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Formulation of a full dynamic transport model for heterojunction devices

Anoushiravan Arman
University of Nevada, Las Vegas

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Formulation of a full dynamic transport model for heterojunction devices

Arman, Anoushiravan, M.S.
University of Nevada, Las Vegas, 1991
FORMULATION OF A FULL DYNAMIC TRANSPORT MODEL
FOR HETEROJUNCTION DEVICES

by

Anoushiravan Arman

A thesis submitted in partial fulfillment
of the requirements for the degree of

Master of Science

in

Electrical Engineering

Department of Computer Science and
Electrical Engineering
University of Nevada, Las Vegas
December, 1991
The thesis of Anoushiravan Arman for the degree of Master of Science in Electrical Engineering is approved.

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University of Nevada, Las Vegas
December, 1991
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I would like to acknowledge members of my examining committee, professor A. Iyer, professor S. Singh, professor S. Cloud, and Dean Ronald Smith for their time, and the Department of Electrical Engineering, and the University of Nevada for providing this opportunity for me. I would like to acknowledge the Army Research Office for providing the research grant.

Last but not least, I would like to thank my wife for her unceasing love, support, and understanding.
A new numerical approach for solving problems of the heterostructure p-n junction is presented in this work by using a Full Dynamic Transport Model (FDTM).

Most numerical models have been based on simplified dynamic transport models such as the Energy Transport Model or the Drift Diffusion Model. These models do not accurately predict the behavior of a heterostructure.

In this thesis a Full Dynamic Transport Model is presented which consists of the Momentum Conservation Equation (MCE), Energy Conservation Equation (ECE), Particle Conservation Equation (PCE), and Poisson's Equation. In our model carrier velocity and electron energy are taken as variables and have been found using electron concentration and electrostatic potential.

The results of the simulation of a one-dimensional p-n heterojunction are presented, which include electron concentration, electrostatic potential, electric field, carrier velocity, and electron energy distribution throughout the device for two different doping levels. Also presented are the I-V characteristics of the device. The effect of variation in doping levels on I-V characteristics of the device has also been studied.

It has been found that by increasing the doping from $10^{16} \text{cm}^{-3}$ to $5 \times 10^{17} \text{cm}^{-3}$, the built-in voltage of an $Al_{0.3}Ga_{0.7}As/GaAs$ heterojunction increases from 1.33V to 1.54V which is consistent with the results reported by others [1]–[4]. Maximum velocity of electrons changes from $2.5 \times 10^{7} \text{cm/sec}$ to $1.8 \times 10^{7} \text{cm/sec}$, which is due to the increased collision of electrons with doping impurities. This is also the reason for increased electron average en-
ergy from 270\textit{mev} to 640\textit{mev}. This increase in energy is believed to be due to the hot-electron phenomenon. The results obtained are in good agreement with the existing experimental values reported by others [1] \textendash{} [6].
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<tr>
<td>$\epsilon$</td>
<td>Permittivity</td>
<td>(F/cm)</td>
</tr>
<tr>
<td>$\Phi$</td>
<td>Work function</td>
<td>(ev)</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Total scattering rate</td>
<td>(sec$^{-1}$)</td>
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<tr>
<td>$\psi$</td>
<td>Electrostatic potential</td>
<td>(V)</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Charge density</td>
<td>(C cm$^{-3}$)</td>
</tr>
<tr>
<td>$\mu_n$</td>
<td>Electron mobility</td>
<td>(cm$^2$V$^{-1}$sec$^{-1}$)</td>
</tr>
<tr>
<td>$\mu_p$</td>
<td>Hole mobility</td>
<td>(cm$^2$V$^{-1}$sec$^{-1}$)</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Relaxation time</td>
<td>(sec)</td>
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<tr>
<td>$\tau_w$</td>
<td>Energy relaxation time</td>
<td>(sec)</td>
</tr>
<tr>
<td>$\tau_m$</td>
<td>Momentum relaxation time</td>
<td>(sec)</td>
</tr>
<tr>
<td>$\nabla$</td>
<td>Del operator ($\frac{\partial}{\partial z}$)</td>
<td>(cm$^{-1}$)</td>
</tr>
<tr>
<td>$\nabla_k$</td>
<td>Del operator in momentum space ($\frac{\partial}{\partial k}$)</td>
<td>($\frac{sec}{Kg \text{cm}}$)</td>
</tr>
<tr>
<td>$a$</td>
<td>Known constants derived from linearizing</td>
<td></td>
</tr>
<tr>
<td>$C$</td>
<td>Net doping concentration</td>
<td>(cm$^{-3}$)</td>
</tr>
<tr>
<td>$D$</td>
<td>Diffusion constant</td>
<td>(cm$^2$/sec)</td>
</tr>
<tr>
<td>$D_n$</td>
<td>Electron diffusion constant</td>
<td>(cm$^2$/sec)</td>
</tr>
<tr>
<td>$E$</td>
<td>Electric field</td>
<td>(V/cm)</td>
</tr>
<tr>
<td>$E_x$</td>
<td>Electric field in x direction</td>
<td>(V/cm)</td>
</tr>
<tr>
<td>$E_y$</td>
<td>Electric field in y direction</td>
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</tr>
<tr>
<td>$E_c$</td>
<td>Energy band gap at the conduction band</td>
<td>(ev)</td>
</tr>
<tr>
<td>$E_f$</td>
<td>Fermi energy level</td>
<td>(ev)</td>
</tr>
<tr>
<td>$E_v$</td>
<td>Energy band gap at the valence band</td>
<td>(ev)</td>
</tr>
<tr>
<td>$f$</td>
<td>Non-equilibrium distribution function</td>
<td></td>
</tr>
</tbody>
</table>
\( f^0 \)  
Constant function

\( f^{k-1} \)  
Constant function from last iteration

\( F \)  
Applied force

\( F_{1/2} \)  
Fermi-Dirac integral

\( h \)  
Planck's constant  \((J\text{-sec})\)

\( H \)  
Hamiltonian function

\( J \)  
Current density  \((A/cm^2)\)

\( J_n \)  
Electron current density  \((A/cm^2)\)

\( J_p \)  
Hole current density  \((A/cm^2)\)

\( k \)  
Boltzmann constant  \((J/K)\)

\( m_n \)  
Effective mass of electron  \((Kg)\)

\( m_p \)  
Effective mass of hole  \((Kg)\)

\( n \)  
Electron concentration  \((cm^{-3})\)

\( n_i \)  
Intrinsic electron concentration  \((cm^{-3})\)

\( N_c \)  
Density of states in conduction band  \((cm^{-3})\)

\( N_v \)  
Density of holes in valence band  \((cm^{-3})\)

\( p \)  
Hole concentration  \((cm^{-3})\)

\( P \)  
Momentum  \((Kg \text{ cm/sec})\)

\( P_f(t) \)  
Probability density

\( q \)  
Electronic charge  \((C)\)

\( Q_T \)  
Heat flow rate  \((J/sec)\)

\( r \)  
Space vector

\( t \)  
Time  \((sec)\)

\( T \)  
Lattice temperature  \((K)\)

\( T_e \)  
Effective electron temperature  \((K)\)

\( v(r,k) \)  
Group velocity  \((cm/sec)\)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$v_n$</td>
<td>Electron velocity</td>
<td>(cm/sec)</td>
</tr>
<tr>
<td>$v_p$</td>
<td>Hole velocity</td>
<td>(cm/sec)</td>
</tr>
<tr>
<td>$V_c$</td>
<td>Applied voltage</td>
<td>(V)</td>
</tr>
<tr>
<td>$V_b$</td>
<td>Built-in voltage</td>
<td>(V)</td>
</tr>
<tr>
<td>$w_n$</td>
<td>Average electron energy</td>
<td>(ev)</td>
</tr>
<tr>
<td>$w_p$</td>
<td>Average hole energy</td>
<td>(ev)</td>
</tr>
<tr>
<td>$w_0$</td>
<td>Initial electron energy</td>
<td>(ev)</td>
</tr>
<tr>
<td>$W$</td>
<td>Local kinetic energy</td>
<td>(ev)</td>
</tr>
<tr>
<td>$x$</td>
<td>Position in x direction</td>
<td>(cm)</td>
</tr>
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</table>
Chapter 1

Introduction

In recent years heterostructure devices have been the subject of intensive research for their high speed advantage [1] – [10]. Accurate modeling of the heterojunction is an important tool in simulation of many heterojunction devices such as Heterojunction Bipolar Transistors (HBT). The main feature of heterojunction device operation is the confinement of holes at the center of the space charge region just inside of the p-region, which allows high injection efficiencies of electrons from the p- to the n- side of the device. The heterojunction is usually made of GaAs and AlGaAs, as seen in Figure (1.1) [8]. The confinement of holes is due to a potential barrier at the junction which opposes hole injection into the n-region. At the same time, the lack of a barrier for electrons allows higher injection into the p-region [11]. This feature means that it is not necessary to have a device that is more heavily doped in the n-region than the p-region to achieve high injection ratios, as is necessary in homojunctions. The most important variables in improving the performance of heterojunctions are velocity and energy of electrons and holes.

