Finite Difference Time Domain Simulation of Subpicosecond Semiconductor Optical Devices

by

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(ABSTRACT)

An efficient numerical method to simulate a subpicosecond semiconductor optical switch is developed in this research. The problem under studying involves both electromagnetic wave propagation and semiconductor dynamic transport, which is a nonlinear phenomenon. Finite difference time domain (FDTD) technique is used to approximate the time dependent Maxwell's equations for full-wave analysis of the wave propagation. The dynamic transport is handled by solving the balance equations using the energy and momentum relaxation time approximation. Based on the structure of the device, a physical semi-analytical model is also developed for preliminary analysis. Simulation results in the device's subpicosecond responses including nonlinearity and overshoot. The validity of the method is verified by comparing the simulation with the published experimental results. The method can be extended to other devices as well.
"We are in the ordinary position of scientists of having to be content with piecemeal improvements: we can make several things clearer, but we cannot make everything clear."

_Frank Plumton Ramsey_
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Chapter 1

Introduction

1.1. Objective and Contributions of the Dissertation

The main objective of this dissertation is to investigate propagation of an ultrafast pulse in a planar transmission line environment with GaAs semiconductor material as the propagation medium. An optical switch is used as an example for simulation based on solving the time dependent Maxwell's equations and the semiconductor transport equations using the finite difference time domain (FDTD) technique. The method used in this research can be extended into other similar devices such as pulse forming devices and optical sampling devices. The main contributions of this dissertation include:

1. Successfully obtained simulation responses of an optical switching device to an ultrafast pulse excitation, hence resulting in a careful investigation of the characteristics of the optical device. The simulation results agreed qualitatively with the experimental results. The method developed in this research is efficient and can be extended to other semiconductor devices as well as microwave devices;
2. Successfully simulated the interaction of the electromagnetic phenomena and the nonlinear dynamic transport in the optical device;

3. Developed a semi-analytical macroscopic model for an optical switch. The model can be used to preliminarily and efficiently estimate responses of the device.

1.2. Review of High Speed and High Frequency Devices [1,2]

Two major areas of semiconductor integrated circuits, Monolithic Microwave Integrated Circuit (MMIC) and High Speed Integrated Circuit (HPIC), have made great advances for the past two decades. Two important candidate semiconductor materials for these applications are the binary compound Gallium Arsenide (GaAs) and the elemental semiconductor silicon (Si). GaAs possesses five times greater electron mobility than Si and has excellent semi-insulating properties, which make it an excellent candidate for MMIC and HPIC to satisfy high frequency and high speed data rate requirements. Although Si is still a major material for medium and low speed digital circuits due to its mature technology and low cost in volume production, GaAs has become a major candidate in HPIC fabrication such as high speed DRAM's and CPU's used in modern high speed supercomputers.

Applications of MMIC technology include military, commercial, and consumer applications. Major applications of MMICs have been military applications. These
applications include electronic warfare, radar, as well as smart weapons, which require high speed and high frequency operations. For example, an advanced military radar must possess a wide operating bandwidth, rapid and accurate tracking of multiple targets. In order to achieve these requirements, one approach is to build an active-element phased-array radar, which consists of thousands of individual transmit-receive (T/R) modules. So far, GaAs MMIC technology is the prime candidate to realize such a radar system. It is predicted that a modern radar receiver can cover a wide frequency range extending from a frequency below 1 GHz up to 100 GHz by the year 2000. GaAs MMIC technology also offers significant improvement of components performances employed in modern high-data-rate fiber link communication systems. The systems implemented with GaAs MMICs can have data rates as high as 5 Giga bits/s.

In commercial and consumer applications, GaAs MMIC technology can offer analog and digital circuits to meet requirements ranging from UHF to millimeter-wave frequencies. These circuits are used in instruments and communication equipment such as frequency synthesizers, network analyzers, RF receivers, optoelectronic transceivers, and other applications.

MMIC is a circuitry combining various active device functions and passive device functions such as amplification, switching, filtering and others, on a single semiconductor substrate, a III-V binary compound material in this case. Active devices and passive
devices in MMICs include single-gate field effect transistors (FET), dual-gate field effect transistor, Schottky diode, resistors, and capacitors. All these devices are fabricated at the same time on a common semiconductor substrate using the same processing technology, a molecular beam epitaxy technique with diffusion capability [3].

Planar transmission lines are important in MMICs since they provide the base for laying out the devices as well as provide the necessary interconnections between the various devices. The transmission line configuration mostly used is the microstrip line because of its compatibility with the processing technology. Also, it provides transmission path interconnecting one MMIC circuit to another one. Therefore, GaAs semiconductor material not only serves as a material on which the devices are fabricated, but also is medium in which microwave signals can propagate [4].

1.3. Applications of Modern Optical Devices [5,6]

As GaAs technology is pushing the frequency range to the 100 GHz range, one problem concerning GaAs MMIC measurements arises. The problem is that currently available testing equipment are far behind both the desired bandwidth and the frequency range of GaAs devices and circuits that have been realized by modern processing technology. This problem has motivated research work to explore new electrical testing methods. One approach under investigation is the electro-optic sampling testing method.
In the electro-optic sampling testing method, a time domain step-like waveform is
generated by injecting a laser beam onto a GaAs MMIC substrate. As a result of this
optical excitation, the optical absorption in the GaAs substrate results in the generation of
an electric pulse in the vicinity of a conductor. The generated electrical pulse is a step-like
waveform with a transition time of the order of 1 ps or less, which implies a bandwidth of
greater than 100 GHz.

Traditionally, photoconductors have been used to convert optical signals into
electrical signals. As great advancement of ultrafast optical sources, typically laser
sources, many optoelectronic devices based on the same principles of photoconductors are
being developed. These devices include photoconducting electrical pulse generators,
photoconducting electrical sampling gates, and photoconductive switches. Their
applications are mainly in measurements of extremely high speed integrated circuits.
These devices in structure are combined with broadband transmission lines in their
applications. Physically, an ultrafast electrical pulse generated by an ultrafast optical pulse
propagates as a guided wave in a transmission line.

The frequency spectrum covered by ultrafast electrical pulses can be as high as
many hundreds of gigahertz, in some cases even terahertz. Transmission lines such as
coaxial lines, microstrip lines, slot lines as well as coplanar lines are the transmission
structures for ultrafast electrical pulses. The main concern in this regard is that the
transmission lines used with optical devices result in dispersion and loss of the signal. Although a coaxial line has good bandwidth, low dispersion, and low loss, it is difficult to combine a coaxial structure with a planar structure, which is usually of a photoconductor structure. Microstrip, coplanar, and slot line structures are all compatible with semiconductor microelectronics fabrication technology and have good frequency characteristics for ultrafast pulse transmission. Therefore, optical devices are practically integrated into transmission line structures.

1.4. Considerations of Modeling Optical Devices

As mentioned previously, a photoconductor made from a semiconductor material acts as an optical-to-electrical converter. When an optical pulse is injected onto the photoconductor, carriers are excited within the semiconductor material. The excitation process is very short (of the order of less $10^{-15}$ s), being considered as simultaneously. The photo-excited carriers move with a certain velocity along the direction of the electric field applied to the photoconductor. The carriers can be regarded as individual particles and move according to Newton's law of motion under the influence of the applied electric field. This process is referred to carrier transport and can be studied by the Monte Carlo (MC) method [7,8,9]. Since there is an extremely great number of carriers that need to be simulated one by one, the cost of computation time are extremely high. Thus, the MC method is fairly limited in that sense.
As an alternative method to the MC method, the movement (transport) of the carriers is governed by the transport equations such as Boltzmann equation, continuity equation, and current equation [10]. It is well known that the velocity of the carriers in a typical semiconductor material such as GaAs is electric field dependent. A velocity overshoot phenomenon exists when the electric field varies rapidly due to carrier relaxation process, implying nonlinear phenomena. Although solving Boltzmann and the associated equations is relatively less costly as compared to the MC method, it is still a very costly process.

When a photoconductor is integrated into a transmission line structure and the structure is excited by an ultrafast optical pulse [11], two kinds of phenomena occur. Photo-excited carriers are generated within the semiconductor underneath the transmission line on one hand, and electromagnetic wave propagates along the transmission line on the other hand. A proper model should be able to describe these two phenomena, particularly the interaction between the photo-excited carriers and the electromagnetic wave propagation.

It is well known that wave propagation is governed by Maxwell's equations. To describe propagation of an ultrafast pulse on a transmission line, the best way would be to directly and analytically solve the time dependent Maxwell's equations. Unfortunately, it is
prohibitive so far to do that in most practical problems because the time dependent Maxwell's equations are coupled partial differential equations. The time dependent Maxwell's equations can be solved, however, using numerical approximation techniques, like many other engineering problems. In particular, when modern computers are able to provide high computation speed and large amount of memory, numerical approximate solutions to the time dependent Maxwell's equations have become a practical alternative way.

One popular numerical method to approximate the time dependent Maxwell's equations is the finite difference time domain (FDTD) method [12,13,14]. In that method, derivatives in the Maxwell's equations with respect to both time and space are approximated by finite differences. As a result, the original time dependent Maxwell's equations are converted into a set of finite difference equations, which can be solved relatively easily. Usually, intensive computation time, computation speed, and computer memory are needed to solve the finite difference equations.

1.5. Summary and Dissertation Organization

The above discussion indicates that there is an urgent need to understand the fundamental characteristics of wave propagation in semiconductors. It has also been indicated that difficulties encountered in solving wave equations and semiconductor
transport equations together, and these difficulties are so great that dealing with this topic in an efficient manner becomes a great challenge.

This dissertation is organized into seven Chapters. Chapter 1 serves as an introduction, in which needs of modeling semiconductor subpicosecond switch are discussed. Literature review is to be presented in Chapter 2. Using the FDTD method to solve the time dependent Maxwell's equations as well as the issues of concern are analyzed in Chapter 3. Chapter 4 focuses on the implementation of FDTD with a verification example presented. Chapter 5 is devoted to solving semiconductor transport equations using the relaxation approximation. Chapter 6 constitutes the most important part of this dissertation, where combination of the FDTD technique in solving the Maxwell's equations and the relaxation time approximation of the transport equations, simulation, and analysis of the simulated results are presented in Chapter 6. The simulation results are also verified by comparing to the published experimental data in Chapter 6. Finally, summary and conclusions are provided in Chapter 7.
Chapter 2

Literature Survey

2.1. The FDTD Method

A space-grid time domain technique, later called the finite difference time domain (FDTD), was first proposed to solve numerically the time dependent Maxwell's equations by K.S. Yee in 1966 [12]. In his paper, the Maxwell's vector equations were decomposed into a set of scalar coupled equations in a rectangular coordinate system. The spatial derivatives of the curl operators and time integration were approximated using finite difference method. In the finite difference equations, the scalar E-field and H-field components were arranged in a regular interleaved Cartesian space meshes such that each of them was shifted half of discrete point. In this genius arrangement of the field components in the discrete space, the finite difference equations not only retained a clear picture of the original physics of the Maxwell's equations, but also had a second order accuracy both in space and time, which was the so-called leapfrog scheme in numerical sense. Yee used the technique to investigate TE and TM waves in a two dimensional scattering problem, which has an enclosed conducting boundary. He also discussed numerical stability criteria for the technique. The simulation results gave rise to clear
illustration of propagating waves in time domain. Yee also compared his simulation with the known results and found a good agreement with each other. Yee's paper, in particular the arrangement of field components in the interleaved meshes, built a foundation of the later FDTD technique which is used nowadays by many researchers. The paper has been recognized as a landmark paper and is being referred in almost every paper concerning this technique.

Yee's paper was not brought to researchers' attention until 1975 when Taflove and Brodwin used Yee's algorithm to simulate a 2-D EM scattering problem all the way to the steady state [13]. In their paper, Taflove and Brodwin treated an irradiating cylindrical scatterer as an initial value problem. The scattering by an incident plane wave with a frequency $f$ was simulated by solving finite difference form of the time dependent Maxwell's equations at each discrete point. The time domain method they used gave a result with accuracy of only about 10%, not as good as other frequency domain methods. They attributed the poor accuracy to the coarse meshes used in order to save computation time. Details concerning the use of FDTD in scattering problem were discussed in the paper. In addition, they derived correctly a numerical stability criterion for the Yee's numerical algorithm.

