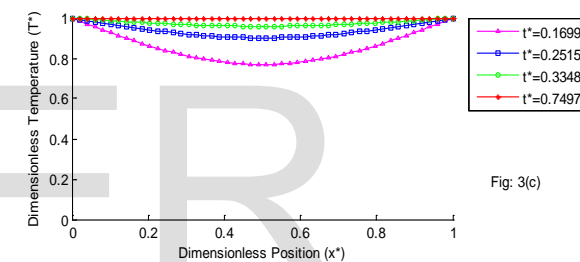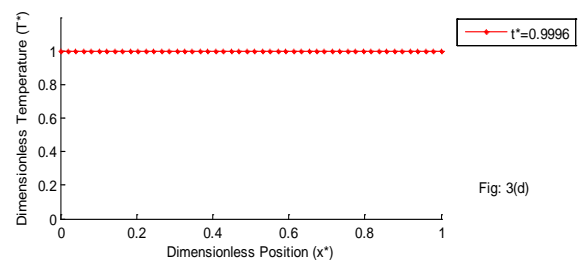

Fig: 3(a)

Fig: 3(b)

Fig: 3(c)

Fig: 3(d)

Fig.3. Non-Fourier DPL heat conduction solutions from the starting time t =0 for F$_T$ = 0.45 predicted by FDM computation-al method at different instants of time (a) t*=0.0000, 0.0049, 0.0183 (b) t*=0.0266, 0.0433, 0.0599 (c) t*=0.1699, 0.2515, 0.3348, 0.7497 (d) 0.9996.

expressed only in terms of the conducting medium's thermo-physical properties (α, $\tau_q \& \tau_T$) and computational spatial & time increments ($\Delta x \& \Delta t$) remains constant.

The convergence history of the dimensionless temperature T* variable at the spatial dimensionless position x* = 0.2245 for the FDV computational method is as shown in Fig.4. The x* = 0.2245 is the 12th grid point from the left boundary of the 1-D computational domain which is designated as the 1st grid

point. The temperature distributions in the thin silicon film were also used to estimate the needed to reach the steady state condition as shown in Fig.1 (d). The iteration process continues until the desired steady state results with following convergence criteria:

$$\left|(\Delta T^*)_i^{n+1}\right| \leq \varepsilon \qquad (26)$$

Where $(\Delta T^*)_i^{n+1} = (T^*)_i^{n+1} - (T^*)_i^n$

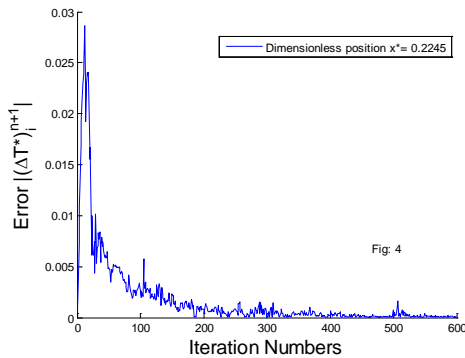and in the present work, the preselected error $= 10^{-5}$.

Fig.4. Convergence history of dimensionless temperature T* variable for the FDV computational method.

4 CONCLUSION

On characterizing and resolving the non-Fourier DPL heat conduction equation (3) by the FDV computational method, the numerical simulation of the transient temperature field distributions in the one dimensional thin silicon film *resembling a micro-electronic structure* subjected to spontaneously applied spatial temperature gradient at both boundary ends predicted a finite speed heat wave propagation in contrast with the classical parabolic heat conduction. Consequently a finite difference / finite element scheme based on FDV methodology can now be utilized as an alternative to the existing computational methods for non-Fourier DPL heat conduction numerical simulations in micro / nano electronic devices & structures in semiconductor industry.

Also true to its built-in nature, the character of the 1st order FDV parameters to resemble the field (temperature) contour distributions reappeared on applying FDV method to non-Fourier / *non- classical* DPL heat transfer problems. This further demonstrates the extension capabilities of FDV method to characterize and resolve non-Fourier / *non- classical* heat conduction.