In recent works most models have been based on thermal equilibrium
approximations such as the Drift-Diffusion Model (DDM) [3],[6],[19],[20]. None of these models is ideal for device design due to their excessive computation time and the problem of incorporating a successful recombination-generation mechanism. DDM is a linear velocity model in which the electrons are assumed to be subject to a drift force and a diffusive force, and the electron velocity is:

\[ v_n = -\mu_n E - \frac{D_n}{n} \nabla n \]  

(1.1)

where \( v_n \) is electron velocity, \( \mu_n \) is electron mobility, \( D_n \) is diffusion coefficient for electrons, \( n \) is electron concentration, and the del operator \( \nabla \) is \( \frac{\partial}{\partial x} \). The first term in the right hand side of Eq. (1.1) is the drift component and the second term is the diffusion component, hence, the Drift-Diffusion approximation. The main difficulty with this model is the estimation of accurate values for electron mobility and diffusion constants [21],[22]. Also, in DDM, the effects of high field electron dynamics are neglected due to the thermal equilibrium assumption.

Full Dynamic Transport Model (FDTM), on the other hand, is a non-linear model involving carrier velocity and average energy, which will eliminate the necessity of calculating the mobility and diffusion constants. It is an accurate model of electron velocity which is not only a function of electron density and electric field, as seen in Eq. (1.1), but also a function of electron energy, \( w \). In this work a Full Dynamic Transport Model consisting of the Momentum Conservation Equation (MCE), the Energy Conservation Equation (ECE), the Particle Conservation Equation (PCE), and Poisson's Equation is employed. The conservation equations are all derived from the Boltzmann Transport Equation (BTE). The applicability of the BTE to heterostructure semiconductors has been discussed by many researchers.
The theory is valid within the position dependent effective mass model and under the assumption that variation of potentials over a lattice unit cell is small compared to the crystal potential. The important hot electron phenomena, such as velocity overshoot, may be accounted for by including the third moment of the BTE, which provides for energy conservation. In recent works, only a simplified FDTM system of equations has been applied in a one dimensional model [18], [23] – [25].

In this thesis, we propose a solution for the Full Dynamic Transport Equations, which will not use Drift-Diffusion approximation. Furthermore, this model does not need knowledge of carriers' mobility or diffusion constants. Our model is applied to a one-dimensional representation of a heterojunction device, and will use a finite difference scheme to calculate the solution of the system of equations.

In the next chapter, a literature review on numerical modeling related to semiconductor devices is presented. Different models such as Drift-Diffusion, Monte Carlo, and Full Dynamic Transport Model and their general characteristics, are discussed.

Chapter 3 presents the derivation of the system of equations that form the Full Dynamic Transport Model. Also, a full one dimensional model and a simplified one-dimensional model which are used in our program, are discussed.

In Chapter 4 our numerical approach for solving the system of equations has been presented and includes discretization method and boundary conditions. The results of the computer program are presented in Chapters 5 and 6.
Chapter 2

Literature Review on Numerical Modeling

2.1 Numerical Modeling

Numerical modeling is defined as producing a representation or simulation of a problem or a process that cannot be subject to an exact analysis. Numerical modeling of semiconductor devices are based on partial differential equations which describe the transport of carriers in different regions of the device. There are many different modeling methods for device simulation, but they all originate from two methods, the Monte Carlo simulation and an iterative solution of Boltzmann's Transport Equation in conjunction with solution of the Poisson's Equation. These solution must accurately take device geometry and carrier dynamics into account to give a self-consistent solution.

There have been several attempts to develop simpler models for studying carrier transport effects in small devices, which are based on moments of Boltzmann's Equation; their accuracy and CPU time strongly depend on the simplifying assumption on which their derivation is based [23] – [25].
2.2 Drift-Diffusion Model

Drift-Diffusion Model follows the classical Boltzmann Equations. The Drift-Diffusion approximation is derived by assuming that the average electron energy is uniform, that is \( \nabla w_n \) is zero, and the electron temperature gradient is negligible. Also, it assumes that there is at least an order of magnitude difference between the device and circuit responses, which implies steady-state operation, hence \( \frac{\partial V_{	ext{xn}}}{\partial t} \) is zero. Furthermore, the time variation of the external forces is neglected which implies a slowly varying applied electric field. Such a model cannot determine the time-dependent conductivity phenomena, such as velocity overshoot.

In Drift-Diffusion Modeling, one does not use velocity as a variable. Instead, one uses the Particle Continuity Equations for electrons and holes. The Current Density Equations, after incorporation of the above assumptions, yield the current density equation for electrons [21],[22]:

\[
J = (q n \mu_n(E) E) + (q D_n(E) \nabla n)
\]

(2.1)

The difficulty in using Eq. (2.1) is obtaining an accurate estimate of the field dependent mobility, \( \mu_n(E) \), and the diffusion constant, \( D_n(E) \). The diffusion coefficient \( D_n(E) \), is usually defined using the well known Einstein relationship:

\[
D(E) = \frac{\mu_n(E) k T}{q}
\]

(2.2)

where \( k \) is the Boltzmann constant, \( T \) is the lattice temperature, \( q \) is electron charge, \( n \) is the electron concentration, \( E \) is the electric field, and \( \mu_n(E) \) is the field dependent mobility.
2.3 Monte Carlo Model

The Monte Carlo method is a statistical numerical technique for solving mathematical and physical problems and is used to simulate device operation. A typical Monte Carlo method involves the generation of a sequence of random numbers according to a given probability distribution. Monte Carlo analysis of transport in semiconductors is done by following the motion of one or more particles, subject to the action of external forces. These forces on the particles consist of applied electric and magnetic fields, and scattering mechanisms. The velocity, energy, and position of each particle continuously changes during a free-flight. If the particle was last scattered at \( t = 0 \), then the probability of the particle being scattered between time, \( t \), and time \( t + dt \), is determined by [29]:

\[
P_f(t) \ dt = \lambda[w(t)] \exp\left[- \int_0^t \lambda[w(t')] \ dt' \right] \ dt
\]

where \( P_f(t) \) is the probability density of scattering at time \( t \), and \( \lambda[w(t)] \) is the total scattering rate determined from scattering mechanisms namely, electron-electron, and electron-hole scattering. \( w(t) \) is electron energy at time \( t \), and the notation of \( (t') \) is for time after collisions.

All the relevant physical quantities such as velocity and energy are computed and recorded throughout the course of simulation. From the history of these quantities, one can extract information of interest by computing the appropriate statistical averages [4][30].

The strength of Monte Carlo models lies in the ability to simulate transport phenomena at the microscopic level. Any complicated phenomenon can be studied by including the elementary processes in the simulation, and the
implementation is usually relatively straightforward in comparison to other methods such as the analytical techniques, or other numerical techniques. The treatment leads to a more accurate solution of the Boltzmann Equation, which can not be obtained from other techniques [4], [25], [29].

However, there are important limitations to the Monte Carlo method. Since the simulation involves interaction of carriers with the crystal lattice and with other carriers, a good knowledge of the energy band structure, lattice temperature, definition of the applied external fields, and a set of initial conditions are required in order to give an accurate treatment of the scattering processes. Also, the convergence of these processes is usually slow and long computation time is required. Furthermore, phenomena with long transient time are difficult to simulate because the number of scattering events is drastically reduced, and the program steps needed to go from one collision solution to another increases, resulting in even longer computational time.

2.4 Full Dynamic Transport Model

Full Dynamic Transport Model is derived from Boltzmann Transport Equation by taking its first, second, and third moments. This yields expressions for Particle Conservation, Momentum Conservation, and Energy Conservation Equations respectively [26], [27], [29]. The FDTM contains classical equations which assume instantaneous elastic collisions between two particles. It is also necessary to assume that the external forces acting on the carriers are constant over a distance comparable with lattice spacing which is about $0.03\mu m$. Particle interactions between electron-electron, hole-hole, and electron-hole are assumed to be small. The important advantage of this
model is its accuracy for predicting the electron behavior in the submicron regime, where the Drift-Diffusion approximation may not be applicable. It provides a more acceptable CPU time for the device engineer by not using mobility as one of its variables, which takes most of the computational time. One of the limitations of this model is the need to have accurate values for the effective mass of the electron, $m_e$, momentum relaxation time, $\tau_m$, energy relaxation time, $\tau_w$, and boundary conditions to begin the solution of system of equations.

There are four basic equations. In FDTM, the first three have to be written for both electrons and holes, which will give us six equations and the Poisson's Equation. If one wants to solve these in two or three dimensions, one has twelve or eighteen equations plus the Poisson's Equation respectively, which are very difficult, if not impractical, to solve as a coupled or self-consistent system.

