Solar cells with energy bandgaps engineered for the optimal collection of photogenerated carriers have the potential to yield higher efficiencies than conventional cells. Much of the numerical simulation of bandgap engineered solar cells has been concentrated on modeling the popular AlₓGa₁₋ₓAs/GaAs material system.

In this work, the development and the results of the application of a numerical analysis program for the simulation of variable composition AlₓGa₁₋ₓAs/GaAs and (AlₓGa₁₋ₓ)₀.₄₇In₀.₅₃As/InP bandgap engineered solar cells is presented. A review of the numerical simulation of variable composition devices, including derivations of the discretized forms of the basic semiconductor equations applicable to the modeling of variable composition devices, and a discussion of material parameter modeling are also provided.

Simulation results, the first presented for (AlₓGa₁₋ₓ)₀.₄₇In₀.₅₃As/InP solar cells, suggest that conversion efficiencies approaching 18 percent for p-n
(AlGa)InAs/InP cells with heavily doped emitters are possible, but that efficiencies for n-p cells may be limited by a large valence band spike barrier. Results for AlGaAs/GaAs cells are similar to those reported elsewhere.

It was found that when modeling variable composition devices, the carrier saturation velocity must be properly accounted for in regions where varying material composition introduces large effective fields. Neglecting saturation velocity modeling in graded emitter regions was found to yield excessively high efficiencies, and the wrong trend in efficiency with emitter width.
Numerical Simulation of
$\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ and $(\text{Al}_x\text{Ga}_{1-x})_{0.47}\text{In}_{0.53}\text{As}/\text{InP}
$ Bandgap Engineered Solar Cells

by

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In addition, I would like to express my gratitude to Louie McCrady, not only for his moral support, but for the innumerable consultations I received from him in the area of personal computer programming. Special thanks, for the most basic reasons, go out to my parents. But foremost, I would like to thank Caroline Koff, my wife, for her patience and support, and to whom this thesis is dedicated.
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$\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ and $(\text{Al}_x\text{Ga}_{1-x})_{0.47}\text{In}_{0.53}\text{As}/\text{InP}$

Bandgap Engineered Solar Cells

Chapter One

INTRODUCTION

The attainment of highly efficient solar cells is the driving force behind the compound semiconductor solar cell effort. It has long been known that a larger bandgap than that of silicon is required for the design of optimally efficient solar cells under solar irradiation [1]. Many compound semiconductors can provide not only larger bandgaps than silicon, but also greater carrier mobilities. One such compound semiconductor is GaAs.

The efficiencies of early GaAs solar cells were suppressed by excessive surface recombination [2]. It was found that by using a wider gap AlGaAs "window" layer as the top layer of the solar cell, more optical generation would occur around the collection junction, contributing to greater efficiency, and less would occur near the surface [3]. An extension of this idea is to use doping and composition gradients to produce electric and effective electric fields to draw generated carriers toward the collection junction and thereby increase collection efficiency [4]. This progression is shown in Fig. 1-1.
Fig. 1-1. Progression of solar cell design. Minority carrier spacing is proportional to the optical generation rate. (a) Uniform composition. (b) Non-uniform composition (heterojunction) without composition grading. (c) Nonuniform composition with composition grading.

In accordance with their energy band diagram representations, solar cells
of the type shown in Fig. 1-1c are referred to as bandgap engineered solar cells. Accurate modeling of bandgap engineered devices cannot be accomplished analytically, due to the introduction of many position dependent material parameters. However, these position dependent parameters can be accounted for by numerical simulation.

Numerical simulation of bandgap engineered devices is no longer a purely academic exercise. Recent advances in fabrication technology, such as molecular beam epitaxy (MBE) and metalorganic chemical vapor deposition (MOCVD), have made the bandgap engineering of semiconductor devices a reality, and provided an extra degree of freedom for the device designer. Numerical modeling, then, becomes a valuable tool for the investigation of device behavior and the optimization of device design.