As more and more researchers recognized the use of the FDTD technique based on Yee's algorithm in simulating practical scattering problems in an open space, difficulties
arose concerning limited computer memory and time. It became necessary to limit a practically infinite space of interest to a finite simulation region or simulation domain without losing accuracy. A so-called absorbing boundary condition is required at the boundaries of the finite simulation domain. Although a simple extrapolation method and an average process were proposed in [13,15] as absorbing boundary conditions to simulate outgoing waves, an accurate and numerically stable absorbing boundary condition for Yee's algorithm was derived by Mur [16] in 1981. Mur's method, based on a more general method proposed by Engquist and Majda [17], was specifically developed for the field arrangement in Yee's grid. The absorbing boundary condition was a second order one and can be reduced to first order easily, if necessary. Mur also gave a finite difference form of the absorbing boundary condition and discussed in detail the stability of the method. A case was selected where an exact solution existed for simulation of the absorbing boundary condition. Compared with the exact solution, the absorbing boundary condition gave rise to very accurate results.

In the early time of its application, the FDTD technique was used mainly in scattering problems. Mei et al applied this technique to the simulation of discontinuities in planar microstrip lines [18,19]. Since a microstrip line itself was dispersive, effects of numerical dispersion in the FDTD technique were investigated [20,21]. A microstrip line open-end was simulated as a typical dispersive discontinuity using the FDTD technique. A Gaussian pulse was used as an excitation and enforced at the launching port of the
microstrip. It was assumed that only the dominant mode was left to propagate down the line after the pulse traveled a certain distance. The incident waveform to the open-end and the reflected waveform from the open-end were recorded. Then, these waveforms were transformed into the frequency domain to calculate the reflection coefficient $S_{11}$, which was in turn used to obtain a dispersive lumped model of the open-end. A superabsorbing boundary condition was also developed specially for planar microstrip lines [18].

2.2. Simulation of Optoelectronic Devices

The picosecond optical switches made in transmission lines were analyzed and modeled by lumped circuit elements [11]. The gap of an optical switch was modeled as a capacitance. The photo-excited carriers injected by a laser pulse were represented by a time-varying conductance, in parallel with the gap capacitance embedded in a transmission line. The author of the paper analyzed the effects of the gap capacitance on the speed of the responses of the devices. However, this macroscopic circuit model did not take time-varying electromagnetic fields into consideration, ignoring any electromagnetic wave phenomena associated with the device structure. Thus, such an approximation was only valid when the geometrical dimension of the gap and the transmission line cross section of the device were small compared to the distance an electromagnetic pulse travels in the shortest time interval of interest.
The first paper appeared in 1990 in which picosecond optoelectronic switches were modeled by incorporating a self-consistent Monte Carlo charge transport model of Gallium Arsenide (GaAs) into a 3D FDTD solver [7]. In their paper, El-Ghazaly et al pointed out that a problem like modeling of switching transients in an optoelectronic switch could not be dealt with properly in frequency domain because of involvement of opto-excited carrier transport, which is a nonlinear phenomenon. Ensemble Monte Carlo (EMC) methods were used to simulate the transport of opto-excited carriers within GaAs materials. Since the optoelectronic switch under simulation had a planar microstrip line structure, the FDTD technique was used to directly solve the time dependent Maxwell's equations. Although the EMC method in modeling carrier transport was claimed to be very accurate, it presented a major obstacle that it was too expensive in terms of computer memory and computation time. Because of the constraint in computer resources, much smaller number of carriers were actually simulated (e.g. 9000 out of $3\times10^{16}$/cm$^3$ were simulated in the case being discussed). Also, there were several other unresolved problems such as boundary conditions concerning utilization of EMC with FDTD techniques. The authors concluded their paper by pointing out the complication of the problem and hoped for further investigation using other methods.
2.3. Semiconductor Transport

The negative differential mobility of GaAs was initially observed and reported in 1963 [22]. Since then, a great deal of experimental and theoretical investigation into the transport properties of this material have been done [23 - 25]. Accurate results were obtained by using a Monte Carlo method in [8,26,27]. In this method, the motion of one electron was simulated in momentum space through a large number of scattering processes. The times were recorded that the electron spent in each element of momentum space during its flight and these times were proportional to the distribution function, from which the relationship between drift velocity and applied electric field was found. The drift velocity was found to be a function of the electric field in relatively low field intensity, then reach a maximum value and finally exhibit a saturation value in high field region. The simulation results further confirmed the experimental observation on the field dependent transport properties.

In the early days of modeling semiconductor devices, steady state and static approximations were basic assumptions. These approximations were questionable when device geometries became small and operating frequencies became high. The nonstationary electron dynamics of field effect transistors (FET) was investigated in 1972 [28]. A thorough investigation of the electron dynamics using Monte Carlo methods was reported in 1982 by Molestue [29]. In his method, detailed transport of a large number
of electrons was simulated and histories of the transport were recorded to calculate
dynamic parameters such as electron populations in various valleys, drift velocity versus
time which was in the order of ps. Many physical processes such as interaction between
carriers and lattice, carrier generation and recombination, avalanche effects, trapping as
well as tunneling were included in the simulation. Therefore, results given in his paper
were believed to be accurate. Particularly interesting to other researchers was the
phenomenon of drift velocity overshoot, meaning that electron drift velocity could not
reach instantaneously at the moment when an electric field was applied to the electron.
There was a transition process during which an electron attained a large value of drift
velocity at relatively short time and then "relaxed" to a steady state value. This
phenomenon correctly described the electron dynamics in a time scale of ps.

Other than the Monte Carlo method, a method called full dynamic transport model
was proposed in 1982 by Rolland et al [30] to study a transferred-electron devices over
100 GHz. The method involved in solving the particle conservation equation, the
momentum conservation equation, the energy conservation equation, and the Poisson's
equation to account for the electron dynamic transport properties. Although the method
was shown to be effective in simulating the electron dynamics, it was very complicated in
its algorithm.
2.4. Summary

As a summary, the literature survey indicates that the FDTD technique has been an
effective technique in solving the time dependent Maxwell's equations in simulating
scattering problems and planar microstrip line problems. The steady state and dynamic
transport properties have been studied theoretically and confirmed experimentally.
Simulation of propagation of photogenerated carriers in optoelectronic device with both
electromagnetic and transport considerations in subpicosecond time scale involves in a
nonlinear problem. The conventional frequency domain methods cannot be applied. The
research work of using Monte Carlo methods as well as the FDTD method was reported
the paper [7]. The method of [7] is too expensive to be used in many practical
engineering problems. Consequently, a method more efficient than that is necessary.
Chapter 3

The FDTD Numerical Method for Solving
the Time Dependent Maxwell's Equations

3.1. Introduction

The FDTD method is a direct way to solve the time dependent Maxwell's equations using finite differences to approximate derivatives both in space and time. In this chapter, the time dependent Maxwell's equations, represented in vector form and scalar form, and the Yee's arrangement of the field components are introduced. Based on the Yee's arrangement, a second order center-to-center finite difference approximation of Maxwell's equations is derived. Critical issues such as stability requirements and numerical dispersion concerning the use of the FDTD method are discussed in this chapter. Necessity of application of absorbing boundary condition is also briefly discussed in order to handle open space problems.
3.2. The Time Dependent Maxwell's Equation

To describe propagation in the time domain, the time dependent Maxwell's equations need to be solved. The 3-Dimensional time dependent Maxwell's curl equations are given by:

\[ \nabla \times \vec{E} = -\partial \vec{B} / \partial t \quad (3-1) \]

\[ \nabla \times \vec{H} = \partial \vec{D} / \partial t + \vec{J} \quad (3-2) \]

where \( \vec{D} \) is the electric flux density (displacement vector) in Coulombs per meter\(^2\), \( \vec{E} \) is the electric field intensity in Volts per meter, \( \vec{B} \) is the magnetic flux density in Webers per meter\(^2\), \( \vec{H} \) is the magnetic intensity in Amperes per meter, and \( \vec{J} \) is the current density in Amperes per meter\(^2\). The following equations relate \( \vec{D} \) to \( \vec{E} \) and \( \vec{B} \) to \( \vec{H} \), respectively:

\[ \vec{D} = \varepsilon \, \vec{E} \quad (3-3) \]

and

\[ \vec{B} = \mu \, \vec{H} \quad (3-4) \]

where \( \varepsilon \) and \( \mu \) are the electric permittivity and the magnetic permeability of the medium, respectively.
The vector form of the curl equations (3-1) and (3-2) can be decomposed into a system of six coupled scalar equations:

\[-\partial B_x/\partial t = \partial E_x/\partial y - \partial E_y/\partial z \quad (3-5a)\]

\[-\partial B_y/\partial t = \partial E_y/\partial z - \partial E_z/\partial x \quad (3-5b)\]

\[-\partial B_z/\partial t = \partial E_z/\partial y - \partial E_y/\partial x \quad (3-5c)\]

\[\partial D_x/\partial t = \partial H_z/\partial y - \partial H_y/\partial z - J_x \quad (3-5d)\]

\[\partial D_y/\partial t = \partial H_x/\partial z - \partial H_z/\partial x - J_y \quad (3-5e)\]

\[\partial D_z/\partial t = \partial H_y/\partial x - \partial H_x/\partial y - J_z \quad (3-5f)\]

These coupled scalar equations are the basis of the Finite Difference Time Domain (FDTD) method for electromagnetic wave propagation in 3-D space.

3.3. Yee's Arrangement [12]

The use of the FDTD method to solve a system of scalar equations is based on the Yee's algorithm. Yee's algorithm possesses several features such as:
a) Solving for both electric field and magnetic field in time and space simultaneously rather than for only one at a time.

b) Arranging the E-field and H-field components in space in such a way that every E-field component vector is surrounded by four H-field components and every H-field component vector is also surrounded by four E-field components. This arrangement gives rise to a very clear picture of physical meaning of Faraday's Law and Ampere's Law in space.

c) Approximating the derivatives both in space and time in the scalar equations with a central differences, which has second order accuracy as well as the so-called leapfrog arrangement in time evolution.

The region or the simulation domain in space is first discretized into a number of basic building blocks: cubic cells. The whole region is filled with these building blocks. For each cubic cell, Yee's arrangement of the field components are illustrated in Figure 3.1.
3.4. Finite Difference Approximation

Based on Yee's arrangement, Maxwell's equations, equations (3-5a) through (3-5f), for a homogeneous region are discretized into finite difference equations using the central-to-central scheme both in space and time:

\[
E_x^{n+1}(i,j,k) = E_x^n(i,j,k) + \frac{\Delta t}{\varepsilon} \left[ \frac{H_{z}^{n+1/2}(i,j,k+1) - H_{z}^{n+1/2}(i,j,k)}{\Delta y} \right] - \frac{H_{y}^{n+1/2}(i,j,k + 1) - H_{y}^{n+1/2}(i,j,k)}{\Delta x} - J_x^n(i,j,k) \tag{3-6a}
\]

\[
E_y^{n+1}(i,j,k) = E_y^n(i,j,k) + \frac{\Delta t}{\varepsilon} \left[ \frac{H_{x}^{n+1/2}(i,j,k+1) - H_{x}^{n+1/2}(i,j,k)}{\Delta z} \right] - \frac{H_{z}^{n+1/2}(i+1,j,k) - H_{z}^{n+1/2}(i,j,k)}{\Delta x} - J_y^n(i,j,k) \tag{3-6b}
\]

\[
E_z^{n+1}(i,j,k) = E_z^n(i,j,k) + \frac{\Delta t}{\varepsilon} \left[ \frac{H_{y}^{n+1/2}(i+1,j,k) - H_{y}^{n+1/2}(i,j,k)}{\Delta x} \right] - \frac{H_{x}^{n+1/2}(i,j+1,k) - H_{x}^{n+1/2}(i,j,k)}{\Delta y} - J_z^n(i,j,k) \tag{3-6c}
\]
\[ H_x^{n+1/2}(i,j,k) = H_x^{n-1/2}(i,j,k) - \frac{\Delta t}{\mu} \left[ \frac{E_x^n(i,j,k) - E_x^n(i,j,k-1)}{\Delta z} \right. \]

\[ - \frac{E_y^n(i,j,k) - E_y^n(i,j,k-1)}{\Delta y} \left. \frac{E_z^n(i,j,k) - E_z^n(i-1,j,k)}{\Delta x} \right] \quad (3-6d) \]

\[ H_y^{n+1/2}(i,j,k) = H_y^{n-1/2}(i,j,k) - \frac{\Delta t}{\mu} \left[ \frac{E_y^n(i,j,k) - E_y^n(i,j,k-1)}{\Delta z} \right. \]

\[ - \frac{E_x^n(i,j,k) - E_x^n(i-1,j,k)}{\Delta x} \left. \frac{E_z^n(i,j,k) - E_z^n(i,j-1,k)}{\Delta y} \right] \quad (3-6e) \]

\[ H_z^{n+1/2}(i,j,k) = H_z^{n-1/2}(i,j,k) - \frac{\Delta t}{\mu} \left[ \frac{E_z^n(i,j,k) - E_z^n(i-1,j,k)}{\Delta x} \right. \]

\[ - \frac{E_x^n(i,j,k) - E_x^n(i,j-1,k)}{\Delta y} \left. \frac{E_y^n(i,j,k) - E_y^n(i-1,j,k)}{\Delta z} \right] \quad (3-6f) \]

where \( \Delta x \), \( \Delta y \), and \( \Delta z \) are the space discretization units in x, y, and z direction, respectively, and \( \Delta t \) is the time interval. The subscript indices i, j, and k correspond to the coordinates of the discretized space and \( n \) denotes the order of time instant. It is seen that the electric field components are computed at the time \( n\Delta t \), while the magnetic field components are computed at the time \( (n+1/2)\Delta t \), indicating a leapfrog operation.
3.5. Stability Requirement [31,32]