Numerous analytical and numerical methods have been developed for semiconductor modeling using one-dimensional FDTM [18], [23] — [25]. In our work we use a one-dimensional model of FDTM for electrons without using the Drift-Diffusion approximation or mobility. Instead, we use the second moment of the BTE to calculate the velocity of carriers and the third moment of the BTE to calculate the energy of carriers, which gives us more accurate results. We assume a steady-state case, therefore all the terms that are in the form $\frac{d}{dt}$ are neglected. We neglect the gradient of heat flow, $Q_T$, by assuming that the electron distribution function is symmetrical in momentum space. We eliminate the convective term, $v \nabla v$, and the terms with the kinetic energy, $\frac{1}{2}mv^2$, because of their negligible effects.

This analysis will start with a description of the heterostructure modeled
and derivation of FDTM from BTE. In the subsequent chapters the Energy, Charge, and Momentum Conservation Equations are developed, followed by a discussion and conclusion of sample results.
Chapter 3

Full Dynamic Transport Model

3.1 Device Structure and Operation

A heterojunction is defined as a junction formed between two dissimilar semiconductors, such as n-type AlGaAs and p-type GaAs. The two semiconductors have different energy bandgap, $E_g$, dielectric permittivities, $\epsilon$, and work functions, $\Phi$. When the two dissimilar semiconductors are joined together, the barrier height for the carrier injection is increased by the difference in the bandgap, $E_g$, as shown in Figure (3.1) [22]. By matching of the lattices, hole injection from the n-type to the p-type will be suppressed and this will result in increased injection efficiency [31].

The conduction band spike suppresses electron injection from the p-type to n-type. A compositional grading, a few hundred angstroms wide, is frequently employed to eliminate the spike (see Figure (3.2) [35]). Compositional grading does increase electron injection, but it also increases recombination in the space charge region (both in the bulk and at the perimeter of the junction). Furthermore, heterojunction devices can be operated at a high temperature ($350^\circ K$), because of its large bandgap and can be operated...
down to liquid helium temperature (4°K), because of its shallow impurity levels [33].

3.2 System of Equations

In this section, the system of equations of a Full Dynamic Transport Model (FDTM) is discussed. This system consists of the Momentum Conservation Equation (MCE), Energy Conservation Equation (ECE), Particle Conservation Equation (PCE), and the Poisson’s Equation.

3.2.1 Boltzmann Transport Equation

The total force $F(r, k)$ experienced by the carriers in a crystal is given by [29]:

$$F(r, k) = F_E + F_I \tag{3.1}$$

where $F_E$ is the force due to external electromagnetic fields, and $F_I$ is due to internal crystal forces.

The classical Hamiltonian for electrons is given by:

$$H(r, k) = E_c(r) + W(r, k) \tag{3.2}$$

In other words, the carriers energy in a crystal is due to the crystal potential and external fields represented by $E_c(r)$ which is the conduction band energy level, and $W(r, k)$, the local kinetic energy. Applying Hamilton’s Equations yields the electron group velocity:

$$v(r, k) = \frac{\partial H}{\partial P} = \frac{1}{\hbar} \nabla_k W(r, k) \tag{3.3}$$

and the force term is given by:

$$F(r, k) = \nabla . H(r, k) = \nabla . E_c(r) + \nabla . W(r, k) \tag{3.4}$$
$F(r, k)$ is the force applied to the carriers, $v(r, k)$ is the average velocity of electrons, $P$ is the momentum, $\hbar$ is reduced Planck's constant, and the del operator $\nabla_k$ is $\frac{\partial}{\partial k}$ for the momentum space.

The Boltzmann Transport Equation (BTE) is given by [27]:

$$\frac{\partial f}{\partial t} + v \cdot \nabla f + \frac{F}{\hbar} \cdot \nabla_k f = \frac{\partial f}{\partial t} |_{\text{coll}}$$  \hspace{1cm} (3.5)

where the non-equilibrium distribution function, $f$, must satisfy the following condition:

$$f \Rightarrow 0 \quad , \quad \text{as} \quad |k| \Rightarrow \infty$$  \hspace{1cm} (3.6)

The left hand side of Eq. (3.5), is the total derivative for the distribution function, $f$, which comes from conservation of density in phase space ($\frac{\partial f}{\partial t} = 0$). The second term accounts for the position dependence of the distribution function, and the third term is due to the fact that the acceleration is velocity dependent. Finally, the last term ($\frac{\partial f}{\partial t} |_{\text{coll}}$) accounts for the scattering due to collisions.

The collision term can be simplified by the relaxation time approximation given by [29]:

$$\frac{\partial f}{\partial t} |_{\text{coll}} = \frac{-(f - f^\circ)}{\tau(r, W, F)}$$  \hspace{1cm} (3.7)

Where $f^\circ$ is the equilibrium distribution function and the quantity $\tau$ shows the rate of return to the state of equilibrium from the disturbed state; it is termed the relaxation time. The relaxation time approximation implies that upon removal of the external applied fields the non-equilibrium distribution function relaxes to its equilibrium value with a time constant $\tau(r, W, F)$. 
The BTE is valid within the position dependent effective mass model, and under the assumption that variation of potentials over a lattice unit cell is small compared to crystal potential. The limitations of the BTE model requires device structure dimensions to be greater than approximately 0.03 \( \mu m \), below which quantum transport processes become important.

### 3.2.2 Momentum Conservation Equations

The second moment of the BTE is obtained by multiplying the BTE with \( \hbar k \) and integrating over \( k \)-space. Substituting Eqs. (3.3) and (3.4) in Eq. (3.5), taking the integral in turn for the electron momentum equation, and after manipulation of terms, we have the Momentum Conservation Equation (MCE):

\[
\frac{\partial P}{\partial t} + q E + \frac{2}{3n} \nabla (nW) + v \nabla . P - \frac{1}{3n} \nabla (nv.P) = \frac{\partial P}{\partial t}|_{\text{coll}} \quad (3.8)
\]

with the mean momentum density \( P \) satisfying the relation \( P = mv \), and \( W \) being the local total energy. Using the collision term from Eq. (3.7), with \( f = mv \) and \( f^o = 0 \), (due to the fact that electron average velocity approaches zero with no external force applied), Eq. (3.8) yields:

\[
\frac{\partial mv}{\partial t} + q E + \frac{2}{3n} \nabla (nW) + v \nabla . (mv) - \frac{1}{3n} \nabla (mnu^2) = \frac{-mv}{\tau(r, W, F)} \quad (3.9)
\]

Dividing Eq. (3.9) by mass, \( m \), and assuming effective mass is constant with respect to position in a crystal, and rearranging the terms, yields Eq. (3.10) for electrons:

\[
\frac{\partial \nu_n}{\partial t} = -\frac{q E}{m_n} - \frac{2}{3m_n n} \nabla (nw_n) - \nu_n \nabla . \nu_n + \frac{1}{3n} \nabla (nv_n^2) + \frac{\nu_n}{\tau_m} \quad (3.10)
\]
Eq. (3.10) is the general formula for the electron velocity, with subscript \( (n) \) representing the variables associated to electrons; \( \omega_n \) is the total local energy of electrons in the \( W \) term of Eq. (3.9), and \( \tau_m \) is the momentum relaxation time. The first term, \(-\frac{\mathbf{F}}{m_n}\), gives the acceleration due to the crystal potential and the external electric field. The second term, \(-\frac{2}{3m_n\nu_n} \nabla (n\omega_n)\), represents the diffusive acceleration, which forces electrons to move in the direction that minimizes the concentration and energy of electrons. The third term, \(-\nu_n \nabla . \omega_n\), causes convective electron flow, giving electrons a tendency to move to an area where electrons move the fastest. The fourth term, \(-\nabla \nabla (n\omega_n^2)\), is due to the kinetic energy of electrons. The last term, \(-\frac{\omega_n}{\tau_m}\), is due to collisions.

### 3.2.3 Energy Conservation Equations

The third moment of the BTE provides the Energy Conservation Equation (ECE) and is obtained by multiplying the BTE by \( \frac{\hbar^2 k^2}{2m} \) and integrating over \( k \)-space.