In this thesis the performance of bandgap engineered Al$_x$Ga$_{1-x}$As/GaAs and (Al$_x$Ga$_{1-x}$)$_{0.47}$In$_{0.53}$As/InP solar cells, based on one-dimensional numerical simulation, is investigated. The importance of the Al$_x$Ga$_{1-x}$As material system in solar cell design is derived from its near optimal bandgap of 1.424 eV, and near perfect lattice match for all aluminum concentrations, and is verified empirically with highly efficient cells having been measured [5][6]. One-dimensional numerical simulations of Al$_x$Ga$_{1-x}$As/GaAs solar cells based on Boltzmann and Fermi-Dirac statistics have been reported in [7][8] and [9], respectively. A two-dimensional numerical simulation of Al$_x$Ga$_{1-x}$As/GaAs solar cells with constant composition layers has also been reported [10].

Properties of the (Al$_x$Ga$_{1-x}$)$_{0.47}$In$_{0.53}$As/InP material system suggest that it is also a likely candidate for solar cell design. InP has a wide bandgap of 1.34
eV and high electron mobility. \((\text{Al}_x\text{Ga}_{1-x})_{0.47}\text{In}_{0.53}\text{As}\) is lattice matched to InP for all compositions \(x\), and has a large bandgap swing (giving the bandgap engineer something to work with). Even so, at least to the author's knowledge, \((\text{Al}_x\text{Ga}_{1-x})_{0.47}\text{In}_{0.53}\text{As}/\text{InP}\) solar cells have neither been fabricated nor simulated. Investigating the potential of this material system for solar cell design, as compared to that of \(\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}\), is the goal of this thesis.

The \(\text{AlGaAs}/\text{GaAs}\) and \((\text{AlGa})\text{InAs}/\text{InP}\) solar cell simulations discussed herein were performed with a solar cell simulation program developed and written by the author. The remainder of this thesis is summarized as follows.

A general discussion of the numerical simulation of variable composition semiconductor devices, based on Boltzmann statistics, is presented in Chapter Two; including the finite difference discretization of the nonuniform semiconductor device equations and their boundary conditions, and the matrix representation for simultaneous and sequential solution methods. In Chapter Three, specifics of the solar cell simulation program, as related to the general numerical simulation issues of Chapter Two, are given. Material parameter modeling, and program architecture and interface are also discussed. In Chapter Four, one- and two-dimensional simulation results are presented and discussed. Conclusions and recommendations for further work are given in Chapter Five. Finally, for purposes of reference, appendices are given which detail certain derivations.
Chapter Two

NUMERICAL SIMULATION OF SEMICONDUCTOR DEVICES

The numerical analysis of a semiconductor device involves the application of numerical techniques to the solution of the semiconductor equations which describe the device. This can be accomplished through the following four basic steps:

1. Physical modeling: The determination of differential equations and boundary conditions that accurately represent the physics of the device over the simulation geometry, and the determination of models, either theoretical or empirical, for any material parameters present in the device equations.

2. Partitioning of the domain: The domain, which represents the simulation geometry, is partitioned into subdomains; the geometry of the subdomains, rectangular or triangular, is dependent on the method of discretization, finite difference or finite element, respectively. The selection of discretization method may be influenced by overall device geometry. The finer the partitioning, the better the resulting approximation to the exact solution.

3. Discretization of equations: Once a discretization method has been chosen and the domain partitioned, the differential equations are approximated in each subdomain by algebraic difference equations. The unknowns of the resulting algebraic equations are approximations to the values of the continuous dependent variables of the differential equations at discrete points in the subdomains. Since the partitioning is fine and the
differential equations are, in general, nonlinear, this process yields a large system of nonlinear algebraic equations.

4. Solution of nonlinear algebraic system: A numerical solution technique is applied. In general, only iterative methods are applicable to the solution of a system of nonlinear algebraic equations. Of the iterative methods, Newton's method (where each iteration requires the linearization and solution of the resulting linear system) is the most popular [11].

Each of these four steps are investigated in this chapter. How numerical modeling has been applied to solar cells is also reviewed.

2.1 Physical Modeling

Physical modeling of a semiconductor device starts with an investigation of the physics that control the device behavior. This allows the derivation of basic equations, including boundary conditions, that describe (model) the physics of the device, or allows the association of the device with a proper set of previously derived equations.