To understand concerns involved in the FDTD scheme, consider the general one

dimensional (1-D) scalar wave equation:

$$\frac{\partial^2 f}{\partial t^2} = c^2 \frac{\partial^2 f}{\partial x^2}$$  \hspace{1cm} (3-7)

where \( f(x,t) \) represents a physical field quantity and \( c \) is the propagation velocity. One can verify that a general solution to the above equation is given by the following equation,

$$f(x,t) = F(x+ct) + G(x-ct)$$  \hspace{1cm} (3-8)

where \( F \) and \( G \) are arbitrary functions.

The space and time are discretized into a finite number of increments, \( \Delta x \) and \( \Delta t \), respectively. \( f^n_i \) denotes a wave or field quantity at \( x_i = i\Delta x \) and at time \( t_n = n\Delta t \). The central-central finite difference scheme is to expand \( f(x,t) \) around \( x_i \) while \( t_n \) is fixed:

$$\left( \frac{\partial^2 f}{\partial x^2} \right)_{x_i,t_n} = \frac{f_{i+1}^n - 2f_i^n + f_{i-1}^n}{(\Delta x)^2} + O((\Delta x)^2)$$  \hspace{1cm} (3-9)

Similarly, \( f(x,t) \) is expanded around \( t_n \) while \( x_i \) is fixed:
\[
\left( \frac{\partial^2 f}{\partial t^2} \right)_{x_i,t_n} = \frac{f_{i+1}^{n+1} - 2f_i^n + f_{i-1}^n}{(\Delta t)^2} + O[(\Delta t)^2]
\]  

(3-10)

where \( O[] \) indicates the higher order terms of the approximation. Substituting equations (3-9) and (3-10) into equation (3-7) and neglecting the higher order terms lead to a finite difference equation for the wave equation:

\[
f_{i+1}^{n+1} = \left( \frac{c \Delta t}{\Delta x} \right) [f_{i+1}^n - 2f_i^n + f_{i-1}^n] + f_i^n - f_i^{n-1}
\]

(3-11)

For a given \( \Delta x \), the selection of \( \Delta t \) is mainly determined by the stability requirement or the Courant, Fredrich, and Levy (CFL) condition. In numerical computation concerning an initial value problem, errors such as truncations are unavoidable. If these errors grow as time evolves, the numerical computation would overflow. To study the stability of the finite difference scheme, one can follow the classical method known as Von Neumann's method. Assume that the solution at the discrete point \( x_i = i \Delta x \) and at the time \( t_n = n \Delta t \) is given by

\[
f_i^n = e^{an} e^{bi \Delta x}
\]

(3-12)
where $\alpha$ is a growing factor and $\beta$ is a phase factor. Substituting (3-12) into the finite difference equation (3-11) gives rise to

$$e^{\alpha \Delta t} = 1 - 2\alpha^2 \sin^2 \left( \frac{\beta \Delta x}{2} \right) \pm 2\alpha \sin \left( \frac{\beta \Delta x}{2} \right) \left[ \alpha^2 \sin^2 \left( \frac{\beta \Delta x}{2} \right) - 1 \right]^{1/2} \quad (3-13)$$

where $\alpha = (c\Delta t/\Delta x)$. As the von Neumann stability condition requires that $|e^{\alpha \Delta t}| \leq 1$, one can have

$$\alpha^2 \sin^2 \left( \frac{\beta \Delta x}{2} \right) \leq 1 \quad (3-14)$$

The above equation can then lead to the CFL stability condition:

$$\Delta t \leq \frac{\Delta x}{c} \quad (3-15)$$

This condition implies that $\Delta t$ is selected such that any errors due to the numerical process are constrained locally and do not grow or propagate to the next time step. A similar procedure can be followed to obtain the stability conditions for the 2-D and 3-D cases, respectively, as given by [33]

$$\Delta t \leq \frac{1}{c} \frac{1}{\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}} \quad (3-16)$$

and
\[ \Delta t \leq \frac{1}{c \sqrt{3}} \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}} \]  \hspace{1cm} (3-17)

3.6. Numerical Dispersion [31 - 34]

Dispersion is defined as the variation of wavelength \( \lambda \) (or wavenumber \( k = 2\pi/\lambda \)) with frequency \( f = \omega/2\pi \). For a continuous sinusoidal travelling plane wave \( f(x,t) = e^{i(\omega t - kx)} \), a dispersion relation can be obtained for the 1-D wave equation as

\[ k = \pm \frac{\omega}{c} \]  \hspace{1cm} (3-18)

The phase velocity is given by

\[ v_p \equiv \frac{\omega}{k} = \pm c \]  \hspace{1cm} (3-19)

When the propagation velocity is a frequency independent constant, the propagation is dispersionless, implying every frequency component has the same propagation velocity.

For the same wave equation, numerical dispersion is introduced if the solution is achieved by using the finite difference approximation. For a sinusoidal wave, the finite difference gives rise to

\[ f'_n = e^{i\omega n \Delta t - ki \Delta x} \]  \hspace{1cm} (3-20)
where \( k' \) is the numerical wavenumber presented in the finite difference grid. The difference between \( k' \) and \( k \) is due to the numerical errors which lead to the numerical dispersion.

Substituting (3-20) into equation (3-11), one can obtain the following equation

\[
\cos(\omega \Delta t) = \left( \frac{c \Delta t}{\Delta x} \right)^2 [\cos(k' \Delta x) - 1] + 1
\]

(3-21)

Based on this equation, three cases can be analyzed:

Case (1). Conditions \( \Delta t \to 0 \) and \( \Delta x \to 0 \)

Since

\[
\cos(\omega \Delta t) \approx 1 - \frac{1}{2}(\omega \Delta t)^2
\]

(3-22)

and

\[
\cos(k' \Delta x) \approx 1 - \frac{1}{2}(\omega \Delta x)^2
\]

(3-23)

then, one can have

\[
k' = \pm \frac{\omega}{c}
\]

(3-24)

In this case, \( k' \) is the same as that in the continuous case. This is logically correct because when \( \Delta t \to 0 \) and \( \Delta x \to 0 \), the finite differrence solution approaches the continuous solution.
Case (2). Condition \((c\Delta t/\Delta x) = 1\)

Under this condition, equation (3-21) becomes

\[
\cos(\omega \Delta t) = \cos(k'/\Delta x) \tag{3-25}
\]

then, the wavenumber is given by

\[
k' = \pm \frac{\omega \Delta t}{\Delta x} = \pm \frac{\omega}{c} \tag{3-26}
\]

\(k'\) in this case is the same as the exact solution. This is a very significant outcome that if \((c\Delta t/\Delta x)\) is selected to unity, the finite difference solution gives rise to an exact solution.

Case (3). \(\Delta t\) and \(\Delta x\) are finite and \((c\Delta t/\Delta x) \neq 1\)

This is a general case where the dispersion exists. The dispersion relation is derived from (3-21) and given by

\[
k' = \frac{1}{\Delta x} \cos^{-1}\left\{ 1 + \left(\frac{\Delta x}{c\Delta t}\right)[\cos(\omega \Delta t) - 1] \right\} \tag{3-27}
\]

Case (2) indicates that there is no dispersion if \((c\Delta t/\Delta x) = 1\). However, this condition is also the upper limit of the stability requirement, which cannot be used
practically. Therefore, \((c\Delta t/\Delta x)\) which is slightly less than but very close to unity should be used so that the numerical operation is stable while the dispersion minimized.

3.7. Absorbing Boundary Conditions [16,17,34]

For a practical problem, the space where electromagnetic fields are computed is usually an infinite domain. It is obvious that no computer can have enough memory and speed to handle the infinite space. The problem has to be solved in a limited space called a simulation domain. In other words, artificial boundaries need to be enforced. The artificial boundary conditions are called absorbing boundary conditions, which mean that they absorb any reflection of the outgoing propagating wave to an acceptable level and at the same time are compatible with the FDTD algorithm.

The compatibility of a useful absorbing boundary condition for the FDTD that uses Yee's arrangement is concerned about the fact that the central-to-central finite difference is utilized. At the boundary, computation of the field components requires the information outside the boundary. Therefore, the absorbing boundary conditions must provide the lacking information for the field components at the boundary while suppressing the reflection from that boundary.

For simplicity, one can consider a 2D wave equation given by
\[ \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} - \frac{1}{c^2} \frac{\partial^2 f}{\partial t^2} = 0 \]  

(3-28)

where \( f = f(x,y,t) \) represents a propagating scalar field component. If one uses the following symbols:

\[ D_x^2 \equiv \frac{\partial^2}{\partial x^2} \quad D_y^2 \equiv \frac{\partial^2}{\partial y^2} \quad D_t^2 \equiv \frac{\partial^2}{\partial t^2} \]  

(3-29)

then,

\[ L \equiv D_x^2 + D_y^2 - \frac{1}{c^2} D_t^2 \]

\[ = \left[ D_x + \frac{D_t}{c} \sqrt{1 - \left( \frac{D_y}{D_t/c} \right)^2} \right] \left[ D_x - \frac{D_t}{c} \sqrt{1 - \left( \frac{D_y}{D_t/c} \right)^2} \right] \]  

(3-30)

It has been proven [34] that the operator in the first parenthesis absorbs the wave travelling toward the right boundary while the second one absorbs the wave travelling toward the left boundary. In equation (3-30), if one approximates the term inside the square root, that is

\[ \sqrt{1 - \left( \frac{D_y}{D_t/c} \right)^2} \approx 1 - \frac{1}{2} \left( \frac{D_y}{D_t/c} \right)^2 \]  

(3-31)
then, approximate analytical absorbing boundary conditions for the propagation in $+x$
direction and $-x$ direction are given, respectively, by

$$D_x D_y f + \frac{1}{c} D_t^2 f - \frac{c}{2} D_y^2 f = 0$$
(3-32)

and

$$D_x D_y f - \frac{1}{c} D_t^2 f + \frac{c}{2} D_y^2 f = 0$$
(3-33)

Similarly, one can obtain approximate absorbing boundary conditions for the propagation
in $+y$ direction and $-y$ direction as given, respectively, by

$$D_y D_x f + \frac{1}{c} D_t^2 f - \frac{c}{2} D_x^2 f = 0$$
(3-34)

and

$$D_y D_x f - \frac{1}{c} D_t^2 f + \frac{c}{2} D_x^2 f = 0$$
(3-35)

The derivatives in equations (3-32) through (3-35) can then be approximated by
center-to-center finite difference to make it compatible with the FDTD approximation of
the Maxwell's equations.
3.7. Summary

The time dependent Maxwell's equations can be solved using the FDTD numerical method. Yee's arrangement of the field components in the discretized space provides a second-order approximation in both time and space. The FDTD scheme should satisfy the stability requirement. The numerical dispersion can be minimized by selecting \((c\Delta t/\Delta x)\) close to unity. In order to apply the FDTD method in open space problems, absorbing boundary conditions are usually needed. In the next chapter, Chapter 4, a simulation of a Gaussian pulse propagating on a microstrip line is provided for a demonstration of the FDTD technique.
Figure 3.1  The Yee's arrangement of electric field and magnetic field components for the FDTD simulation.
Chapter 4

Simulation of a Wideband Pulse Propagation on a Microstrip Line Using the FDTD Method

4.1. Introduction

The FDTD method for solving the time dependent Maxwell's equations can be used to simulate wave propagation on a microstrip line, including those lines that have discontinuities. The method provides a clear picture of propagation of a time domain pulse and the distortion of the pulse. The frequency domain parameters can also be derived from the recorded time domain waveforms based on the Fourier correlation between time domain and frequency domain signals.