ECE is used to calculate \( \omega_n \) which is the electron average energy. Integrating BTE (Eq. (3.5)) over momentum space \( k \), we obtain: [26].

\[
\frac{\partial \omega_n}{\partial t} = -q(\nu_n \cdot E) - \nu_n (\nabla \omega_n) - \frac{2}{3n} \nabla \cdot (n\nu_n (\omega_n - \frac{m_n}{2} \nu_n^2)) - \frac{\nabla}{n} Q_T - \left( -\frac{\partial \omega_n}{\partial t} \right)_{coll}
\]

\((3.11)\)

The left-hand side of Eq. (3.11) is the total rate at which energy changes within a differential volume element of electron gas as it moves along the direction of electron flow. The right hand side describes how individual forces contribute to changes in the total energy of the volume element. In the right hand side, the first term, \(-q(\nu_n \cdot E)\) corresponds to the contribution
of applied electric field, and the second term, \(-v_n(\nabla w_n)\) is due to the convection of energy flow. The third term, \(-\frac{2}{3n} \nabla \cdot (nv_n(w_n - \frac{m_n}{2}v_n^2))\), is a combination of the second and fourth terms in Eq. (3.10). Therefore, the relationship between these two terms can be described as the total energy, \(W\), minus the total kinetic energy, \(\frac{1}{2}mv^2\), which is the same as total potential energy. It has been assumed that \(-\frac{\nabla Q_T}{n}\) = 0, this assumption is shown to be valid when the distribution function is symmetrical about some mean value in the momentum space, which implies that the temperature is constant throughout the device [25]. The main effect of gradient of heat flow rate, \(Q_T\), in the simulation is to smooth abrupt corners and abrupt changes in average energy \(w\). The last term, \(-\frac{d}{dt}(\frac{w_0}{\tau_w})\), in Eq. (3.11) is the change in energy due to collisions, and can be represented by \(\frac{w-w_0}{\tau_w}\), where \(\tau_w\) is the energy relaxation time, and \(w_0\) is the initial average electron energy equal to \(\frac{3}{2}kT_0\), and \(T_0\) is the effective electron temperature.

### 3.2.4 Particle Conservation Equations

Particle Conservation Equations (PCE), can be derived from the first moment of BTE [29],[32]:

\[
\frac{\partial n}{\partial t} + \nabla \cdot (nv) = -R
\]  
(3.12)

Where \(R\) is the net rate of generation or recombination of electrons, positive \(R\) is recombination and negative \(R\) is generation. The left hand side of Eq. (3.12) describes the change of the total electron density that moves in and out of a given volume of space, and the net generation or recombination of electrons in that same volume of space.

PCE can also be derived by using Particle Continuity Equation and
Carrier Transport Equation. Particle Continuity Equation is derived from the first Maxwell Equation:

\[ \nabla \cdot (\nabla \cdot H) = \nabla \cdot J + \frac{\partial \rho}{\partial t} = 0 \]  

(3.13)

where \( H \) is the Magnetic field, \( \rho \) is the electron charge density, and \( J \) is the conduction current density. This equation is for both electron and hole densities. Using \( J = J_n + J_p \), and \( \rho = p - n \), Eq. (3.13) can be separated into two equations, one for electrons and one for holes, which for electrons is:

\[ \nabla \cdot J_n - q \frac{\partial n}{\partial t} = q R \]  

(3.14)

and carrier transport equation for electrons is:

\[ J_n = -qn v_n \]  

(3.15)

by replacing \( J_n \) in Eq. (3.14) with (3.15), and rearranging the terms, one can obtain Eq. (3.12).

3.2.5 Poisson’s Equation

Poisson’s Equation is the third Maxwell Equation [21], [22]:

\[ \nabla \cdot D = \rho \]  

(3.16)

replacing electric displacement vector, \( D \), with the electric field vector, \( E \), \( D = \epsilon E \), where \( \epsilon \) is the permittivity , Eq. (3.16) changes to :

\[ \nabla \cdot (\epsilon E) = \rho \]  

(3.17)
replacing $\rho$ with $q(p - n + C)$, where $C$ is the net doping concentration, and assuming that $\epsilon$ is a scalar quantity, the final form of the Poisson's Equation is:

$$\nabla E = \frac{q}{\epsilon}(p - n + C)$$  \hspace{1cm} (3.18)

### 3.3 Description of Equations in 1-Dimension

In this thesis, we are going to use a one dimensional model to solve the FDTM, due to the fact that a two dimensional model will require fourteen equations to be solved simultaneously. The computational time required for a two-dimensional system is substantial and the high sensitivity of the system to the initial guess and boundary conditions make it very difficult to obtain convergence to a solution.

Due to the complexity of the system of equations, in all of the previous numerical models using FDTM, considerable assumptions have been made in order to obtain the results, namely, one dimensional modeling, decoupling of the electron velocity, $v$, and energy, $w$, neglecting $\frac{1}{2}mv^2$, $\frac{\nabla}{n}$ $Q_T$, and $\nabla vn$ terms, and using relaxation time approximation to evaluate collision terms [18][23] — [25]. In our work we use a one-dimensional model of FDTM for electrons without using the Drift-Diffusion approximation or mobility. Instead, we use the second moment of the BTE to calculate the velocity of carriers and the third moment of the BTE to calculate the energy of carriers, which gives us more accurate results. We assume a steady-state case, therefore all the terms that are in the form $\frac{d}{dt}$ are neglected. We neglect the gradient of heat flow rate, $Q_T$, by assuming that the electron distribution function is symmetrical in momentum space. We eliminate the convective
term, $v \nabla v$, and the terms with the kinetic energy, $\frac{1}{2}mv^2$, because of their negligible effects.

3.3.1 Momentum Conservation Equation

After expanding Eq. (3.10), by using $\nabla = \frac{d}{dx}$ in a one dimension space, multiplying all the terms by mass $m$, we have:

$$\frac{m_n}{\tau_m} v_{nx} + qE_x + \frac{2}{3n} d(nw_n) dx + m_n v_{nx} \frac{dv_{nx}}{dx} - \frac{m_n}{3n} \frac{d(nv_{nx}^2)}{dx} + m_n \frac{\partial v_{nx}}{\partial t} = 0 \quad (3.19)$$

Expanding the derivatives in the third and fifth terms of Eq. (3.19) yields:

$$\frac{m_n}{\tau_m} v_{nx} + qE_x + \frac{2}{3} \frac{d(w_n)}{dx} + \frac{2}{3n} \frac{d(n)}{dx} + m_n v_{nx} \frac{dv_{nx}}{dx} - \frac{2m_n v_{nx}^2}{3} \frac{d(n)}{dx} - \frac{m_n v_{nx}^2}{3n} \frac{d(n)}{dx} + m_n \frac{\partial v_{nx}}{\partial t} = 0 \quad (3.20)$$

3.3.2 Energy Conservation Equation

Substituting the del operator $\nabla$ for $\frac{d}{dx}$, assuming $-\frac{\nabla}{n} Q_T = 0$, replacing the collision term with $\frac{w_n - w_0}{\tau_w}$, Eq. (3.11) yields:

$$q v_{nx} E_x + v_{nx} \frac{dw_n}{dx} + \frac{2}{3n} \frac{d(nv_{nx}(w_n - \frac{m_n}{2} v_{nx}^2))}{dx} + \left(\frac{w_n - w_0}{\tau_w}\right) + \frac{\partial w_n}{\partial t} = 0 \quad (3.21)$$

3.3.3 Particle Conservation Equation

After expanding Eq. (3.12), by the del operator, $\nabla = \frac{d}{dx}$, and expanding the derivative, we have:

$$\frac{\partial n}{\partial t} + v_{nx} \frac{dn}{dx} + n \frac{dv_{nx}}{dx} = -R \quad (3.22)$$
3.3.4 Poisson’s Equation

Using $\nabla = \frac{d}{dx}$, replacing the electric field, $E$, with the gradient of electrostatic potential, $\psi$, using $E = -\frac{d\psi}{dx}$, and substituting these into Eq. (3.18) yields:

$$\frac{d}{dx} \left( \frac{d\psi}{dx} \right) = \frac{q}{\epsilon}(n - p - C) \quad (3.23)$$

3.4 Simplified Equations in 1-Dimension

3.4.1 Assumptions

In this section we will discuss the assumptions used in our model. In this thesis, we study a steady-state case only, therefore all the terms that are in the form $\frac{\partial}{\partial t}$ are neglected. In order to make the system of equations simpler, we have neglected the convective term, $\nu \nabla \psi$, and the terms with the kinetic energy, $\frac{1}{2}mv^2$. Similar assumptions are usually made by other researchers [23] – [25]; one reason for neglecting $\frac{1}{2}mv^2$ is that the total energy is the sum of thermal and kinetic energy:

$$w = \frac{3}{2}kT_o + \frac{1}{2}mv^2 \quad (3.24)$$

and at room temperature the value of the kinetic energy is negligible compared to the thermal energy.

Using these assumptions we have a relatively simple set of equations for MCE and ECE.