2.1.1 Semiconductor Device Equations

Homogeneous Materials

The standard semiconductor equations for devices made of a homogeneous material can be found in most texts on semiconductor devices [12], and are given as follows:
Current Density

\[ J_p = -qD_p \nabla p - q\mu_p p \nabla \psi \] \hspace{1cm} (2-1)

\[ J_n = qD_n \nabla n - q\mu_n n \nabla \psi \] \hspace{1cm} (2-2)

Current Continuity

\[ \frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot J_p + G_p - U_p \] \hspace{1cm} (2-3)

\[ \frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot J_n + G_n - U_n \] \hspace{1cm} (2-4)

Poisson

\[ \nabla^2 \psi = \frac{q}{\varepsilon} \left( N_d - N_a + p - n \right) \] \hspace{1cm} (2-5)

These equations, along with their boundary conditions, are adequate to model and account for the following important aspects of devices made of a homogeneous material:

* Drift and diffusion currents.
* Position-dependent doping.
* Doping-dependent mobility.
* Bulk and surface carrier generation and recombination.
Heterogeneous Materials

When a device has a spatially varying composition, several other position-dependent parameters must be taken into account:
* Position-dependent bandgap.
* Position-dependent electron affinity.
* Position-dependent mobility, dielectric constant, and absorption coefficient.

The device equations that model these additional factors are derived from the same basic principles as (2-1) to (2-5), only with fewer simplifying assumptions being made. The general expressions for current density are

\[ J_p = \mu_p p \nabla E_{Fp} \]  \hspace{1cm} (2-6)

\[ J_n = \mu_n n \nabla E_{Fn} \]  \hspace{1cm} (2-7)

Expressions for the quasi-Fermi levels are derived in Appendix A. Subtitution yields

\[ J_p = \mu_p p \left[ -q \nabla \psi - \nabla \chi_c - \nabla E_g - \frac{kT}{p} \nabla p + \frac{kT}{N_v} \nabla N_v \right] \]  \hspace{1cm} (2-8)

\[ J_n = \mu_n n \left[ -q \nabla \psi - \nabla \chi_c + \frac{kT}{n} \nabla n - \frac{kT}{N_c} \nabla N_c \right] \]  \hspace{1cm} (2-9)
Equations (2-8) and (2-9) are then used in the standard current continuity equations of Eqs. (2-3) and (2-4). It should be noted that these expressions are based on Boltzmann statistics. A derivation of transport equations based on Fermi-Dirac statistics can be found in [13][14][15][16]. In Appendix B, a general Poisson equation is derived from Gauss's law:

\[ \nabla^2 \psi = -\frac{q}{\varepsilon} (p - n + C) - \frac{1}{\varepsilon} \nabla \psi \cdot \nabla \varepsilon \]  

(2-10)

where \( C = N_{d^+} - N_{a^-} \).

Modeling of carrier recombination and generation terms in the continuity equations should include the effects of Shockley-Read-Hall (SRH), radiative, and Auger generation/recombination, and impact ionization. A discussion of how to model these processes is given in [11]. Usually, only those processes expected to dominate are included in the modeling. When optical generation is important, such as in solar cells, the contributing position-dependent generation rate for heterogeneous materials is modeled by [7]

\[ g(y) = \sum_{\lambda} T(\lambda) N(\lambda) \alpha(C(y), \lambda) \exp \left( -\int_0^y \alpha(C(y), \lambda) \, dy \right) \]  

(2-10i)

where \( T(\lambda) \) is the antireflection layer transmission coefficient, \( N(\lambda) \) is the incident photon density per wavelength interval, \( C(y) \) is the composition profile, and \( \alpha(C(y), \lambda) \) is the absorption coefficient.
2.1.2 Boundary Conditions

Three basic types of boundaries are encountered in semiconductor device simulation: Boundaries between semiconductor and contact metal, boundaries between semiconductor and insulator, and "artificial" boundaries between semiconductor and semiconductor along the edge of a desired simulation domain. The boundary conditions that apply to these boundaries are described below.

Semiconductor-Metal Boundaries:

Metal contacts are either ohmic or non-ohmic. This discussion only pertains to the ohmic contact. A discussion of the non-ohmic Schottky contact can be found in [11].