In this chapter, the FDTD method is used to simulate a microstrip line open end. The simulation serves as an example to demonstrate the use of the method in the simulation of planar structures involving microwave devices. The simulation also verifies the FDTD program developed in this dissertation research.
4.2. A Microstrip Line for Simulation

A microstrip line is a typical transmission line used in high speed optical devices as well as planar microwave circuits due to its compatibility to planar fabrication technology. However, microstrip lines suffer phase distortion \([35,36]\). Microstrip lines are dispersive because signals propagate in more than one medium. In other words, the propagation velocity is frequency dependent. Therefore, understanding propagation of time domain signals on a microstrip line is an important step in high speed and high frequency circuit design.

As illustrated in Figure (4.1), the simulated problem is that of an open ended microstrip line on a dielectric substrate. All conductors used in the structure were assumed to be perfect while the dielectric material was assumed lossless with a relative dielectric constant \( \varepsilon_r = 3.1 \). The structure geometrical parameters are chosen as,

- thickness of the substrate = 2.0 mm
- width of metal strip = 1.0 mm
- thickness of metal strip = 0.0
length of metal strip = 8.0 mm

4.3. Selection of Parameters for FDTD Simulation

A major consideration in FDTD simulation is to define the simulation domain, which encloses the original problem by proper boundary condition. For the simulation problem being considered, the boundaries of the simulation domain include the front and back planes along the $z$-direction, the side plane in the $x$-direction, and the top plane in the $y$-direction (note that the bottom is the ground plane). Since the microstrip line possesses a guiding nature, most of the energy is propagated along the $z$-direction. Therefore, an absorbing boundary condition is appropriate to use at the positions of $z=0$ and $z = Nz \Delta h$.

Unlike in the $z$-direction, the propagation direction is not in the normal direction with the boundaries of the side and the top. The wave propagation is in the form of evanescent wave. The absorbing boundary condition is not suitable at these boundaries. Actually, real situation in these boundaries is rather complicated and there is no simple available solution. A solution to this is to assume that perfect conductors are placed at these boundaries, where the tangential fields are set to zero. The enforcement of these boundary conditions changes the original problem into a problem of a shielded microstrip line. Efficient simulation takes advantage of the symmetrical structure of the microstrip
line along the center of the signal strip and only half of the simulation domain is necessary. A magnetic wall is applied at the symmetrical plane.

In order to ensure good spatial resolution, the incremental spacings in x, y, and z were chosen to equal, Δx = Δy = Δz = Δh = 0.1 mm. The corresponding number of the intervals in the x, y, and z directions were chosen as Nx = 30, Ny = 40, and Nz = 100, respectively. The time stepping interval Δt, determined by the stability criterion equation (3-14), was selected as 4.0x10^-14 s. The selection of Nx, Ny, and Nz is based on considerations of limited computer resources (memory and computation time) as well as possibly close approximation between the shielded microstrip line and the original problem. The computer memory used in the simulation, for example, may be estimated. For one field component, about 0.5 Megabytes (30 x 40 x 100 x 4 = 0.48 Megabytes) is needed for single precision computation. At least 4 Megabytes memory is needed for total six field components plus other variables.

One additional issue needed to be considered is the interface between the air and the dielectric substrate, where the tangential field components are E_x and E_z. Due to the requirement of the continuity of the tangential fields at the interface, it can be proved [18] that the average value of the two dielectric constants, air and substrate, should be used to calculate these field components at the interface. Since it is assumed that the permeability
is the same throughout the simulation domain, there is no need to have special treatment for the calculation of the magnetic field components at the interface.

4.4. FDTD Simulation

In the finite difference numerical simulation, the smoothness of the excitation signal is desirable to reduce numerical errors. This is because the finite difference approximation assumes the existence of the higher order (higher than second order, for example, in the leapfrog scheme) derivatives of the original function in the partial differential equation. A Gaussian pulse, as shown in Figure 4.2a, is known to have the required smoothness. It is a suitable candidate for the excitation source. However, the major drawback of the Gaussian pulse is that it starts from negative infinity and ends at positive infinity, implying its non-physical and non-causal nature. Although fully understanding of the validity of the simulation resulted from the gaussian pulse remains to be investigated, so far it has been the only wideband excitation pulse used in the FDTD simulations.

To reduce the effects of the non-physical nature on the simulation, the original pulse (the maximum is located at \( t = 0 \)) needs to be modified. The maximum point is shifted to a certain positive value \( t_0 \) which is large compared to the width of the pulse. In
other words, the pulse is truncated at \( t = -t_0 \) first and then assumed to start at that point, as shown in Figure 4.2b and given by

\[
E_y(x, y, z = 0, t) = \exp \left[ -\left( \frac{t - t_0}{T} \right)^2 \right]
\]  

(4-1)

where \( t_0 \) is the time at which the Gaussian pulse reaches its maximum and \( T \) is a parameter that determines the width of the pulse. The excitation is given to the field components \( E_y \) underneath of the metal strip at the front plane while all other field components are set to zero. The field component \( E_y(x, y, z=0, t) \) is distributed uniformly at the excitation plane and translated into the simulation domain, as shown in Figure 4.2c. To ensure a wideband spectrum and avoid significant truncation error, \( t_0 = 200 \Delta t \) and \( T = 30 \Delta t \) are used in the simulation. The selection of the values for \( t_0 \) and \( T \) leads to the truncated value \( E_y(x, y, z=0, t =0) = 5.0 \times 10^{-20} \), which is small enough to be negligible.

4.5. Simulation Results and Discussion

The simulation program flow-chart is given in Figure 4.3. The simulated time domain waveforms of the field component \( E_y \) just below the metal strip are shown in Figure 4.4 - 4.6. These graphs present the 3D plots. The pulse just reaching the open-end is shown in Figure 4.4. When the pulse reaches the open end, a reflection response occurs. The reflection is added to the incident wave, resulting in a higher magnitude
waveform, as illustrated in Figure 4.5. After the pulse goes through the open end, it travels back to the excitation end, as shown in Figure 4.6.

It can be observed that after the pulse leaves the excitation front, there are oscillations tailing the pulse. The longer the pulse travels, the larger the oscillations. This is the dispersion or phase distortion to the original pulse. As pointed out in the previous Chapter, the microstrip line is dispersive in nature due to the wave propagation in multilayer dielectric media, which lead to frequency dependent velocity. The simulation results agree with the results reported in [18], in which a similar structure was used for simulation. The distortion nature to the microstrip lines also agrees with the observation resulted from more thorough study of the dispersion of the microstrip lines [37].

As the pulse travels along the strip, most of the energy is guided by the strip. However, a small amount of surface wave can be seen, indicating the full wave analysis ability of the FDTD method. It can also be observed that at the edge of the metal strip, the field intensity is higher. This is due to the fringing phenomenon that the electric fields tend to concentrate at the place having rapid geometrical change such as the edges of the conductor strips.

The frequency domain parameters such as the S-parameters and the frequency-dependent effective dielectric constant can be derived from the time domain
waveforms. This was done by recording the time domain waveforms at every time step at specified locations and then carrying out the Fourier transformations of the waveforms [18,19]. It should be pointed out that good absorbing boundary conditions are needed in order to obtain accurate frequency domain data, since the Fourier transform is very sensitive to errors or noise of the recorded waveforms. In addition, selection of the time intervals and the number of time steps is made to result in suitable resolution in the frequency domain data.

4.6. Summary

A microstrip line open-end is simulated using the FDTD method. The resulted time domain waveforms illustrate wave propagation on the microstrip line and the open-end. The results also show phenomena associated with a microstrip line such as the phase distortion, leading to oscillations tailing the travelling pulse, the fringing fields and the surface wave. The simulation results agree well with the previously reported results. The simulation of the microstrip line indicates the utility of the FDTD method as well as the validity of the simulation program.
Figure 4.1. An open-ended microstrip line for the FDTD simulation. The simulation domain is indicated by the dot lines.
Figure 4.2. (a) An original gaussian pulse with the maximum at $t=0$; (b) A shifted gaussian pulse with the maximum at $t=200$; (c) Illustration of the incident pulse at the launching port.
Figure 4.3. The flow-chart of the FDTD simulation.
Figure 4.4. The propagating pulse (E_y underneath the conductor strip) approaching the open end.
Figure 4.5. The propagating pulse (Ey underneath the conductor strip) with the peak signal at the open end. The shown pulse is superposition of the incident and the reflected pulses.
Figure 4.6. The propagating pulse (Ey underneath the conductor strip) reflecting back from the open end.
Chapter 5

Relaxation Time Approximation of
Semiconductor Balance Equations

5.1. Introduction

When a semiconductor material like GaAs is used in devices such as an optical switch or other microwave applications, the material serves as a propagation medium, optical-to-electrical conversion as well as conduction medium.

In this Chapter, fundamentals of semiconductor are first introduced, including the current density equation, the continuity equation, and the Boltzmann equation. Physical backgrounds of the transport properties, time dependent and equilibrated, are provided in order to understand the nonlinearity of the drift velocity. Two methods, solving the coupled Boltzmann equations and the Monte Carlo method, are briefly described. Then, concepts of the energy relaxation time and the momentum relaxation time are introduced as the basis on which the nonlinearity of the electron transport is analyzed and obtained.
5.2. Fundamentals of semiconductors [38,39]

In a semiconductor, charged carriers include both electrons and holes. However, in a doped semiconductor (p-type doping or n-type doping), the majority of the carriers are either electrons for the n-type doping or holes for the p-type doping. Concerning the conduction properties of a bulk semiconductor, only the majority carriers are necessarily considered because the condition always holds that the number of majority carriers are much larger than the number of minority carriers. Throughout the following analysis, an n-type doped semiconductor is assumed.

When an external electric field is applied to a piece of semiconductor, conduction current within the semiconductor consists of two types of currents; the drift current and the diffusion current. The drift current is due to the applied electric field exerted upon the electrons while the diffusion current is attributed to a non-uniform distribution of the electrons. The current density without considering the diffusion current is given by

\[ J = qvn \]  

(5-1)

where \( q \) is the electric charge, \( v \) is the average velocity of the electrons, and \( n \) is the concentration of the electrons. Note that both the velocity and the concentration of the
electrons are functions of the electric field and time so that the current density is also a function of these two factors.

Under the influence of the applied electric field, an electron absorbs energy from the electric field and drifts in the direction of the electric field. Since a semiconductor is a crystallized solid, the electron experiences scattering or interaction with the atoms and other electrons when it drifts a certain distance. When a scattering event occurs, the electron loses (or dissipates) its energy to the scattering process and changes its moving direction. The electron drifts again right after the scattering until its next scattering. One can imagine that the motion of the electron is a zigzag process. Therefore, the velocity of the electrons is a statistically average process and is determined by several factors including the electric field (the force applied to electrons), the concentration of the electrons, and the scattering mechanisms within the semiconductor (the environment of the electrons' motion).

5.3. Transport Properties

Transport properties are described by the Boltzmann Transport Equation (BTE) given by [39]
\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{qE}{h} \frac{\partial f}{\partial k} = \int_{k'} d k' \left[ f(k')W(k', k) - f(k)W(k, k') \right]
\] (5.2)

where \( f(r,k,t) \) is the distribution in momentum \( k \)-space and geometrical \( r \)-space, \( \mathbf{v} \) is the drift velocity, \( W \) is the scattering probability function, \( E \) is the electric field, \( q \) is the electric charge, and \( h \) is the Planck's constant. The drift velocity is related to the energy band structure \( \xi(k) \) of the semiconductor material by the equation

\[
\mathbf{v} = \frac{1}{h} \frac{\partial \xi}{\partial k}
\] (5.3)

As seen from the above equations, the necessary parameters to solve the Boltzmann equation are the scattering probability function and the electric field. The average quantities such as \( \langle \xi \rangle \) and \( \langle \mathbf{v} \rangle \) can be deduced from the distribution function \( f \).