3.4.2 Momentum Conservation Equation

$$\frac{m_n}{\tau_m} v_{nx} + qE_x + \frac{2}{3} \frac{d(w_n)}{dz} + \frac{2w_n}{3n} \frac{d(n)}{dz} = 0 \quad (3.25)$$
Moving the first term to the right hand side, multiplying all the terms by momentum relaxation time, \( \tau_m \), dividing by mass \( m \), and dropping the prefix for electrons in the \( x \) direction, \( f_{nx} = f \), Eq. (3.25) yields the following expression for the average velocity:

\[
v = -\frac{\tau_m}{m} \left[ qE + \frac{2}{3} \frac{d(w)}{dx} + \frac{2w}{3n} \frac{d(n)}{dx} \right]
\]  

(3.26)

### 3.4.3 Energy Conservation Equation

Using the same assumptions as in section 3.3.3, one can expand Eq. (3.21), to form an expression for the electron energy, \( w \), as follows:

\[
qvE + v \frac{dw}{dx} + \frac{2}{3n} \frac{d(nw)}{dx} + \left( \frac{w - w_o}{\tau_w} \right) = 0
\]  

(3.27)

after expanding second and third terms;

\[
qvE + v \frac{dw}{dx} + \frac{2}{3} \frac{d(v)}{dx} w + \frac{2}{3} v \frac{d(w)}{dx} + \frac{2}{3n} \frac{d(n)}{dx} w + \frac{w}{\tau_w} - \frac{w_o}{\tau_w} = 0
\]  

(3.28)

rewriting the equation in terms of variable \( w \) and \( \frac{dw}{dx} \), on the left side and other terms that do not depend on energy on the right side of equation we have:

\[
\left( \frac{5}{3} v \right) \frac{dw}{dx} + \left( \frac{2}{3} \frac{d(v)}{dx} + \frac{2}{3n} \frac{d(n)}{dx} + \frac{1}{\tau_w} \right) w = \left( \frac{w_o}{\tau_w} - qvE \right)
\]  

(3.29)

### 3.4.4 Particle Conservation Equation

To simplify the problem further we used an analytical solution to calculate the electron and hole concentration. This simplification was needed to
decouple the energy and velocity terms in ECE and MCE from the Poisson's Equation and PCE. Boltzmann statistics were used to relate the electron and hole concentration to the electrostatic potential, $\psi$ [22]. These assumptions are valid for nondegenerate semiconductors with parabolic band structures at thermal equilibrium, such as Si and Ge. For GaAs and AlGaAs semiconductors, which have two or more parabolic bands, the validity of these assumptions is questionable. In spite of this, because of lack of a better understanding of the physics of these devices, we have used the above assumptions. Also, the velocity of electrons is assumed to be an instantaneous function of the electric field, which is not true in practice. Due to the complexities in solving the system of equations we had to find a way to decouple the system of equations for the results to converge to a solution. The advantage of this simplified approach for calculating electron and hole concentrations is that convergence can be achieved rather easily.

In order to obtain an analytical form for the carrier concentrations, we can integrate the density of states function, $\rho_c(E)$, multiplied with the corresponding carrier distribution function, $f_n(E)$, over the energy space [21],[22].

$$n = \int_{E_c}^{\infty} \rho_c(E) f_n(E) \, dE$$  \hspace{1cm} (3.30)

where $E_c$ is the energy at the bottom of the conduction band. If we assume the distribution function, $f$ to be a Fermi-Dirac distribution :

$$f_n(E) = \frac{1}{1 + e^{\frac{E-E_F}{kT}}}$$  \hspace{1cm} (3.31)

combining Eqs. (3.30) and (3.31) yields:
The asymptotic behavior of $F_\frac{1}{2}(x)$ (Fermi-Dirac integral of the order of $\frac{1}{2}$), for large negative argument ($x << -1$), can be an analytical function \cite{22,29}:

$$F_\frac{1}{2}(x) = \frac{\sqrt{\pi}}{2} e^x$$ (3.33)

then, an analytical expression for $n$ becomes:

$$n = N_c e^{\frac{E_f-E_c}{kT}}$$ (3.34)

replacing the Fermi energies, $E_f$, with $q\psi$ yields:

$$n = N_c e^{\frac{q(\psi-(V_c+V_b))}{kT}}$$ (3.35)

$$p = N_v e^{\frac{q(\psi-(V_c+V_b))}{kT}}$$ (3.36)

for electron and hole concentrations, which is valid for nondegenerate semiconductors. Where $N_c$ and $N_v$ are the effective density of states in the conduction and valence band, respectively. $\psi$ represents the electrostatic potential, $V_c$ represents the applied voltage, and $V_b$ is the built-in voltage.

### 3.4.5 Poisson’s Equation

Using the above assumptions, Eq. (3.23) yields:

$$\frac{d}{dx} \left( \frac{d\psi}{dx} \right) = \frac{q}{\epsilon} \left( -C - N_v e^{\frac{q(\psi-(V_c+V_b))}{kT}} + N_c e^{\frac{q(\psi-(V_c+V_b))}{kT}} \right)$$ (3.37)
Chapter 4

Our Numerical Approach

The system of differential equations which is used in our numerical approach is:

\[ \frac{d}{dx} \left( \frac{d\psi}{dx} \right) = \frac{q}{\epsilon} \left( -C - N_v e^{\frac{\psi - (V_v + V_n)}{h}} + N_c e^{\frac{\psi - (V_v + V_n)}{h}} \right) \] (4.1)

\[ n = N_c e^{\frac{\psi - (V_v + V_n)}{h}} \] (4.2)

\[ p = N_v e^{\frac{\psi - (V_v + V_n)}{h}} \] (4.3)

\[ v = -\frac{\tau_n}{m} [qE + \frac{2}{3} \frac{d(w)}{dx} + \frac{2w d(n)}{3n dx}] \] (4.4)

\[ \left( \frac{5}{3} v \right) \frac{dw}{dx} + \left( \frac{2}{3} \frac{d(v)}{dx} + \frac{2}{3n} \frac{d(n)}{dx} + \frac{1}{\tau_w} \right) w = \left( \frac{w_0}{\tau_w} - qvE \right) \] (4.5)

These five equations cannot be solved analytically; the solution must be calculated by means of numerical approach for the five unknowns, \( \psi, n, p, v, \) and \( w \). Any numerical approach for the solution of such a system consists essentially of three parts: 1) defining the domain, which is the simulation
geometry of the device. 2) Approximating the differential equations in the domain by discretizing the equations, which involves only values of the continuous dependent variables at discrete points in the domain. 3) Iteratively solving the discretized equations.

4.1 Discretization Scheme

A finite-difference scheme is employed to solve the set of nonlinear first and second-order partial differential equations, where the domain is partitioned into subregions by mesh points as seen in Figure (4.1). These nonlinear differential equations have to be approximated by difference equations which involve only values of the continuous dependent variables at discrete points in the domain of the system. The nonlinearity originates from the dependencies of various coefficients $\tau_m$, $m$, and $\tau_w$ on the electric field and the coupling of the variables $n$, $p$, $E$, $v$, and $w$.

The partial differential equations are written as a set of finite-difference equations at each point of a non-uniform mesh over the entire one-dimensional simulation domain. Since much of the change in values of variables takes place in and close to space charge regions, a high concentration of mesh points are placed near the heterojunction, resulting in very small mesh spacing in that region. These finite-difference equations are derived from truncated Taylor series with the assumption that the functions involved and their derivatives are continuous and single-valued [21]. For a scalar quantity $f_i$ defined at the major mesh points $i$, the first derivative is defined as:

$$\frac{\partial f_i}{\partial x} = \frac{f_{i+1} - f_i}{x_{i+1} - x_i} \quad (4.6)$$

where $x_i$ is the distance position in the x-direction for the mesh point $i$,.
and $x_{i+1}$ is the next position for the mesh point $i$. The second derivative is defined at the major mesh points as:

$$\frac{\partial^2 f_i}{\partial x^2} = \frac{2}{(x_{i+1} - x_{i-1})} \left[ \frac{f_{i+1} - f_i}{x_{i+1} - x_i} - \frac{f_i - f_{i-1}}{x_i - x_{i-1}} \right]$$  \hspace{1cm} (4.7)

Poisson’s Equation is discretized into the form:

$$\frac{\psi_{i+1}^k - \psi_{i-1}^k}{x_{i+1} - x_{i-1}} - \frac{\psi_i^k - \psi_{i-1}^k}{x_i - x_{i-1}} = \frac{q}{\epsilon} (-C - N_v \ e^{\frac{q(v_{i+1} + v_{i-1})}{kT}} + N_c \ e^{\frac{q(v_{i}^{k-1} - (v_{i+1} + v_{i-1}))}{kT}})$$  \hspace{1cm} (4.8)

$$n_i = N_c \ e^{\frac{q(v_{i}^{k-1} - (v_{i+1} + v_{i-1}))}{kT}}$$  \hspace{1cm} (4.9)

$$p_i = N_v \ e^{\frac{q(v_{i+1} + v_{i-1})}{kT}}$$  \hspace{1cm} (4.10)

where $\psi^{k-1}$ is the value of electrostatic potential from the last iteration, and for the first iteration an initial guess is taken for charge density, $\rho$, which is all the terms in the right hand side of Eq. (4.8).