The carrier concentrations at ohmic contact boundaries are identically determined by assuming thermal equilibrium and space-charge neutrality. These two conditions are modeled by the following two equations, respectively:

\[ np - n_i^2 = 0 \]  \hspace{1cm} (2-11)

\[ p - n + C = 0 \]  \hspace{1cm} (2-12)

Equations (2-11) and (2-12) are solved simultaneously for the majority carrier concentration at a boundary. The thermal equilibrium condition provides the minority concentration. Depending on the doping type, the following Dirichlet boundary conditions result [11]:
For contacts to n-type material

\[ n = \frac{C}{2} + \sqrt{\left(\frac{C}{2}\right)^2 + n_i^2} \]  \hspace{1cm} (2-13)

\[ p = \frac{n_i^2}{n} \]  \hspace{1cm} (2-14)

For contacts to p-type material

\[ p = -\frac{C}{2} + \sqrt{\left(\frac{C}{2}\right)^2 + n_i^2} \]  \hspace{1cm} (2-15)

\[ n = \frac{n_i^2}{p} \]  \hspace{1cm} (2-16)

The Dirichlet boundary condition for the potential at an ohmic contact is determined by requiring that the potential difference between any two contacts is equal to the sum of any built-in potential and the applied bias between the two points, with the potential values adjusted to some reference potential. A method for determining the built-in potential is given in Appendix A.

Semiconductor-Insulator Boundaries:

Whereas the ohmic contact provided Dirichlet boundary conditions, the
semiconductor-insulator interface is modeled by assuming that the basic semiconductor equations hold, but are subject to certain Neumann boundary conditions (in the sense that they include derivatives of the unknown variables) [11]. The continuity equations are subject to the condition that the current component perpendicular to the boundary is equal to the surface recombination current at the boundary.

\[
J_n \cdot n = - qR_s \tag{2-17}
\]

\[
J_p \cdot n = qR_s \tag{2-18}
\]

where [11]

\[
R_s = \frac{n p - n_1^2}{n + n_1 + p + p_1} \frac{1}{s_p + s_n} \tag{2-19}
\]

Equation (2-19) is simply the Shockley-Read-Hall recombination equation with bulk capture rates replaced by surface recombination velocities.

Poisson's equation at the boundary is subject to Gauss's law in differential form:

\[
\varepsilon_{sem} \frac{\partial \psi_{sem}}{\partial n} - \varepsilon_{ins} \frac{\partial \psi_{ins}}{\partial n} = Q_{int} \tag{2-20}
\]

Artificial Boundaries:

If it can be physically justified, artificial boundaries can conveniently be modeled by assuming zero spatial variation across and perpendicular to the
boundary in the values of the basic unknown variables.

\[ \frac{\partial p}{\partial n} = 0, \quad \frac{\partial n}{\partial n} = 0, \quad \frac{\partial \psi}{\partial n} = 0. \]  

(2-21 abc)

2.1.3 Parameter Modeling

Accurate numerical semiconductor device simulation not only depends on the use of proper device equations and boundary conditions, but on the accurate modeling of material parameters. These parameters include

* Doping and composition-dependent mobility.
* Doping and composition-dependent bandgap.
* Composition-dependent electron affinity.
* Composition-dependent dielectric constant.
* Composition-dependent absorption coefficient.

These parameters are best modeled by analytical fits to, or interpolation of, experimental data. When experimental data is not available, theoretical expressions can be used.
2.2 Discretization of the Semiconductor Equations

The way the domain is partitioned, and the type of algebraic approximations used to approximate the differential equations in each subdomain, depend on the method of discretization; namely, the finite difference method, or the finite element method. Since it has been found that the finite difference method works well for the semiconductor equations (the majority of the literature in this field is based on this method), and since this method is exclusively employed herein, only the finite difference method is discussed. Discussions of the finite element method can be found in [17][18].

2.2.1 Partitioning the Simulation Domain (Mesh Design)

For a two-dimensional analysis, the simulation geometry is partitioned into rectangles by a mesh of horizontal and vertical lines. The intersections of these lines give points where approximate solutions to the differential equations are found. A generalized point on the grid is represented by a pair of indices \((i, j)\), as shown in Fig. 2-1. As seen, the mesh lines are closer together near interfaces and contact edges. These are areas where the unknown variables tend to vary greatly and finer partitioning is required for accurate approximation.
2.2.2 Finite Difference Approximations of the Semiconductor Device Equations