Based on the BTE, one can study the influence of the size of a device and the operating condition of the device on the transport properties. If variation of the electric field during the mean free time between two collisions is negligible, the partial derivative with respect to the space in the BTE vanishes. For a steady state, time variation in the distribution is so weak that the derivative of the distribution with respect to time can be negligible. However, in small size devices and very high frequency operating conditions, these two cases are no longer valid [40,41]. Therefore, transient transport properties have to be considered.
Consider that a step function of electric field is applied to a multivalley semiconductor material. Carriers in the central valley, where the carriers possess higher mobility, absorb energy from the electric field and are accelerated. After a short time (in the order of 0.5 ps or less), the carriers are transferred to the lower-mobility upper valleys of the band structure. These physical processes cause the so-called velocity overshoot, implying that the velocity increases to a maximum value in a very short time and then decays to a steady state value or saturated velocity.

Usually, transport properties are referred to as the velocity relation with the electric field (v-E relation) and the transient (time dependent) phenomena. Methods to obtain the v-E relation include an iteration method of solving the BTE [10] and the Monte Carlo simulation [8,9,26,29]. The iteration method is basically to solve the BTE numerically using finite differences. The Monte Carlo method simulates the carriers' motion under the influence of the electric field and various scattering events. The Monte Carlo method provides accurate description of the transport phenomena and therefore gives rise to accurate results of the v-E relation. However, it is very costly in computation.

5.4. Monte Carlo Method

The Monte Carlo method used in obtaining characteristics of the dynamic transport in semiconductors is to simulate the motion of one or more charged carriers
under the influence of the applied electric field, the magnetic field, and the given scattering mechanisms. There are two processes involved in the simulation of the motion. One is the free flight process while another is the occurrence of the scattering events. The free flight is the time duration of two successive collisions. During the time period of the free flight, the carriers' motion simply follows the Newton's Law for a particle subjected to an external force. The microscopic processes of the scattering events are described by the given scattering probabilities. Both the free flight time and the scattering events are randomly selected. As a result, generation of sequences of random numbers with the given distribution probabilities is essential to the Monte Carlo method. The generation of the random numbers can be accomplished by a computer.

To achieve the transport characteristics of the steady-state and homogeneous phenomena, it is sufficient to simulate one carrier over a long time. This is because of the assumption that one single carrier traveling over a long path contains information on the behavior of all other carriers as a whole. However, a large number of carriers have to be simulated one by one in order to achieve nonstationary dynamic behaviors. Histories of every one of the simulated carriers are recorded. The desired information can be extracted from the recorded histories. Compared to the simulation of the steady-state situation, the simulation of nonstationary situation is much more computationally costly.
5.5. Balance Equations

GaAs is a III-V compound semiconductor material, which has upper energy valleys and low energy valleys [38]. The drifting velocity of carriers in the upper energy valley is different from that in lower energy valleys due to the dependence of the drifting velocity of electron average energy. In the lower energy valleys, electrons have higher velocity which is proportional to the electric field. When the electric field is increased to a level, called threshold value, the electrons have enough energy to be transferred to upper energy valleys, where the electrons have relatively low drifting velocity. This physical background explains a basic characteristic relation between the drifting velocity and the applied electric field.

To describe the dynamic characteristics of the transport, that is time dependent velocity under the influence of an electric field, the momentum and energy balance equations as an alternative method to the Monte Carlo method can be used and are given for one dimensional case by [42,43]

\[
\frac{d(m^*v)}{dt} = qE \frac{m^*v}{\tau_m(\xi)}
\]  
(5-4)

\[
\frac{d\xi}{dt} = qEv - \frac{\xi - \xi_0}{\tau_{\xi}(\xi)}
\]  
(5-5)
where \( v = v(t) \) is the time dependent drifting velocity, \( E \) is the electric field, \( m^* = m^*(\xi) \) is the effective mass of the electron, \( q \) is the electric charge, \( \xi = \xi(t) \) is the time dependent mean energy of the electrons, \( \xi_0 \) is the thermal-equilibrium energy, \( \tau_m(\xi) \) and \( \tau_\xi(\xi) \) are the momentum relaxation time and the energy relaxation time, respectively. Both relaxation times are energy-dependent.

These two equations have classical meanings. For the first equation, the first term on the right hand side is an applied force upon a particle while the second term implies a frictional effect. For the second equation, the first term represents the power that electrons acquire from the applied force while the second term illustrates the loss of energy. In GaAs material, the frictional effect against the electron drifting velocity is due to the randomization of the moving direction of electrons after collisions. The energy loss is attributed to energy exchange between electrons and phonons during collisions.

5.6. Relaxation Time Approximation of the Balance Equations

In steady-state conditions, which are equivalent to \( d(m^*v)/dt = 0 \) and \( d\xi/dt = 0 \), the drift velocity \( v_s \) in equation (5-4) is given by [42,43]

\[
\nu_s = \frac{q\tau_m(\xi)}{m^* (\xi)} E_s(\xi)
\]  

(5-6)
where $E_s$ is the steady-state electric field. Notice that both momentum and energy relaxation time constants are functions of energy. Since the energy of the carriers is an instantaneous function of the electric field, the relaxation time constants can be given by

$$
\tau_m(\xi) = \frac{m * (\xi) v_s(\xi)}{qE_s(\xi)} \tag{5-7}
$$

$$
\tau_e(\xi) = \frac{\xi - \xi_0}{qE_s(\xi)v_s(\xi)} \tag{5-8}
$$

where $v_s(\xi)$ and $E_s(\xi)$ are the steady-state values of the drift velocity and the electric field, respectively, corresponding to the energy under consideration. Substitution of equation (5-7) and (5-8) into equation (5-4) and (5-5), respectively, leads to the following equations

$$
\frac{d(m * v)}{dt} = q[E - \frac{v}{v_s(\xi)}E_s(\xi)] \tag{5-9}
$$

$$
\frac{d\xi}{dt} = q[Ev - E_s(\xi)v_s(\xi)] \tag{5-10}
$$

Equation (5-9) and (5-10) can describe the electron dynamics knowing the steady-state values of $v_s(\xi)$ and $E_s(\xi)$. They can be solved either analytically or numerically, depending on the given relations of $v_s(\xi)$ and $E_s(\xi)$ versus $\xi$. These relations are usually obtained using the Monte Carlo simulation.
Direct outputs from a Monte Carlo simulation are $v_s(E_s)$ and $\xi_s(E_s)$, from which the relations $v_s(\xi)$ and $E_s(\xi)$ can be easily obtained. Typical curves of $v_s(E_s)$ and $\xi(E_s)$ are shown in Figure 5.1 and Figure 5.2 [8,9,43]. Nonlinearities of the velocity and the energy are obviously seen. In particular, the steady-state energy increases as the electric field increases. The steady-state velocity also increases at relatively low electric field, but behaves a decreasing function in the high field range, implying a negative differential mobility.

5.7. Finite Difference Algorithm Solving the Balance Equations

Based on the knowledge of $v_s(E_s)$ and $\varepsilon(E_s)$, equations (5-9) and (5-10) can be solved numerically for $v(t)$ and $\varepsilon(t)$ by a finite difference method. A solving procedure is given as follows: at $t = 0$, initial conditions $v(t) = 0$ and $\xi(t) = \xi_0$ are assumed. At any time instant $t$, $\xi_s = \xi(t)$ is used because of the assumption that the energy is an instantaneous function of the electric field. With a known $\xi_s$, $E_s$ and in turn $v_s$ can be obtained. These values are then used to obtain $RHS_v$ and $RHS_\varepsilon$, the right-hand sides of equation (5-9) and (5-10), respectively. Using the finite difference approximation, the updated velocity $v(t)$ and energy $\xi(t)$ are given by

$$m * v(t + \Delta t) = m * v(t) + \Delta t * RHS_v$$

(5-11)
\[ \xi(t + \Delta t) = \xi(t) + \Delta t \cdot RHS_{\xi} \]  \hspace{1cm} (5-12)

This process repeats until the steady-state or the specified time period is reached. The achieved \( v(t) \) with respect to different applied electric fields are shown in Figure 5.3. The terminated time period is 3 ps, at which the steady-state velocity and the equilibrium energy are reached. From the shown figure, it is clearly seen that the velocity overshoot is very significant at the high electric fields while there is no velocity overshoot at the low electric field. Examining both Figure 5.1 and Figure 5.3, one can find that the electric field values which do not cause the velocity overshoot in Figure 5.3 correspond to the electric field values lying in the linear region in Figure 5.1. The velocity overshoot is caused by the negative differential mobility.

The momentum and energy relaxation time method has been compared with the Monte Carlo method [43]. Results obtained by both methods have rather good agreement. The attractive advantage of the relaxation time method over the Monte Carlo method is the time saving. The former method requires much less simulation time than the later (approximately 1 min. to 10 hours). Also, the programming is much simpler for the relaxation time method than the Monte Carlo method.
5.8. Summary

The dynamic transport properties of semiconductor materials can be obtained either by Monte Carlo method or by solving the balanced equations. The Monte Carlo method is very expensive in computation time while numerically solving the balanced equations using finite difference scheme provides an efficient way. The simulation results of the dynamic transport properties illustrate the overshoot in the carrier velocity, which needs to be taken into consideration in order to accurately simulate transport phenomena in small dimension devices. The solution of the balanced equations can be replaced by empirical formulas to further increase the computation efficiency.
Figure 5.1. The drift velocity of GaAs material versus the applied electric fields [8,9,43].
Figure 5.2. The mean energy of GaAs material versus the applied electric fields [8,9,43].
Figure 5.3. The drift velocity of GaAs material versus time at the different applied electric fields, resulted from the simulation of the balance equations using the relaxation time approximation.
Chapter 6

Simulation of a Subpicosecond
Semiconductor Optical Switch

6.1. Introduction

Application of the FDTD method to simulation of the propagation of a wideband
time domain pulse on a microstrip line and derivation of relaxation time method for the
semiconductor transport equation have been described in the previous chapters. In this
chapter, we shall deal with that combination of these two methods to simulate a problem
which involves both transport of charged particles and wave propagation phenomena.

A modern laser can generate a gaussian-like optical pulse with a full duration at
half maximum (FDHM) in the subpicosecond range. A photoconductor is a typical device
used to convert the optical pulse into an electrical pulse. The conversion process includes
absorption, drifting, and diffusion within the semiconductor materials. The electrical pulse
achieved in this way is usually much slower than the exciting optical pulse since the drift
and diffusion are slow processes. However, a fast response can be obtained if the
photoconductor has a transmission-line-like configuration. Simulation of such a
photoconducting device constitutes the main theme of this chapter, so as to demonstrate
the usefulness of the technique introduced by this research.

6.2. Problem Statement

An optical switch is a transmission-line-like photoconductor, as shown in Figure
6.1. It consists of a metal microstrip line deposited on a GaAs substrate. Metalization is
also realized on the back of the substrate to form a ground plane. At the middle of the
microstrip line, there is a small gap. The gap is used as an active region into which a laser
pulse is injected.

In its normal operation, one of the microstrip lines of the switch is grounded while
the other one is connected to a DC voltage $V_b$. The ground plane and the coupled
microstrip line are also grounded. At the beginning, a DC electric field is built up between
the gap due to the biased voltage. It is assumed that the conductivity of the substrate is
very small and can be negligible. When a laser pulse is injected into the active region,
photo-excited carriers are generated. These carriers are immediately being influenced by
the initial electric field and move away from the gap by drift and diffusion. The biasing
voltage is selected so high that the drifting motion under the influence of the electric field
is dominant. The drift velocity is governed by the transport dynamic characteristics, which depend on the electric field.

The photo-generation process lasts a short period of time, during which two other physical phenomena are involved at the same time. The photo-generated carriers drift to the metal contacts of the microstrip line and are absorbed there. Recombination of the photo-generated carriers takes place due to various recombination centers. The time before the carriers are being recombined is called the carrier life time. A typical lifetime of the carriers in the GaAs material is about 100 ps. As a result of recombination, some of the photo-generated carriers do not make contribution to the current flowing into the signal conductor strip.