In the next step, the Momentum Conservation Equation, Eq. (4.4), is solved for the average electron velocity, $v_i$:

$$v_i^k = \frac{\tau_m}{m} \left[ qE_0^i + \frac{2}{3} \frac{d(w_{i}^{k-1})}{dx} + \frac{2w_{i}^{k-1} d(n_i^0)}{3n_i^0} \frac{d(n_i^0)}{dx} \right]$$  \hspace{1cm} (4.11)

where $E_0^i$ is the value of the electric field, and $n_i^0$ is the electron density from the solution of Poisson’s Equation, Eq. (4.8), and $w_{i}^{k-1}$ is the value from the last iteration of ECE.

Discretizing the Energy Conservation Equation and using the average electron velocity, $v_i$, of the same iteration, $k$ yields:
\[
\left(\frac{5}{3} v_i\right) \frac{w_{i+1} - w_i}{x_{i+1} - x_i} + \left(\frac{2}{3} \frac{d(v_i)}{dx} + \frac{2}{3n_i^q v_i} \frac{d(n_i^q)}{dx} + \frac{1}{\tau_w}\right) w_i = \left(\frac{w_0}{\tau_w} - q v_i E_i^p\right) \quad (4.12)
\]

rearranging the terms for \( w_i \) and \( w_{i+1} \):

\[
\frac{5v_i}{3(x_{i+1} - x_i)} w_{i+1} + \left(\frac{2}{3} \frac{d(v_i)}{dx} + \frac{2}{3n_i^q v_i} \frac{d(n_i^q)}{dx} + \frac{1}{\tau_w} - \frac{5v_i}{3(x_{i+1} - x_i)}\right) w_i = \left(\frac{w_0}{\tau_w} - q v_i E_i^p\right) \quad (4.13)
\]

From Eq. (4.13) we can define the next iteration value for the electron energy as follows:

\[
w_{i+1} = a(1)w_i + a(2) \quad (4.14)
\]

where \( a(1) \) and \( a(2) \) are described as:

\[
a(1) = -\left[\frac{2}{3} \frac{d(v_i)}{dx} + \frac{2}{3n_i^q v_i} \frac{d(n_i^q)}{dx} + \frac{1}{\tau_w} - \frac{5v_i}{3(x_{i+1} - x_i)}\right] / \left[\frac{5v_i}{3(x_{i+1} - x_i)}\right] \quad (4.15)
\]

\[
a(2) = -\left[\frac{w_0}{\tau_w} - q v_i E_i^p\right] / \left[\frac{5v_i}{3(x_{i+1} - x_i)}\right] \quad (4.16)
\]

4.2 Domain and Boundary Conditions

To solve the set of discretized equations, we need to start with a set of initial guesses for the variables as well as boundary values for the boundaries of the simulation domain. Shown in Figure (4.1) are all the boundaries that need boundary values. These boundary conditions are presented in this section.
4.2.1 Boundary Conditions for $\psi$

We assume that the ohmic contacts are purely voltage controlled [1]:

$$\psi - \psi_{bi} - \psi_c = 0$$  \hspace{1cm} (4.17)

where $\psi_c$ is the externally applied bias, and $\psi_{bi}$ is the built-in potential. Also, we assume that the ohmic contacts are ideal contact, which means that there is no voltage drop across them. With $p$-side grounded, and the applied voltage on the $n$-side at $x = L$, where $L$ is the length of the device, we have two boundary conditions:

$$\psi(0) = 0 \hspace{1cm} \psi(L) = \psi_{bi} + \psi_c$$  \hspace{1cm} (4.18)

4.2.2 Boundary Conditions for Velocity

At position $x = 0$, which is the ground, the electron velocity is very low because the electric field is almost zero. The highest electric field is inside the space charge region, and far from position $x = 0$, any velocity that electrons have is due to thermal energy. Therefore:

$$v(0) = 1 \text{ cm/sec}$$  \hspace{1cm} (4.19)

The value of $1 \text{ cm/sec}$ was chosen because we can not take the value of zero, because there are terms in Eq. (4.16) that have velocity in the denominator. Compare to the values of velocity in the space charge region which is in the order of $10^6$ to $10^7 \text{ cm/sec}$ the value of $1 \text{ cm/sec}$ is almost zero.

4.2.3 Boundary Conditions for Energy

At position $x = 0$, which is the ground, the electron velocity is almost zero, and from Eq. (3.24) we have:
\[ w(0) = \frac{3}{2} kT_0 \] (4.20)

which is the boundary condition for \( w \).

### 4.3 Initial Guess for \( n, p, \) and \( v \)

For the carrier concentrations an initial guess of \( n - p = 0 \) was assumed in order to calculate the charge density, \( \rho \) in the Poisson's Equation. Also for the initial guess of the electron velocity, \( v \), a constant value of \( 10^6 \text{cm/sec} \) has been assumed.
Chapter 5

Results

5.1 Flow Chart of the Computer Program

In this chapter, sample results of our numerical model for a device using the simplified one-dimensional Full Dynamic Transport Model are presented. A Fortran program, \( PNP.f \), was written on SUN Sparc Station 1 computer. A flow chart of the program is shown in Figures (5.1), and (5.2). In the first step of the program, device parameters are entered which specify constants such as temperature, energy relaxation time, momentum relaxation time, and effective mass of electrons and holes. An initial guess for the charge density \( \rho \) is used to calculate the electrostatic potential, \( \psi \), by using Poisson Equation (Eq. (4.8)). Then, from the calculated value of \( \psi \), the electron concentration \( n \), and hole concentration \( p \) are calculated using Eqs. (4.9) and (4.10). If convergence is not achieved, the charge density, \( \rho \) is recalculated from the new \( \psi \), \( n \), and \( p \), and then Poisson Equation is solved again. When convergence is achieved (with the current value of variables being within 1% of the previous iteration), we proceed to calculate an initial value for the electron velocity, \( v_i \), and the electron energy \( w_i \), from the previously calculated \( \psi \) and \( n \). Then, the Momentum Conservation Equation
(Eq. (4.11)), is solved to calculate the electron velocity which is used to calculate the electron energy by solving the Energy Conservation Equation (Eq. (4.14)). If convergence is not achieved, the last iteration is repeated to calculate \( v \) and \( w \). In Figure (5.3) the convergence of energy to a value of 816 meV is shown. Once the convergence is achieved (with the current value of variables being within 1 \% of the previous iteration), the data is written into a file.

In order to implement the model, a \( n - p \), AlGaAs-GaAs heterojunction device is used with parameters given in Table 1. The structure and dimensions of the device are shown in Figure (4.1), where the \( n \)-region is AlGaAs, and the \( p \)-region is GaAs with equal lengths. The voltage is applied to the \( n \)-region with the \( p \)-region grounded. The spacing of the mesh points are nonuniform with more mesh points close to the width of the space charge region to obtain higher accuracy. The initial guess for the charge density \( \rho \) along the length of the device is shown in Figure (5.4). \( \rho_i \) is calculated by using \( N_D - N_A \) and assuming that \( p - n \) is negligible. The net donor density \( N_D \) and the net acceptor density \( N_A \) in the heterojunction device are inputs to the program.

### 5.2 Distribution of the Variables

Figures (5.5) and (5.6) show the electrostatic potential, \( \psi \), throughout the device for different applied voltages (from 2.2 V to -1.2 V). As expected, the width of the space charge region decreases as the applied voltage increases. The right hand side of the \( p \) section is ground, and the voltage on the \( n \) side represents \( V_{bi} - V_c \), with \( V_{bi} \) being the built-in voltage and \( V_c \), the applied voltage. Also, there is no discontinuity of \( \psi \) at the heterojunction.
The charge density $\rho$ along the length of the device is shown in Figure (5.7); for reverse bias voltages. As can be seen, the assumption that the charge density can be approximated as a step function for an initial guess is valid. Nevertheless, for large forward voltages, $(V_c < -1V)$ the step function behaves more as a triangular function. For this reason the depletion approximation becomes invalid at high forward bias voltages, and the convergence is achieved with significantly more iteration cycles. Taking the negative derivative of $\psi$ we have electric field, $E$, which is shown in Figure (5.8). We can observe that the electric field reaches a maximum value of $7.5 \times 10^4 V/cm$ at the center of the space charge region. In our model a forward bias is represented by a negative voltage, and a reversed bias is represented by a positive voltage applied to the $n$ side of the device, because of the circuit biasing (see Figure (4.1)). Also, the width of the space charge region increases as the applied voltage decreases from a forward voltage of $-1.2V$, to a reverse voltage of $2.2V$.