In order for the semiconductor equations to be discretized, they must be written in a form specific to the coordinates used to represent the device geometry. In two dimensional cartesian coordinates the basic semiconductor equations become
Current Continuity

\[
- \frac{1}{q} \left( \frac{\partial J_{px}}{\partial x} + \frac{\partial J_{py}}{\partial y} \right) - R + G = 0 \quad (2-22)
\]

\[
\frac{1}{q} \left( \frac{\partial J_{nx}}{\partial x} + \frac{\partial J_{ny}}{\partial y} \right) - R + G = 0 \quad (2-23)
\]

Poisson

\[
\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\frac{q}{\varepsilon} (p - n + C) - \frac{1}{\varepsilon} \left( \frac{\partial \psi}{\partial x} \frac{\partial \varepsilon}{\partial x} + \frac{\partial \psi}{\partial y} \frac{\partial \varepsilon}{\partial y} \right) \quad (2-24)
\]

In the finite difference method each partial differential equation is approximated by a system of algebraic difference equations, where each difference equation is obtained by substituting difference approximations for the differential terms in the differential equation. Usually, a finite difference approximation to a derivative of a variable with respect to a coordinate axis is based on the differences in the value of the variable at the mesh point and at its two opposing neighbors along the same coordinate direction.

The difference approximations for the first and second derivatives have the following forms:

\[
\frac{\partial u}{\partial x} \bigg|_{i,j} \approx \frac{u_{i+1/2,j} - u_{i-1/2,j}}{h_i + h_{i-1}} \approx \frac{u_{i+1,j} - u_{i-1,j}}{h_i + h_{i-1}} \quad (2-25)
\]
The basic semiconductor equations are discretized using these approximations:

**Discretized Current Continuity**

\[
\frac{1}{q} \frac{J_{px,i-1/2,j} - J_{px,i+1/2,j}}{h_i + h_{i-1}/2} + \frac{1}{q} \frac{J_{py,i,j-1/2} - J_{py,i,j+1/2}}{k_j + k_{j-1}/2} - R_{i,j} + G_{i,j} = 0 \tag{2-27}
\]

\[
\frac{1}{q} \frac{J_{nx,i+1/2,j} - J_{nx,i-1/2,j}}{h_i + h_{i-1}/2} + \frac{1}{q} \frac{J_{ny,i,j+1/2} - J_{ny,i,j-1/2}}{k_j + k_{j-1}/2} - R_{i,j} + G_{i,j} = 0 \tag{2-28}
\]

**Discretized Poisson**

\[
\frac{\psi_{i+1,j} - \psi_{i,j}}{h_i} - \frac{\psi_{i,j} - \psi_{i-1,j}}{h_{i-1}} + \frac{\psi_{i,j+1} - \psi_{i,j}}{k_j} - \frac{\psi_{i,j} - \psi_{i,j-1}}{k_{j-1}} + \frac{1}{\epsilon} \left[ \frac{\psi_{i+1,j} - \psi_{i-1,j}}{h_{i-1} + h_i} - \frac{\psi_{i,j+1} - \psi_{i,j-1}}{k_{j-1} + k_j} \right] \]

\[
= 0 \tag{2-29}
\]
The discretization of the current density equations can also be accomplished by direct substitution of difference approximations. However, in the case of uniform composition materials it has been found that this direct substitution leads to a numerical instability if the potential between any two mesh points is greater than $2kT/q$ [19]. Scharfetter and Gummel have pointed out [20] that using the current density equations in their integral form eliminates this problem. As a similar situation is expected for the current density equations relating to nonuniform materials, it is recommended that these equations also be employed in their integral form. The discretized integral-form of the current density equations are derived in Appendix C for the one-dimensional problem, and are easily extended to the two-dimensional problem as follows:

\begin{align}
J_{p_{x(i+1/2,j)}} &= \frac{qD_{p_{x(i+1/2,j)}}}{h_i} \left[ B\left(\text{arg}_{p_{x(i,j)}}\right) p_{i,j} - B\left(\text{arg}_{p_{x(i,j)}}\right) p_{i+1,j} \right], \quad (2-30) \\
J_{p_{y(i+1/2,j)}} &= \frac{qD_{p_{y(i+1/2,j)}}}{k_j} \left[ B\left(\text{arg}_{p_{y(i,j)}}\right) p_{i,j} - B\left(\text{arg}_{p_{y(i,j)}}\right) p_{i,j+1} \right], \quad (2-31) \\
J_{n_{x(i+1/2,j)}} &= -\frac{qD_{n_{x(i+1/2,j)}}}{h_i} \left[ B\left(\text{arg}_{n_{x(i,j)}}\right) n_{i,j} - B\left(\text{arg}_{n_{x(i,j)}}\right) n_{i+1,j} \right], \quad (2-32)
\end{align}
\[ J_{ny_{i+\frac{1}{2}}} = -\frac{qD_{n_{i+\frac{1}{2}}}}{k_j} \left[ B(-\arg_{ny_{i,j}})n_{i,j} - B(\arg_{ny_{i,j}})n_{i,j+1} \right], \quad (2-33) \]