One can imagine that the current, caused by the drift carriers, flowing between the gap certainly leads to changes in the electric field and in turn the magnetic field. The alternative changes of the electric and magnetic fields become waves due to the guiding nature of the transmission line. In other words, the photo-generated carriers act as an exciting source of electromagnetic waves propagating on the microstrip lines. Although most of the energy of the electromagnetic waves is propagated along the transmission line, waves also propagate to the sides so that loss occurs during the transmission.
6.3. A Lumped Semi-Analytical Model

Before analyzing the propagation of a photo-generated pulse on the optical switch described in the last section, it is helpful to suggest a lumped model representing the switch, as shown in Figure 6.2. The lumped model is based on the assumption that a wave propagates in the microstrip is a pure TEM mode without any radiation loss. In the lumped model, the microstrip transmission line is represented by its characteristic impedance $Z_0$. A capacitance $C_g$ exists at the gap between the metal-semiconductor contact A and the contact B. The effects between the contact and the ground plane right at the gap can be modeled by a shunt capacitance $C_o$. The photo-generated currents being absorbed at the contact A and the contact B are represented by two current sources $I_a(t)$ and $I_b(t)$. Since the waves excited at the contacts are propagating in both directions, the opposite-propagating waves appear at the other contact after a delay is modeled as current-controlled current sources with a time delay.

The model can be solved for the propagating voltages $v_r(t)$ and $v_i(t)$ by applying basic circuit laws. The following are two cases for the solution, which are to be seen as semi-analytical forms, assuming $I_a(t)$ and $I_b(t)$ are given in numerical forms.
6.3.1. Case 1: The Current Sources Are $I_a(t) = -I_b(t)$

In this case, the circuit model is symmetrical. Therefore, it is only necessary to solve one side, for example, the right-hand side. Applying the well known circuit law leads to the following equations:

$$I_a(t) = -[i_1(t) + i_2(t) + i_3(t)]$$  \hspace{1cm} (6-1)

$$v_i(t) = i_3(t)Z_0$$  \hspace{1cm} (6-2)

$$\frac{dv_i}{dt} = \frac{1}{2} \frac{i_1(t)}{C_g}$$  \hspace{1cm} (6-3)

$$\frac{dv_i}{dt} = \frac{i_2(t)}{C_0}$$  \hspace{1cm} (6-4)

where $i_1(t)$, $i_2(t)$, and $i_3(t)$ are currents flowing into $C_g$, $C_0$, and $Z_v$ respectively, as indicated in Figure 6.2. Simplification of equations (6-1) to (6-4) gives rise to the following equation:

$$\frac{dv_i(t)}{dt} + k_1 v_i(t) = -k_2 I_a(t)$$  \hspace{1cm} (6-5)

Here:

$$k_1 = \frac{1}{Z_v(2C_g + C_0)}$$
and
\[
k_2 = \frac{1}{2C_x + C_0} = k_1 Z_0
\]

The above equation is a standard form of a first-order, linear inhomogeneous differential equation. Its solution is given by

\[
v_{0}(t) = \exp(-k_1 t)[C - \int k_2 I_a(t) \exp(k_1 t) dt]
\]  \hspace{1cm} (6-6)

where \( C \) is a constant determined by the initial condition. The initial condition of \( v_{0}(t) \) is the DC biasing voltage \( V_b \), that is \( v_{0}(0) = V_b \). Substituting the initial condition leads to the final solution for the propagation voltage \( v_{0}(t) \), specifically,

\[
v_{0}(t) = \exp(-k_1 t)[V_b - k_2 \int I_a(t) \exp(k_1 t) dt]
\]  \hspace{1cm} (6-7)

If the current source is given by

\[
I_a(t) = \begin{cases} 
0 & \text{for } t < 0 \\
I_0 & \text{for } t \geq 0 
\end{cases}
\]  \hspace{1cm} (6-8)

then the step response of the optical switch is given by

\[
v_{0}(t) = V_b \exp(-k_1 t) - I_0 Z_0
\]  \hspace{1cm} (6-9)
6.3.2. Case 2: The Current Sources \( I_a(t) \) and \( I_b(t) \) Are Not Equal

In this case, similar circuit equations can be obtained as in case 1. The voltage across the gap \( v_i(t) \) satisfies the following two equations:

\[
\frac{dv_i(t)}{dt} = \frac{i_1(t)}{C_g} = \frac{i_1(t)}{C_g} \tag{6-10}
\]

\[
v_i(t) = v_r(t) + v_i(t) \tag{6-11}
\]

After similar simplification as in case 1, one can obtain the coupled equation for \( v_i(t) \), \( v_i(t) \), and \( v_i(t) \):

\[
C_g \frac{dv_i(t)}{dt} + (C_0 + C_g) \frac{dv_i(t)}{dt} + \frac{v_r(t)}{Z_0} = -I_b(t) \tag{6-12}
\]

\[
C_g \frac{dv_i(t)}{dt} + (C_0 + C_g) \frac{dv_i(t)}{dt} + \frac{v_i(t)}{Z_0} = -I_a(t) \tag{6-13}
\]

\[
(2C_g + C_0) \frac{dv_i(t)}{dt} + \frac{v_i(t)}{Z_0} = -[I_a(t) + I_b(t)] \tag{6-14}
\]
Solving equations (6-12) - (6-14) gives rise to solutions to $v_i(t)$, $v_r(t)$, and $v_t(t)$ as follows:

$$v_i(t) = \exp(-k_1 t) \left[ V_b - \int k_2 (I_a(t) + I_b(t)) \exp(k_1 t) dt \right]$$  \hspace{1cm} (6-15)

$$v_r(t) = \exp(-k'_{1r} t) \int f_1(t) \exp(k'_{1r} t) dt$$  \hspace{1cm} (6-16)

$$v_t(t) = \exp(-k'_{1t} t) \left[ V_b - \int f_2(t) \exp(k'_{1t} t) dt \right]$$  \hspace{1cm} (6-17)

Here:

$$k'_{1i} = \frac{1}{C_0 Z_0}$$  \hspace{1cm} (6-18)

$$f_1(t) = \frac{[-I_b(t) + C_0 d v_i(t) / dt]}{C_0}$$  \hspace{1cm} (6-19)

$$f_2(t) = \frac{[-I_a(t) + C_0 d v_i(t) / dt]}{C_0}$$  \hspace{1cm} (6-20)

Note that initial conditions $v_i(0) = V_b$, $v_r(0) = 0$, and $v_t(0) = V_b$ are used in solution (6-15) - (6-17).
The semi-analytical solutions for the photo-generated propagating voltages derived in this section allow convenient analysis of the optical switch. The integration in the solution can be carried out numerically. The relaxation model described in Chapter 5 can then be implemented into the semi-analytical model. The simulation of the model provides comparison with the FDTD simulation, leading to more thorough understanding of the device.

6.4. Equations for Numerical Simulation

For convenience, some of the equations to be used in the simulation process are rewritten and assembled here. These equations include the time dependent Maxwell's equations and the balanced equations for semiconductor dynamic transport. In addition, the semiconductor transport continuity equation as well as current equation are also needed in the simulation.

The time dependent Maxwell's equations:

\[ \nabla \times \vec{E} = \frac{\partial \vec{B}}{\partial t} \]  

\[ \nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J} \]  

(6-21)  

(6-22)
\[ \vec{D} = \varepsilon \vec{E} \]  \hspace{1cm} (6-23)

\[ \vec{B} = \mu \vec{H} \]  \hspace{1cm} (6-24)

The balance equations:

\[ \frac{d(m \vec{v})}{dt} = q \vec{E} - \frac{m \vec{v}}{\tau_m(\xi)} \]  \hspace{1cm} (6-25)

\[ \frac{d\xi}{dt} = q \vec{E} \cdot \vec{v} - \frac{\xi - \xi_0}{\tau_\xi(\xi)} \]  \hspace{1cm} (6-26)

The above equations, the associated physical quantities, and the discrete finite differenced forms of the equations have been described in Chapter 3 and Chapter 5. In addition to these equations, the continuity equations are given by

\[ \nabla \cdot \vec{J}_n - q \frac{\partial n}{\partial t} = q(R - G) \]  \hspace{1cm} (6-27)

\[ \nabla \cdot \vec{J}_p + q \frac{\partial p}{\partial t} = -(R - G) \]  \hspace{1cm} (6-28)

where \( n \) and \( p \) are the electron and hole concentrations, respectively. \( \vec{J}_n \) and \( \vec{J}_p \) are the electron current density and hole current density, respectively. \( G \) and \( R \) are the generation rate and the recombination rate, respectively. The current equations are given by
\[ \mathbf{J}_n = q(\mathbf{v})_n n + qD_n \nabla n \]  \hspace{1cm} (6-29)

\[ \mathbf{J}_p = q(\mathbf{v})_p p - qD_p \nabla p \]  \hspace{1cm} (6-30)

where \( D_n \) and \( D_p \) are the diffusion constants for electrons and holes, respectively. The subscripts \( n \) and \( p \) in the parenthesis designate the drift velocity for the electrons and holes, respectively. The finite difference forms for the continuity and the current equations can be obtained in similar ways to those used in Chapter 3 and Chapter 5.

6.5. Optical Excitation and Wave Excitation

An optical pulse generated by a laser is the first excitation that is injected into the optical switch, where excess electron-hole pairs are generated due to absorption of the optical energy. Absorption of the optical pulse in a semiconductor material is an exponentially decreasing function of penetration depth. It is also wavelength dependent. For some certain wavelength light sources, absorption occurs only in the very surface layer, while some optical energy can penetrate into deep layers of the material. The excess electron-holes pairs are given by [2]

\[ G(x, y, z, t) = \frac{(1 - \Gamma)\alpha P_{opt}(x, z, t)e^{-\alpha y}}{h\nu} \]  \hspace{1cm} (6-31)
where $\Gamma$ is the reflectivity of the GaAs surface, $\alpha$ is the optical absorption constant, $P_{\text{opt}}$ is the incident optical pulse power density, and $h\nu$ is the energy of one photon. The incident direction is in z-direction while x-y plane is perpendicular to the incident. If the power density is taken to be 1 pJ/pulse, the photon energy 1.55 ev, the full-duration at half-maximum (FDHM) duration 0.3 ps, and the optical pulse is assumed to uniformly cover the gap of the optical switch, the excess carrier concentration generated is about $3 \times 10^{16} / \text{cm}^3$ [7].

Since recombination and drift of the optically-generated carriers occur at the time as the carriers are generated, the actual distribution of the excess carriers is determined by the continuity equation. The lifetime of the optically generated carriers in GaAs is about 100 ps [44]. As mentioned before, the optical pulse is usually a gaussian-like waveform. If the incident pulse is in the subpicosecond time scale, the generation rate $G$ in equation (6-27) and (6-28) is much more significant than the recombination rate $R$ within the time scale (e.g. a few picoseconds) to be concerned. Also, the drift velocity is of the order of $10^5 \text{ M/sec}$. There is no significant change in the distribution of the excess carriers caused by the drift within the subpicosecond time scale. As a result, the current densities flowing into the electrodes or the metal contacts are step-like in the time scale concerned.

When the current flows into the conductor microstrip, an electromagnetic wave is excited and propagates down the transmission line. The discrete space and the discrete
field components at the conductor contact are shown in Figure 6.3. Applying the integral form of the second Maxwell's equation along the rectangular path surrounding the conductor leads to the following approximation

\[-H^1_x \Delta x + H^1_y \Delta y + H^2_x \Delta x - H^2_y \Delta y = \left[J_x + \frac{\partial D_z}{\partial t}\right] \Delta x \Delta y\]

(6-32)

If a perfect conductor is assumed, \(D_z\) vanishes. Furthermore, since the \(\Delta x\) and \(\Delta y\) are taken to be the same, or \(\Delta x = \Delta y = \Delta h\), and the permeabilities both in the air and the semiconductor material are assumed to be the same, the magnetic components excited by the current density are approximately given by

\[|H^1_x| = |H^2_x| = |H^1_y| = |H^2_y| = \frac{1}{4} J_z \Delta h\]

(6-33)

In simulation, these excitation magnetic field components are added onto the field components resulting from the normal FDTD algorithm.
6.6. Numerical Simulation, Results, and Discussions

6.6.1. Simulation

The numerical simulation includes the FDTD fullwave simulation and the simulation of the semiconductor dynamic transport. The dimensions of the optical switch are given as following:

Thickness of the substrate: 50 µm

Width of the metal strip: 60 µm

Width of the gap: 25 µm (gap is located at the middle of the structure)

Length of the substrate: 500 µm

Width of the substrate: 500 µm

Height of the simulation domain: 250 µm

Dielectric constant in GaAs: 13.1
Simulation was carried out in the subpicosecond range. With consideration of available computer resources to the researcher, resolution, and stability requirements, the spatial increment was chosen to be uniform and to be equal to 5 \( \mu \text{m} \). The time increment was then chosen to be \( 5.0 \times 10^{-12} \) sec. The simulation mesh was then 50x50x100, taking advantage of the symmetry of the structure. A DEC alpha workstation and an IBM RICS 6000 workstation were used to carry out the simulation. For a period of simulation time equal to 10 ps, each run took about 8 hours.