Figures (5.9) and (5.10) show the electron concentration, $n$, along the length of the device for different applied voltages (from $2.2 V$ to $-1.2 V$). As expected, the width of the space charge region decreases as the applied voltage increases. There is a discontinuity in the electron density, $n$, at the heterojunction which is due to $\Delta E_c$. The left hand side of the device is $n$-type and the value of electron concentration, $n$, reaches a maximum value of $N_D$, but the right hand side is $p$-type and the value of $n$ depends on the applied voltage. Figures (5.11) and (5.12) show the hole concentration, $p$, along the length of the device for different applied voltages (from $2.2 V$ to $-1.2 V$). There is a discontinuity in the hole density, $p$, at the heterojunction due to $\Delta E_v$, which is smaller than $\Delta E_c$, and therefore causes a lower amount
Figures (5.13) and (5.14) show the electron velocity, \( v \), along the length of the device for different applied voltages (from 2.2 V to -1.2 V). Again, the effect of the applied voltage on the width of the space charge region is seen. Also, the overshoot effect for the electrons can be seen at both ends of the space charge region. These effects are related to the finite time that it takes for an electron to change its energy, and results in boosting the electron velocity to considerably higher levels than the equilibrium values normally observed. There is also a large change in the electron velocity, \( v \), at the heterojunction due to different characteristics of the two materials. Also, as the width of the space charge region decreases, the peak value of the electron velocity in the center of the space charge region decreases due to the fact that electrons do not reach the saturation velocity.

Figures (5.15) and (5.16) show the electron energy along the length of the device for different applied voltages (from 2.2 V to -1.2 V). At the center of the space charge region, the carrier velocity saturates, but the carrier energy increases due to the increase in the electric field, because the total energy of the electrons depends on potential and kinetic energy. The kinetic energy depends on the velocity of the electrons, effects similar to those seen in electron velocity. In particular, the overshoot phenomenon can be seen on the electron energy close to the edge of the space charge region. The potential energy is dependent on the electric field, \( E \), which increases at the center of the space charge region.

The I-V characteristic of Device #1 is shown in Figure (5.17). The turn-on voltage is about 1.0 V, and the current increases exponentially as the voltage increases. Also, the graph crosses at zero-zero, and at negative
voltages the current approaches a small value $I_0$ of about $-1.5A/cm$.

5.3 Doping Effects

We studied two devices with different doping levels. Figures (5.18) through (5.30) are for device #2 with increased doping level; these figures show the same variables as in Figures (5.5) through (5.17). Device #1 has a doping level of $10^{16}cm^{-3}$, and device #2 has a doping level of $5\times10^{17}cm^{-3}$ on both sides of the junction. A comparison of Figures (5.5) and (5.18), shows that the width of the space charge region decreases as the doping level increases; also, the built-in voltage increases from 1.3 V to 1.5 V. As the doping level increases, the saturation velocity is reached at higher reverse voltages. In Figure (5.14), the saturation velocity is reached at 0.4V, but in Figure (5.27) it would be reached at a much higher voltage, because electrons do not have enough time to reach saturation velocity in the short distance of the space charge region. The maximum velocity decreases from $2.5\times10^7cm/sec$ to $1.8\times10^7cm/sec$ at the edge of the space charge region in the GaAs. This is due to the fact that with increased doping levels there will be higher scattering rates which would slow down the electrons. The effect of increased doping levels on the carrier energy can also be seen in Figures (5.16) and (5.29). As the doping level increases the carrier energy increases from $270mev$ to $640mev$. This is due to the fact that as the doping increases, the electron energy becomes more dependent on the electric field than the velocity.

Figure (5.31) shows the I-V characteristics of device #1 and #2. We see that the turn-on voltage increases from 1.0 V to 1.5 V as the doping level increases from $10^{16}cm^{-3}$ to $5\times10^{17}cm^{-3}$. Figure (5.32) shows the I-V
characteristics of device #1, and #2 in an exponential representation by
offsetting the currents by \( I_0 \), which is the negative value that the current
approaches to at large negative voltages. Comparing the I-V characteristics
of device #1, and #2, in Figure (5.32), it can be seen that the I-V character­
istics are of exponential form, because they are linear in an exponential
representation, but with different slopes which causes a turn-on voltage of
1.0 V, for device #1, with a doping level of \( 10^{16} \text{cm}^{-3} \) and a turn-on voltage
of 1.4 V, for device #2 with a doping level of \( 5 \times 10^{17} \text{cm}^{-3} \).

The results obtained from our model are compared to the results pub­
lished by K. Tomizawa [18]. The electron velocity as a function of electric
field reported by Ref. [18] is shown in Figure (5.33) where the overshoot ef­
fect of electrons occurs at 2.0\( kV/cm \) in \( AlGaAs \) with an aluminum fraction of
\( x = 0.3 \). In our model, the overshoot effect of electrons also occurs at about
2.0\( kV/cm \), seen in Figures (5.8) and (5.14). Also, in Figure (5.33), after the
velocity overshoot, the velocity decreases below the final saturation velocity
where the electric field is approximately 8.0\( kV/cm \) for an \( AlGaAs \) with an
aluminum fraction of \( x = 0.3 \) which is comparable to the valley in Figure
(5.14) produced by our model which also occurs at about 8.0\( kV/cm \). This
undershoot effect is not seen in most models due to the simple model used for
mobility. Furthermore, the maximum electron velocity in \( AlGaAs(x = 0.3) \)
with a doping level of \( 1.0 \times 10^{14} \text{cm}^{-3} \) is \( 0.7 \times 10^7 \text{cm/sec} \) and the maximum
electron velocity in \( GaAs(x = 0) \) with a doping level of \( 1.0 \times 10^{14} \text{cm}^{-3} \) is
\( 2.2 \times 10^7 \text{cm/sec} \), seen in Figure (5.33). In our model, the maximum elec­
tron velocity in \( AlGaAs(x = 0.3) \) with a doping level of \( 1.0 \times 10^{16} \text{cm}^{-3} \) is
\( 0.6 \times 10^7 \text{cm/sec} \) and the maximum electron velocity in \( GaAs(x = 0) \) with a
doping level of \( 1.0 \times 10^{16} \text{cm}^{-3} \) is \( 2.5 \times 10^7 \text{cm/sec} \), seen in Figure (5.14) which
agrees with the electron velocity in Ref. [18].

The electron energy reported by K. Tomizawa is shown in Figure (5.34) where the minimum electron energy is about 0.03$\text{eV}$ and the maximum electron energy is about 0.4$\text{eV}$. In our model, comparable results are obtained with a minimum electron energy of 0.13$\text{eV}$ and a maximum electron energy of 0.54$\text{eV}$ shown in Figure (5.16). In both figures, we can observe a sharp drop in the electron energy at the heterojunction. The electron ($n$) and hole ($p$) concentration produced by Ref. [18] are shown in Figure (5.35) where a sharp decrease in the hole concentration is seen going from base to collector and a sharp decrease in the electron concentration is seen going from collector to base. The same characteristic can be observed in Figures (5.10) and (5.12) produced by our model which is due to the diffusion of holes from the $p$-side to the $n$-side and the diffusion of electrons from the $n$-side to the $p$-side.
A system of equations for the Full Dynamic Transport Model (FDTM) was presented in this thesis, which included both electron energy, \( w \), and electron velocity, \( v \), as variables in the numerical model, with the additional parameters that are normally used for device simulation, namely, electron density, \( n \), hole density, \( p \), and the electrostatic potential, \( \psi \). This model predicts the behavior of a \( p - n \) heterojunction device without using the mobility and the diffusion constant or the Drift-Diffusion Model (DDM) approximation.

The FDTM method is valid within the position dependent effective mass model, under the assumption that variation of potentials over a lattice unit cell is small compared to the crystal potential. Comparing with existing dimensions of 1 to 10 \( \mu m \) used in DDM, the limitations of FDTM require the device dimensions to be greater than approximately 0.03 \( \mu m \), because quantum transport processes become important in devices with dimension less than 0.03 \( \mu m \).

In this work a Full Dynamic Transport model consisting of Momentum Conservation Equation (MCE), Energy Conservation Equation (ECE),
Particle Conservation Equation (PCE), and the Poisson's Equation was presented. The important hot electron phenomena, such as velocity overshoot, was accounted for by including the third moment of the BTE, which provides for energy conservation. In recent works, only a simplified FDTM system of equations was applied to solve a one dimensional model [18], [23] – [25].

The results of simulation of a one-dimensional $p-n$ heterojunction were presented, which included electron concentration, electrostatic potential, electric field, carrier velocity, and electron energy distribution throughout the device for two different doping levels. The overshoot effect for the electrons has been seen at both ends of the space charge region. It has also been shown that the width of the space charge region decreases as the applied voltage increases from a forward voltage of $-1.2V$, to a reverse voltage of $2.2V$.

Also presented were the I-V characteristics of the device. The effect of variation in doping levels on I-V characteristics of the device has also been studied. It has been found that by increasing the doping from $10^{16}cm^{-3}$ to $5x10^{17}cm^{-3}$, the built-in voltage increases from $1.33V$ to $1.54V$ which is consistent with the results reported by others [1] – [4]. Maximum velocity of electrons changes from $2.5x10^7cm/sec$ to $1.8x10^7 cm/sec$, which is due to increased collision of electrons with doping impurities. This is also the reason for increased electron average energy from $270mev$ to $640mev$. The results obtained are in good agreement with the existing experimental values reported by others [1] – [6].