where

\[ \arg_{px_{i,j}} = \frac{\psi_{i,j+1} - \psi_{i,j} + \chi_{c_{i,j+1}} - \chi_{c_{i,j}} + E_{g_{i,j+1}} - E_{g_{i,j}}}{V_\tau} \left( N_{v_{i+1,j}} - N_{v_{i,j}} \right), \quad (2-34) \]

\[ \arg_{py_{i,j}} = \frac{\psi_{i,j+1} - \psi_{i,j} + \chi_{c_{i,j+1}} - \chi_{c_{i,j}} + E_{g_{i,j+1}} - E_{g_{i,j}}}{V_\tau} \left( N_{v_{i+1,j}} - N_{v_{i,j}} \right), \quad (2-35) \]

\[ \arg_{nx_{i,j}} = \frac{\psi_{i+1,j} - \psi_{i,j} + \chi_{c_{i,j+1}} - \chi_{c_{i,j}}}{V_\tau} \left( N_{c_{i+1,j}} - N_{c_{i,j}} \right), \quad (2-36) \]

\[ \arg_{ny_{i,j}} = \frac{\psi_{i,j+1} - \psi_{i,j} + \chi_{c_{i,j+1}} - \chi_{c_{i,j}}}{V_\tau} \left( N_{c_{i+1,j}} - N_{c_{i,j}} \right), \quad (2-37) \]

Substituting the discretized current density equations (2-30) to (2-33) into the discretized continuity equations (2-27) and (2-28) yields discretized continuity equations suitable for computer simulation in terms of the three basic unknown variables:

**Hole Current Continuity**
Electron Current Continuity

\[
\frac{D_{p_{i,j}}}{h_{i-1} + h_{i-1} \frac{2}{2}} \left[ B(\arg p x_{i-1,j} p_{i-1,j} - B(-\arg p x_{i-1,j} p_{i,j}) \right]
\]

\[
- \frac{D_{p_{i,j}}}{h_{i} + h_{i-1} \frac{2}{2}} \left[ B(\arg p x_{i,j} p_{i,j} - B(-\arg p x_{i,j} p_{i+1,j}) \right]
\]

\[
\frac{D_{p_{i,j-1/2}}}{k_{j-1} \frac{2}{2}} \left[ B(\arg p y_{i,j-1} p_{i,j-1} - B(-\arg p y_{i,j-1} p_{i,j}) \right]
\]

\[
- \frac{D_{p_{i,j+1/2}}}{k_{j} + k_{j-1} \frac{2}{2}} \left[ B(\arg p y_{i,j} p_{i,j} - B(-\arg p y_{i,j} p_{i,j+1}) \right]
\]

- \( R_{i,j} + G_{i,j} = 0 \) (2-38)
2.2.3 Finite Difference Approximations of Boundary Conditions

When values of the variables can be predetermined on a boundary, there is no need to solve the semiconductor equations on that boundary. Therefore, at Dirichlet boundaries, no discretization is required. However, Neumann boundaries require discretization of the semiconductor equations, and this requires special attention.

When the semiconductor equations are discretized at boundaries using approximations to derivatives like those given in (2-25), the resulting equations contain variables at undefined mesh points outside of the simulation domain. The discretized Neumann boundary conditions at these boundaries also yield equations that relate to the same undefined mesh points. The discretized semiconductor equations and boundary conditions can then be combined to eliminate the undefined variables. A convenient way of discretizing the Neumann boundary conditions [11] is to assume that the undefined meshpoints are equidistant images of the first interior points, and to use the simple interpolation formula

\[ u_{\text{boundary}} = \frac{u_{\text{boundary} + 1} + u_{\text{boundary} - 1}}{2} . \]  

(2-40)
2.3 The Solution of the Semiconductor Equations (Newton's Method)

The solution of the semiconductor equations by Newton's method [21] is discussed in this section. First, a brief summary of Newton's method is given. This is followed by a more detailed look into the important aspects of the method.