The simulation starts with calculation of the static electric field for a given DC bias. The electric field was then used to calculate the drift velocities. The drift current density was then calculated based on the drift velocities and the optically-generated carriers. The magnetic fields and the electric fields were computed according to the FDTD scheme. The process continued for the total simulation time. The simulation flow chart is given in Figure 6.4.

To simulate the semi-analytical model, it is necessary to calculate lumped elements first. For the given structure, a computer program was written using the finite difference method to solve the Poisson equation. The resultant potential was then used to calculate the capacitance \( C_v \), \( C_g \), and the characteristic impedance \( Z_0 \) by applying the Gauss' Law. Note that TEM propagation mode is assumed for the microstrip line when the
characteristic impedance was calculated. The lumped elements were obtained as $C_0 = 5.28 \times 10^{-15} \text{ F}$, $C_g = 4.32 \times 10^{-17} \text{ F}$, and $Z_0 = 37.7 \Omega$.

### 6.6.2 Results and Discussions

In Figure 6.5, responses of the semi-analytical model are shown corresponding to a constant drift velocity equal to $10^5 \text{ M/s}$ and the optical input pulse described in section 6.4. The curve (a) is the one without considering the delayed term in the model while the curve (b) is the total response including the delayed term. The transition time of the response (a) is about 0.3 ps, which is actually the transition time of the input pulse. This is because the time constant of the lumped model is equal to $(C_0 + C_g)Z_0 = 0.2 \text{ ps}$, which is smaller than the transition time of the input pulse. The transition time of the response (b) is about 0.6 ps. For the gap equal to 25 $\mu\text{m}$, the delay time is about 0.3 ps. The longer transition time as well as the higher magnitude are due to the delayed term.

The responses corresponding to nonlinear current sources, which are numerically calculated by solving the balance equation, are shown in Figure 6.6. The curve (a), (b), and (c) represent the responses resulted from the DC bias 5 V, 10 V, and 15 V, respectively. It can be seen that the responses reflect the basic characteristics of the drift velocity as described in Chapter 5. Since the electric field within the gap area close to the metal contact A is larger than that close to the metal contact B, the current source at the
contact A is larger than that at the contact B. Therefore, the basic features of the curves are determined by the larger current source.

It will be helpful to investigate 2D TE mode propagation for the same structures as the 3D full-wave propagation situation. The 2D approximation is assuming that the x-direction extends to infinity. The excitation described in the last section or section 6.4 can excite 2D TE mode, where the magnetic fields component $H_x$, the electric field components $E_z$ and $E_y$ are present. The propagation of electromagnetic energy along the z-direction is the electric component $E_y$ and the magnetic field component $H_x$. Propagating voltage waveforms can be extracted by integrating the electric field component $E_y$ in the y-direction at a specified distance in the z-direction. The 3D simulation, the full wave simulation, include all electric and magnetic field components. The propagating voltages can be obtained by integrating the electric field $E_y$ underneath the metal strip.

(1) Constant drift velocity

The constant drift velocity implies a case where the carriers reach the saturation velocity at no time. Such a case of course is impractical and serves as a reference for comparison only. The voltages corresponding to a constant drift velocity $10^5$ M/s are shown in Figure 6.7A and 6.7B for the 2D and the 3D, respectively. The curves (a) and (b) in the figures illustrate the pulses recorded at $z = 25 \mu m$ and $z = 150 \mu m$, respectively.
The transition time is about 0.85 ps, which is slower than that of the input pulse. Overshoot of the pulses can be observed. The overshoot of the pulse recorded at $z = 150 \mu m$ is larger than the one at $z = 25 \mu m$. Dispersion is believed to be the cause. The dispersion also causes the transition to bend a little, meaning that the transition time is slowed down due to the dispersion.

Since the waves are excited at the gap area, major part of the energy of the waves initially propagate along the propagation direction, the $z$-direction. The wave propagates in this way is known to be TEM mode, which attributes to the rapid transition of the pulse. At the same time, wave also propagates towards the bottom of the substrate, constituting non-TEM mode propagation and slowing down the transition of the pulse. Also, the waves excited at the gap area causes the transition time to be slow due to the delay.

(2) Field and time dependent drift velocity

The nonlinear phenomena are shown in Figure 6.8A and 6.8B for the 2D simulation and the 3D simulation, respectively. The curves (a), (b), and (c) in the figures correspond to the DC biasing voltages $Vb = 5$ V, $10$ V, and $15$ V, respectively. The response with $Vb = 5$ V has little overshoot. The response with $Vb = 15$ V has significant overshoot while the one with $Vb = 10$ V has observable overshoot. Since the
drift velocity is not only field dependent, but also time dependent. The pulses shown in the figure reflect these characteristics. The higher the biasing voltages, the higher the magnitude and the larger the overshoots following the transition. The transition time of the pulse with the larger overshoot is faster than those with smaller overshoot or without overshoot. The magnitudes of the output pulses are not linearly related to the DC bias. A high bias voltage is desirable in order to achieve a high magnitude output pulse. The major limitation to the high biasing voltage is the dielectric breakdown of the substrate. Another concern for the high biasing is the distortion to the pulse shape due the overshoot. A compromise between the high magnitude and less distortion ought to be made to achieve a good quality output step-like pulse.

(3) *The effects of the geometries of the structure*

Note from the above observation and analysis that the DC biasing voltages, the dynamic characteristics of the drift velocity, and the transition time of the input pulse have little effects on the transition time, about 0.85 ps, of the output pulse. It seems that the geometrical structure consisting of the thickness of the substrate, the gap, and the width of the metal strip are the factors to be concerned.

Responses of a structure with a double substrate thickness are shown in Figure 6.9A and 6.9B for the 2D simulation and 3D simulation, respectively. The constant drift
velocity equal to $10^5$ M/s was used in the simulations. The curve (a) and curve (b) correspond to a substrate thickness 50 µm and 100 µm, respectively. It can be seen that the thicker the substrate, the higher the magnitude, but the slower the transition time. These results are consistent with the analysis of the lumped model, where the rise time of the excited pulse is determined by the time constant $\tau = (C_g + C_o)Z_0$ and the magnitude is proportional to the characteristic impedance $Z_0$. The thicker substrate leads to a higher characteristic impedance, which in turn increases the transition time and the magnitude. Therefore, a compromise is also made between the fast transition and the high output magnitude when the substrate thickness is designed. In practical situations, very thin substrate, for example thinner than 50 µm, is hard to be realized.

Effects of the gap on the output pulses are illustrated in Figure 6.10A and 6.10B for the 2D simulation and the 3D simulation, respectively. The responses resulted from a change in the gap from 25 µm to 10 µm, displayed by curve (a) and (b), respectively. It can be observed that the device with the smaller gap results in longer transition time, but has the smoother curve. This is because the smaller gap leads to a larger gap capacitance $C_g$, which in turn causes a longer transition time. Compared to the guided wave propagating around the metal strip, the waves in the gap area has more "distortion". Therefore, the device with the smaller gap gives rise to a pulse with less distortion. In addition, for the same DC biasing voltage, the smaller gap can result in a higher biasing electric field between the gap. However, a too small gap is hard to be realized.
(4) Non-perfect absorption boundary condition

Although the absorption boundary conditions were applied at the front and back planes of the simulation domain, a small amount of reflections are still observed in the later parts of all the simulated responses. The reflection are seen like ripples superpositioned onto the real responses. Compared to the magnitude of the responses, the reflection is only a small percentage. The reflection would be further reduced by using better absorption boundary conditions or increase the length in the z-direction of the simulation domain.

6.6.3 Experimental Verification

Experimental data used for verification in this research were reported by J.A. Valdmanis et al in [45] and by K. Meyer et al in [46]. These data, shown in Figure 6.11 - Figure 6.14, are included in this dissertation solely for purpose of convenience.

Since a pulse generated by an optical switch is extremely fast as seen by the simulation, it is very hard to detect such a fast pulse because the sampling head would have to have a sampling pulse even much faster than the one to be detected. Experimental step-like pulses generated by an optical switch were reported in [45]. In that paper, the author presented step-like pulses generated by the optical switch and detected by a
laser-generated optical probe. The pulses presented in that paper resulted from the responses of the generation and the detection. It was clearly seen that the waveforms of the pulses depended on the sampling system. The transition times of the waveforms was structure dependent. However, a common feature of these pulses was that they were step-like pulses. In other words, the optical switch did generate step-like pulses. The pulses had a transition time about 0.85 ps. The one corresponding to 250 μm substrate thickness and 30 μm gap had much larger distortion than another pulse corresponding to substrate thickness 100 μm.

Compared to the experimental pulses in [45], the simulated pulses in this research is qualitatively consistent. The discrepancy exists mainly in the magnitude of the pulses. The simulated pulses have magnitude in the order of 100 - 200 mV while the experimental ones had only 10 - 20 mV. Note that the conductor strip and the substrate of the device for the simulation is about ten times smaller than the one in the experiment while the gap is the same.

Experimental observations of the overshoot in GaAs subpicosecond optical switch were also reported in [46]. The authors in [46] presented measured responses of the device biased under different DC biasing voltages. The overshoot was observed in the responses when the DC bias was high (the electric field was higher than 5 KV/cm). When the DC bias was moderate and low, an step-like pulse without overshoot was resulted.
Much faster transition times were observed in the transient responses with overshoot. The responses nonlinearly depended on the DC voltages. According the authors, the transient voltages in the experiments were only on the order of 0.01% of the applied DC voltages.

In comparison with the observations in [46], where the dimensions of the experimental device was about the same as those of the one used in the simulation of this research, the simulated responses under different DC biases possesses the same overshoot and nonlinear behaviors. In other words, the simulation results are confirmed by the experiment in [46], although the voltages of the output pulses in the simulation is larger than the experimental ones.

Several reasons may be attributed to the difference in voltages between the simulations and the experiments:

(a) The excitation power. The concentration $3 \times 10^{16} \text{ /cm}^3$ of optically generated carriers was used in the simulation and the carriers with this concentration was assumed to be uniformly distributed in the gap area. This concentration corresponds to a laser optical power of 1 pJ/pulse. There was no indication about the excitation power used for the experiment.
(b) The reflection on the surface of the substrate. In the simulation, a perfect absorption was assumed. The actual reflectivity on the experimental substrate was not known. In other words, the actual concentration of the optically generated carriers may be much smaller than that used in the simulation.

(c) Absorption at the metal contacts. In the simulation, total absorption of the optically generated carriers was assumed at the metal contacts to form the currents following into the metal strip. The actual absorption is not known.

(d) Conductivity of the substrate. In the simulation, the substrate was assumed to be an insulating material. In practical cases, the conductivity may not be zero. The existence of the conducting substrate would lead to loss, resulting in decrease in the magnitude of the pulse.

In spite of the discrepancy in the magnitude, the simulation results do illustrate fundamental characteristics of the optical switch such as the overshoot phenomena, the nonlinear phenomena, the effects of the geometrical parameters, and the distortion characteristics.
6.7. Summary

In this chapter, an optical switch excited by a subpicosecond optical pulse to produce step-like pulses has been simulated. The simulation started with a calculation of the static electric field. The optical pulse injected into the gap area generates carriers, which are drifting under the influence of the electric field between the gap towards the metal strip and being absorbed there. The current flowing into the metal strip excites electromagnetic waves that propagate along the microstrip line and output step-like pulses can then be detected.

A semi-analytical model, which is basically a lumped model, has been developed to describe approximately the responses of the optical switch. The gap area between the two metal contacts was modeled as a gap capacitance $C_g$ and the coupling between the contacts and the ground plane was modeled as a capacitance $C_o$. The microstrip line was seen as a characteristic impedance by the excitation source. The excitation source was modeled as a current source, which could be numerically simulated. The semi-analytical model served as preliminary analysis of the device.