From our results we conclude that this model can be used as a good starting point for future work in using FDTM for modeling heterostructures. Future work should include a more accurate model for electron mass,
$m(E, w, r)$, energy relaxation time, $\tau(E, w, r)$, and momentum relaxation time, $\tau(E, w, r)$, which are dependent on the electric field, $E$, electron energy, $w$, and position in space, $r$. Also, the effects of gradient of heat flow, $Q_T$, in the Energy Conservation Equations, and convective term, $\nu \nabla \nu$, and kinetic energy term, $\frac{1}{2}mv^2$ in the Momentum Conservation Equation could be incorporated.

In the future, higher operation speeds are required for HBT’s. However, the speeds of these devices are primarily limited by extrinsic factors (i.e., junction capacitance), and not by intrinsic delays governed by fundamental transport in the base and collector space charge regions. Decreasing the device dimensions is also crucial for the implementation of HBT’s in complex integrated circuits where both speed and low power consumption are general requirements. Because of the ability of the FDTM to predict the behavior of a heterostructure device at submicron dimensions, it can be used for analyzing new structures.
Table 1: Design parameters of the simulated devices.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Device #1 AlGaAs</th>
<th>Device #1 GaAs</th>
<th>Device #2 AlGaAs</th>
<th>Device #2 GaAs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Doping (cm⁻³)</td>
<td>1.0 x 10¹⁶</td>
<td>1.0 x 10¹⁶</td>
<td>5.0 x 10¹⁷</td>
<td>5.0 x 10¹⁷</td>
</tr>
<tr>
<td>Aluminum concentration</td>
<td>0.3</td>
<td>0.0</td>
<td>0.3</td>
<td>0.0</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>300</td>
<td>300</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>Mass of Holes (Kg)</td>
<td>0.082 m₀</td>
<td>0.082 m₀</td>
<td>0.082 m₀</td>
<td>0.082 m₀</td>
</tr>
<tr>
<td>Mass of Electrons (Kg)</td>
<td>0.092 m₀</td>
<td>0.067 m₀</td>
<td>0.092 m₀</td>
<td>0.067 m₀</td>
</tr>
<tr>
<td>Device Length (µm)</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
</tr>
</tbody>
</table>
Figure 1.1: Energy-band diagram for a p-n heterojunction in equilibrium.
Figure 3.1: (a) Energy-band diagram for two isolated semiconductors in which space charge neutrality is assumed to exist in each region. (b) Energy-band diagram of an ideal p-n heterojunction at thermal equilibrium.
Figure 3.2: (a) Conduction band edge ($E_c$), and valence band edge ($E_v$) under zero bias (solid line) for an abrupt heterostructure case. (b) Conduction band edge ($E_c$), and valence band edge ($E_v$) under zero bias (solid line) for a graded heterostructure case.
Figure 4.1: (a) Simulation domain of the device. (b) The nonuniform mesh spacing used in the simulation.
Figure 5.1: First part of the computer program flow chart.
Figure 5.2: Second part of the computer program flow chart.
Figure 5.3: Convergence of the electron energy, $w$, to a value of 816 meV after 200 iterations, with an error of less than 1% in the program for a fixed point in the simulation domain.
Figure 5.4: Initial guess of the charge density, $\rho$, for an abrupt junction at zero applied voltage.
Figure 5.5: Electrostatic potential, $\psi$, for different applied voltages, in an abrupt junction for device #1.

$N_A = 1.0 \times 10^{16} \text{cm}^{-3}$
$N_D = 1.0 \times 10^{16} \text{cm}^{-3}$

Electrostatic potential, $\psi$, (V)

Distance, $X$, ($x10^{-6}$cm)
Figure 5.6: Expanded view of the electrostatic potential, $\psi$, for different applied voltages, in an abrupt junction for device #1.
Figure 5.7: Expanded view of the charge density, \( \rho \), for different applied voltages, in an abrupt junction for device #1.
Figure 5.8: Expanded view of the electric field, $E$, for different applied voltages, in an abrupt junction for device #1.
Figure 5.9: Electron density, $n$, for different applied voltages, in an abrupt junction for device #1.
Figure 5.10: Expanded view of the electron density, $n$, for different applied voltages, in an abrupt junction for device #1.
Figure 5.11: Hole density, \( p \), for different applied voltages, in an abrupt junction for device #1.
Figure 5.12: Expanded view of the hole density, $p$, for different applied voltages, in an abrupt junction for device #1.
Figure 5.13: Electron velocity, \( v \), for different applied voltages, in an abrupt junction for device #1.

\[
N_A = 1.0 \times 10^{16} \text{cm}^{-3} \\
N_D = 1.0 \times 10^{16} \text{cm}^{-3}
\]
Electron velocity, \( v \), (x 10^6 cm/sec)

\[ N_A = 1.0 \times 10^{16} \text{cm}^{-3} \]
\[ N_D = 1.0 \times 10^{16} \text{cm}^{-3} \]

Figure 5.14: Expanded view of the electron velocity, \( v \), for different applied voltages, in an abrupt junction for device #1.
Figure 5.15: Electron energy, $w$, for different applied voltages, in an abrupt junction for device #1.
Figure 5.16: Expanded view of the electron energy, $w$, for different applied voltages, in an abrupt junction for device #1.
$N_A = 1.0 \times 10^{16} \text{cm}^{-3}$

$N_D = 1.0 \times 10^{16} \text{cm}^{-3}$

Figure 5.17: I-V characteristics for device #1.
Figure 5.18: Electrostatic potential, $\psi$, for different applied voltages, in an abrupt junction for device #2. The space charge region decreases as the doping increases.

$N_A = 5.0 \times 10^{17} \text{cm}^{-3}$

$N_D = 5.0 \times 10^{17} \text{cm}^{-3}$
Figure 5.19: Expanded view of electrostatic potential, \( \psi \), for different applied voltages, in an abrupt junction for device #2, the space charge region decreases as the doping increases.
Figure 5.20: Expanded view of the charge density, $\rho$, for different applied voltages, in an abrupt junction for device #2, with a doping level of $5 \times 10^{17} \text{cm}^{-3}$.  

$N_A = 5.0 \times 10^{17} \text{cm}^{-3}$  
$N_D = 5.0 \times 10^{17} \text{cm}^{-3}$
Figure 5.21: Expanded view of the electric field, $E$, for different applied voltages, in an abrupt junction for device #2.
Figure 5.22: Electron density, $n$, for different applied voltages, in an abrupt junction for device #2.
Figure 5.23: Expanded view of the electron density, $n$, for different applied voltages, in an abrupt junction for device #2.
Figure 5.24: Hole density, $p$, for different applied voltages, in an abrupt junction for device #2.
Figure 5.25: Expanded view of the hole density, $p$, for different applied voltages, in an abrupt junction for device #2.

$N_A = 5.0 \times 10^{17} \text{cm}^{-3}$

$N_D = 5.0 \times 10^{17} \text{cm}^{-3}$
Figure 5.26: Electron velocity, $v$, for different applied voltages, in an abrupt junction for device #2.

$N_A = 5.0 \times 10^{17} \text{cm}^{-3}$
$N_D = 5.0 \times 10^{17} \text{cm}^{-3}$
Figure 5.27: Expanded view of the electron velocity, $v$, for different applied voltages, in an abrupt junction for device #2.

$N_A = 5.0 \times 10^{17} \text{ cm}^{-3}$

$N_D = 5.0 \times 10^{17} \text{ cm}^{-3}$
$N_A = 5.0 \times 10^{17} \text{cm}^{-3}$

$N_D = 5.0 \times 10^{17} \text{cm}^{-3}$

Figure 5.28: Electron energy, $w$, for different applied voltages, in an abrupt junction for device #2.
Figure 5.29: Expanded view of electron energy, $w$, for different applied voltages, in an abrupt junction for device #2.

$N_A = 5.0 \times 10^{17}\text{cm}^{-3}$

$N_D = 5.0 \times 10^{17}\text{cm}^{-3}$
Figure 5.30: I-V characteristics for device #2.

\[ N_A = 5.0 \times 10^{17} \text{cm}^{-3} \]

\[ N_D = 5.0 \times 10^{17} \text{cm}^{-3} \]
Figure 5.31: I-V characteristics for device #1 and #2.
Figure 5.32: Exponential form of I-V characteristics, shifted by +I₀, for device #1 and #2.
Figure 5.33: Velocity-Field curves of electrons calculated for GaAs and AlGaAs published by Kazutaka Tomizawa [18].
Figure 5.34: The average electron energy in Heterojunction Bipolar Transistor, published by Kazutaka Tomizawa [18].
Figure 5.35: The carrier concentration for Heterojunction Bipolar Transistor, published by Kazutaka Tomizawa [18].
Reference