The solution of the semiconductor equations, as arranged in (2-27) to (2-29), is a root-finding problem. Due to its simplicity and speed of convergence, Newton's method is one of the most widely used methods of solving equations by finding their roots. Best described graphically for a single equation in one variable, Fig. 2-2, Newton's method iteratively extrapolates the local derivative (first evaluated at some trial value) to find the next estimate of the root.
Fig. 2-2. Graphically, Newton's method is root-finding by the repeated extrapolation of the local derivative.

The application of Newton's method to the large system of equations that result from the discretization of the semiconductor equations begins with the determination of approximate trial values to the roots of these equations. Since fewer iterations are required to reach the final solution when better trial values are chosen, this step is quite important.

Once trial values have been determined, the Newton iteration process can begin. Each iteration consists of linearizing the nonlinear equations about the trial values, and solving the resulting linear system of equations for corrections to the trial values.

At the end of each iteration, convergence is tested by comparing the magnitude of the correction values to some predetermined "epsilon." If the correction values are too large, the solution is considered not to have converged, and another Newton iteration is performed, each iteration using
the corrected trial values from the previous iteration.

Since Newton's method requires the repeated solution of a large system of linear algebraic equations to obtain correction terms, it is most important that an efficient solution method be used for this task. For relatively small systems, elimination methods can be used. For large systems iterative methods are used. The method used in this work is described in the next chapter on the implementation of the simulation program. Although no attempt is made herein to summarize the vast field associated with the solution of linear systems, the other aspects of Newton's method mentioned above are now described in greater detail.

2.3.1 Trial Values

Essentially, the whole numerical solution process boils down to finding better and better trial values. Trial values determined before entering a Newton iteration process are very important. The closer these trial values are to the actual solution, the fewer Newton iterations are required for convergence; in fact, since Newton's method is not globally convergent, poor trial values may cause divergence.

Trial values for two-dimensional simulations are usually based on the results from one-dimensional simulations in the different boundary regions. Trial values for one-dimensional simulations are based on simplified analytical solutions. When numerical solutions are required at many bias points, the solutions for \( n \) and \( p \) at one bias point can be used as trial values for the next bias point, with the trial potentials determined by interpolation [19].
2.3.2 Linearization and Matrix Representation

The mathematical formulation that allows for the calculation of incremental correction values to the latest approximated values is derived from linearization. In general, the linear approximation of a function in the neighborhood of a point is the Taylor series expansion of the function about the point, with the neglect of nonlinear terms. For a single variable function $F(u)$, linearization about some value $u^k$, where $k$ is the iteration number, yields

$$F(u^{k+1}) \approx F(u^k) + \left[ \frac{\partial F(u)}{\partial u} \bigg|_{u_0}^{u^k} \right] \cdot \delta u^k$$

(2-41)

Since Newton's method is a root-finding method, it is desired that the incremental correction value $\delta u^k$ be calculated such that $F(u^{k+1}) = 0$. Or

$$\left[ \frac{\partial F(u)}{\partial u} \bigg|_{u_0}^{u^k} \right] \cdot \delta u^k = -F(u^k)$$

(2-42)

Equation (2-42) is the basis of Newton's method, and is easily verified graphically with reference with Fig. 2-2. Fully analogous to (2-42), Newton's formulation for multivariable functions becomes:

$$\sum_{i=1}^{N} \left[ \frac{\partial F(u_1, u_2, ..., u_N)}{\partial u_i} \bigg|_{u_1, u_2, ..., u_N}^{u_1^k, u_2^k, ..., u_N^k} \right] \cdot \delta u_i^k = -F(u_1^k, u_2^k, ..., u_N^k)$$

(2-43)
The application of (2-43) to the discretized equations at a generalized mesh point produces equations of the following form:

\[ A_{i,j} \Delta_{i-1,j} + B_{i,j} \Delta_{i,j} + C_{i,j} \Delta_{i+1,j} + D_{i,j} \Delta_{i,j-1} + E_{i,j} \Delta_{i,j+1} = F_{i,j} \quad (2-44) \]