The uniqueness of this FDV algorithm is that for every time step, coefficients ($A_i^n, B_i^n \& C_i^n$) of governing partial differential equation (14) will change as the *local temperature field* changes spatially and temporally and accordingly will modify the same governing FDV equation (14) to numerically solve the appropriate physics of hyperbolic, parabolic or mixed nature that are going on at each grid point. This is in contrast with other existing computational schemes where normally such coefficients [coefficients in the L.H.S of (24) , a case of finite difference scheme] are expressed only in terms of the conducting medium's thermo-physical properties (α, $\tau_q \& \tau_T$) and

computational spatial & time increments (Δx & Δt) remains constant.

Based on local adjacent spatial and temporal temperature field changes, this method provides the best distinct computational scheme for *each grid point* of the computational domain at a given iteration time step when compared to other CFD / CHT schemes for non-classical heat transfer numerical simulation.

Future broad research on FDV methodology will be required to develop local temperature based computational strategies also for the 3-D non-Fourier DPL heat conduction numerical simulation in micro / nano electronic devices with internal heat generation inclusion so as to accurately predict the transient temperature and heat flux distributions in the optimized thermal stability and design of such miniature devices like MOSFETs which has become the building blocks of the semiconductor industry.

The present work based on FDV methodology has initiated the development of such local temperature based computational strategies for non-Fourier DPL heat conduction numerical simulation that will facilitate the optimized thermal stability and design of miniature transistors and circuits in the semiconductor industry.

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l   thickness of silicon film

$t, \Delta t$ time and time step

τ thermal relaxation time

k   total conductivity

T   temperature $=T(x, t)$

k_1 effective thermal conductivity

k_2 elastic conductivity with $k = k_1 + k_2$

ρ mass density

c   specific heat

α thermal diffusivity $= k/\rho c$

a   propagation speed of heat wave or second sound $= (\frac{\alpha}{\tau})^{1/2}$

C   Courant number $= a\,\Delta t/\Delta x$

K   retardation time $= \tau\, k_1/k$

F_T heat conduction model number $\mathbf{K}/\tau$

τ_q phase lag of heat flux

τ_T phase lag of spatial temperature gradient

$\mathbf{F}_i$ convection flux variables column vector

$\mathbf{G}_i$ diffusion flux variables column vector

p   pressure

v_i velocity vector components

O ( )   truncation error

δ_{ij} kronecker delta

τ_{ij} viscous stress tensor

μ dynamic viscosity

$\mu m/\ \mu s$ micro meter / second

$\boldsymbol{U}_{\tau_q}$ $=$ $\mathbf{U}(x, t + \tau_q)$

$\mathbf{G}_{\tau_T}$ $=$ $\mathbf{G}(x, t + \tau_T)$

T_{τ_T} $=$ $T(x,\ t + \tau_T)$

$\Delta\mathbf{U}_{\tau_q}^{n+1}$ $= \mathbf{U}_{\tau_q}^{n+1} - \mathbf{U}_{\tau_q}^{n}$

$\mathbf{b}_i$ diffusion Jacobian

$\mathbf{c}_{ij}$ diffusion gradient Jacobian

s_a, s_b single numerical parameters

s_3 1st order diffusion FDV parameter

s_4 2nd order diffusion FDV parameter

ω user defined specified small number

ε error $\left| (\mathbf{T}^*)_i^{n+1} - (\mathbf{T}^*)_i^{n} \right|$

Superscript

n, n+1   running index in the time direction

Subscript

i, j   co-ordinate dimension counters =1, 2, 3 in a partial differential equation

i-1, i, i+1   running index in the x direction in a finite differenced equation i.e. represent grid points in I-D domain.

NOMENCLATURE

U   conservation solution variables column vector

q   heat flux $= q(x, t)$

$x, \Delta x$ cartesian coordinate and spatial step