The numerical simulation of the optical switch included the FDTD simulation of the electromagnetic waves and the simulation of the semiconductor dynamic transport characteristics. The interaction of these two aspects involved in the optical switch was
realized by the current, formed by the optically generated carriers, and the excitation of the electromagnetic waves due to the current flowing into the metal strip of the microstrip line. The current was field and time dependent due to the drift velocity which was field and time dependent. The simulation was done in 2D and 3D situation for comparison.

The simulated results indicated that the pulses generated by the optical switch were step-like pulses. The transition time of the device with the given structure was about 0.85 ps corresponding to the 0.3 ps FDHM excitation pulse. For the DC biasing voltages equal to 5 V, 10 V, and 15 V, it was observed that the higher the biasing voltages, the higher the magnitude of the output pulses. The relation between the biasing voltages and the output voltages of the pulses was nonlinear. Overshoots of the pulses were clearly observed for the cases of the high DC biasing voltages. The response with the high overshoot had faster transition time than those without the overshoot. The substrate thickness had effects on both the transition time and the magnitude of the pulses. The thicker the substrate, the longer the transition and the higher the magnitude. This was because the thicker substrate resulted in larger characteristic impedance. The dimension of the gap also had observable effect on the transition time and a little effect on the magnitude. A smaller gap, which meant a larger gap capacitance, resulted in longer transition time of the pulses, but gave rise to smoothness of the curve, implying less distortion from the gap area.
The simulation results were compared with the previously published experimental results [45,46]. The simulation agreed with the experiment in several characteristics of the device such as the shape of the pulse (step-like pulse), the overshoot, the nonlinearity, and the transition time. However, discrepancy between the simulation and experiment did exist in the voltage magnitudes. The reasons for the discrepancy in magnitude may be due to unrealistic assumption of the uniform injection of the optical pulse, the estimate of the incident optical power, the use of the total absorption at the metal contacts, and the assumption of insulating GaAs substrate.

In conclusion, the method developed in this research successfully simulated the responses of the optical switch under the excitation of the subpicosecond pulse. The method can efficiently handle the nonlinear dynamic transport characteristics of semiconductor devices involving in electromagnetic waves. The simulations using this method were able to predict characteristics of the subpicosecond optical device such as the step-like responses, the nonlinearity of the responses, the overshoot under the high bias as well as transition time of the responses. The method can be further extended to simulate other devices with similar structure and nonlinear phenomena as the optical switch.
Figure 6.1. An optical switch made on a GaAs substrate. A laser pulse is injected onto the gap between the two conductor strips.
Figure 6.2. A physically-based semi-analytical model of an optical switch.
Figure 6.3. An illustration of excitation of magnetic fields at the metal contact due to the photo-generated current.
Figure 6.4. A flow-chart of the FDTD simulation.
Figure 6.5. Step-like responses of the semi-analytical model resulted from an optical pulse with a FWHM of 0.3 ps, assuming a constant drift velocity equal to $10^3 \text{ M/sec.}$ (a) without considering delayed term; (b) including the delayed term.
Figure 6.6. Step-like responses of the semi-analytical model resulted from an optical pulse with a FWHM of 0.3 ps under different DC biasing voltages. Curves (a), (b), and (c) correspond to the DC voltages 5 V, 10 V, and 15 V, respectively.
(A) Responses of 2D simulation.

(B) responses of 3D simulation.

Figure 6.7. Step-like responses resulted from an optical pulse with a FWHM of 0.3 ps, assuming a constant drift velocity equal to $10^3$ M/sec. The curve (a) was recorded at $z=25\mu m$ and the curve (b) at $z=150\mu m$. 

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(A) Responses of 2D simulation.

(B) Responses of 3D simulation.

Figure 6.8. Step-like responses resulted from an optical pulse with a FWHM of 0.3 ps under different DC biasing voltages. The curve (a), (b), and (c) correspond to DC bias 5 V, 10 V, and 15 V, respectively. All pulses were recorded at the location z=25 μm.
Figure 6.9. Step-like responses resulted from an optical pulse with a FWHM of 0.3 ps with different substrate thickness. The curve (a) and (b) correspond to thickness 50 μm and 100 μm, respectively. All pulses were recorded at the location z=25 μm.
(A) Responses of 2D simulation.

(B) responses of 3D simulation.

Figure 6.10. Step-like responses resulted from an optical pulse with a FWHM of 0.3 ps with different gap dimensions. The curve (a) and (b) correspond to gap width 25 μm and 10 μm, respectively. All pulses were recorded at the location z=25 μm.
Fig. 5. Photograph of the actual display resulting from sampling the impulse response of a 30 μm gap Cr:GaAs photoconductive detector with a 250 μm substrate thickness. An initial rise time of 850 fs is clearly resolved, indicative of a comparable sampling time.

Figure 6.11. Experimental curve showing a step-like pulse reported in [45].
Fig. 6. Photoconductive signal (approximately 20 mV peak) as sampled with 100 μm thick lithium tantalate crystal.

Figure 6.12. Experimental curve showing a step-like pulse with observable overshoot reported in [45].
FIG. 2. Transient photoconductivity results for $\lambda_{\text{cut}} = 620$ nm. The plotted waveform is the transient voltage waveform generated by the photoconductive switch normalized to the applied dc voltage.

Figure 6.13. Experimental curve showing step-like pulses reported in [46]
Figure 6.14. Experimental curve showing step-like pulses reported in [46].
Chapter 7

Summary and Conclusions

7.1. Summary

The main objective of this dissertation is to investigate the generation and the propagation characteristics of an ultrafast (subpicosecond) pulse in a planar transmission line environment with III-V GaAs semiconductor material as the propagation medium. An optical switch is used as an example for simulation based on solving the time dependent Maxwell's equations and the semiconductor transport equations using the finite difference time domain (FDTD) technique. The method used in this research can be extended to other similar devices such as pulse forming devices and optical sampling devices.

The main contributions of this dissertation include:

1. Successfully obtained simulation responses of an optical switching device to an ultrafast pulse excitation, hence resulting in a careful investigation of the characteristics of the optical device. The simulation results agreed qualitatively with the experimental
results. The method developed in this research is efficient and can be extended to other semiconductor devices as well as microwave devices;

2. Successfully simulated the interaction of the electromagnetic phenomena and the nonlinear dynamic transport in the optical device;

3. Developed a semi-analytical macroscopic model for an optical switch. The model can be used to preliminarily and efficiently estimate responses of the device.

Modern high speed devices are now operating at ultrafast speeds in the picosecond and subpicosecond domain. One class of devices of special interest is the optical switch which is typically used in the generation as well as detection of subpicosecond electrical signals. Such devices are constructed as planar transmission lines on top of a semiconductor material. Based on principles of photoconductivity, these devices can be excited by a laser pulse with duration less than 0.1 ps to generate an electrical pulse. The electrical pulse in turn propagates on the planar transmission line. Operation of these devices involves the transport phenomena and the electromagnetic phenomena associated with semiconductor materials. Since these phenomena include nonlinear dynamic transport characteristics of semiconductor carriers, wave propagation, and their interaction, an effective way of device analysis is to solve the associated equations in the time domain.
To analyze electromagnetic propagation, it is necessary to solve Maxwell's equations. The finite difference time domain (FDTD) method is a numerical method of solving the time dependent Maxwell's equations. To apply the FDTD technique, the space is discretized into some basic building blocks. At each block, electromagnetic field components, resulted from the finite differenced Maxwell's equations, are arranged according to Yee's algorithm. Such an arrangement gives rise to second order accuracy both in space and time. Since the wave equations are hyperbolic, the stability requirement has to be satisfied when the time stepping interval is selected. Numerical dispersion would be introduced using finite difference, leading to phase distortion of the propagating waveforms. The dispersion can be minimized by properly choosing the time step. To handle open space problems, an artificial boundary condition or absorbing boundary condition, which can absorb outgoing wave without reflection, is needed to confine the problem within a relatively small space.

The planar transmission line used in these devices is typically a microstrip line. The FDTD method is used to simulate the propagation of a wideband signal (a Gaussian pulse) on the microstrip line. The simulation illustrates some fundamental characteristics of the microstrip such as dispersion, surface wave, and fringing field phenomena.

In semiconductors, the velocity of carriers is a nonlinear function of the applied electric field, especially within a few picoseconds after the electric field is applied. The
relation known as transport characteristic could be achieved numerically by the Monte Carlo method. However, the Monte Carlo method is very costly in computation time and therefore is not suitable for practical engineering applications. An alternative way is to solve the balanced equations using a finite difference numerical scheme. The balanced equations give rise to very accurate results compared to the results of the Monte Carlo method while the computation time is substantially reduced.

When an ultrafast pulse is injected into an optical switch, opto-excited carriers are generated and governed by the semiconductor transport equation. Under the influence of the externally applied biased voltage, the carriers drift onto the transmission line where the opto-generated electrical pulse propagates. The propagation is governed by the Maxwell's equations. To simulate the whole process, the FDTD and the finite differenced balanced equations are applied and properly interacted to result in the device response to the optical excitation.

7.2. Conclusions

The finite difference time domain (FDTD) technique proved to be an useful tool to solve numerically the time dependent Maxwell's equations using the Yee's arrangement of the electric field and magnetic field components. The FDTD technique could properly
describe propagation of an ultrafast pulse on a microstrip line. The simulation results used in this research was consistent with the previously reported results [18].

The semiconductor dynamic transport characteristics were obtained by solving the balance equations using the relaxation time approximation. The finite difference scheme used to solve the balance equations resembled results obtained by much more costly Monte Carlo method [25,26]. The method used in this research was accurate and efficient.

A semi-analytical model, which was basically a lumped model, was developed to describe approximately the responses of the optical switch. In this model, the gap area between the two metal contacts was represented by a capacitance $C_g$ and the coupling between the contacts and the ground plane was modeled as a capacitance $C_0$. The microstrip line was seen as a characteristic impedance by the excitation source. The excitation source was modeled as a current source, which could be numerically simulated. The semi-analytical model served as preliminary analysis of the device.

The simulated results indicated that the pulses generated by the optical switch were step-like pulses. It was observed that the higher the biasing voltages, the higher the magnitude of the output pulses. The relation between the biasing voltages and the output voltages of the pulses were nonlinear. Overshoots of the simulated pulses were clearly observed for the cases of the high DC biasing voltages. The response with the high
overshoot has faster transition time than those without the overshoot. The substrate thickness had effects on both the transition time and the magnitude of the pulses. The thicker the substrate, the longer the transition and the higher the magnitude. This was because the thicker substrate resulted in larger characteristic impedance. The dimension of the gap also had observable effect on the transition time and a little effect on the magnitude. A smaller gap, which meant a larger gap capacitance, resulted in longer transition time of the pulses, but gave rise to smoothness of the curve, implying less distortion from the gap area.

The simulation results were compared with the previously published experimental results [45,46]. The simulation agreed with the experiment in several characteristics of the device such as the shape of the pulse (step-like pulse), the overshoot, the nonlinearity, and the transition time. However, discrepancy between the simulation and experiment did exist in the voltage magnitudes. The reasons for the discrepancy in magnitude may be due to unrealistic assumption of the uniform injection of the optical pulse, the estimate of the incident optical power, the use of the total absorption at the metal contacts, and the assumption of insulating GaAs substrate.

The method developed in this research successfully simulated the responses of the optical switch under the excitation of the subpicosecond pulse. The method can efficiently handle the nonlinear dynamic transport characteristics of semiconductor devices involving
in electromagnetic waves. The simulations using this method are able to predict characteristics of the subpicosecond optical device such as the step-like responses, the nonlinearity of the responses, the overshoot under the high bias as well as transition time of the responses. The method can be further extended to simulate other devices with similar structure and nonlinear phenomena as the optical switch.
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VITAE

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Mr. Jianqing He has an intelligent, kind, and loving wife, Shu Lu, who is currently completing her Ph. D. degree in the same Electrical Department. He is also the father of a beautiful and lovely daughter, Victoria, who is just one year old. He enjoys cooking, fishing, watching everyday's Evening-News, and talking about politics, but he is politically naive. He believes in the creation. He also believes in the fundamental Chinese philosophy: universal harmony.

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