The matrix-vector equations that describe the entire set of mesh points have the form shown in Fig. 2-3.

\[
\begin{bmatrix}
B_{1,1} C_{1,1} & E_{1,1} \\
A_{2,1} B_{2,1} C_{2,1} & E_{2,1} \\
A_{3,1} B_{3,1} C_{3,1} & E_{3,1} \\
A_{4,1} B_{4,1} & E_{4,1} \\
D_{1,2} & B_{1,2} C_{1,2} & E_{1,2} \\
D_{2,2} & A_{2,2} B_{2,2} C_{2,2} & E_{2,2} \\
D_{3,2} & A_{3,2} B_{3,2} C_{3,2} & E_{3,2} \\
D_{4,2} & A_{4,2} B_{4,2} & E_{4,2} \\
D_{1,3} & B_{1,3} C_{1,3} \\
D_{2,3} & A_{2,3} B_{2,3} C_{2,3} \\
D_{3,3} & A_{3,3} B_{3,3} C_{3,3} \\
D_{4,3} & A_{4,3} B_{4,3} \\
\end{bmatrix}
\begin{bmatrix}
\Delta_{1,1} \\
\Delta_{2,1} \\
\Delta_{3,1} \\
\Delta_{4,1} \\
\Delta_{1,2} \\
\Delta_{2,2} \\
\Delta_{3,2} \\
\Delta_{4,2} \\
\Delta_{1,3} \\
\Delta_{2,3} \\
\Delta_{3,3} \\
\Delta_{4,3} \\
\end{bmatrix}
= \begin{bmatrix}
F_{1,1} \\
F_{2,1} \\
F_{3,1} \\
F_{4,1} \\
F_{1,2} \\
F_{2,2} \\
F_{3,2} \\
F_{4,2} \\
F_{1,3} \\
F_{2,3} \\
F_{3,3} \\
F_{4,3} \\
\end{bmatrix}
\]

Fig. 2-3. Matrix-vector system equation for a four row, three column mesh.

Two popular iterative methods for the solution of large linear systems of the form shown in Fig. 2-3 are the block SOR method [19][22] and Stone's strongly implicit method [23].
Convergence Test

Once the linear system equation has been solved, and incremental correction terms are known, a convergence test is performed. A criterion for convergence is that the relative error in the approximated values of all variables is less than some predetermined value. For numerical solutions, the relative error,

\[ \text{Relative error} = \frac{\text{True value} - \text{Approximate value}}{\text{True value}}, \quad (2-45) \]

can be approximated by

\[ \text{Relative error in } u = \frac{u^{k+1} - u^k}{u^{k+1}} = \frac{\delta u^k}{u^{k+1}}. \quad (2-46) \]

2.3.3 Application of Newton's Method

The two usual ways in which Newton's method is applied to the solution of the semiconductor equations are given below.

Sequential Method (Gummel's Algorithm)

A method that has proved very useful for the solution of the semiconductor equations is Gummel's method [24]. In Gummel's method, the sequential solution of Poisson's equation and the two continuity equations is iterated until the unknown variables are solved self-consistently,
to a desired degree of accuracy, through all three equations. A flow chart of Gummel's method is shown in Fig. 2-4.

In order to solve the semiconductor equations sequentially, each equation can only be considered to depend on a single variable during its solution. The other two variables are considered as known, and are replaced by their most recently approximated values. When these equations are discretized using five point discretization, three nonlinear algebraic equations result for each point of the mesh; each with the same five unknowns. If we let \( f_1 \), \( f_2 \), and \( f_3 \) represent Poisson's equation, hole continuity, and electron continuity, respectively, linearization yields equations of the form of (2-44) with the following coefficient definitions:

**Poisson**

\[
A_{i,j} = \frac{\partial f_1}{\partial \psi_{i-1,j}}, \quad B_{i,j} = \frac{\partial f_1}{\partial \psi_{i,j}}, \quad C_{i,j} = \frac{\partial f_1}{\partial \psi_{i+1,j}}, \quad D_{i,j} = \frac{\partial f_1}{\partial \psi_{i,j-1}}
\]

\[
E_{i,j} = \frac{\partial f_1}{\partial \psi_{i,j+1}}, \quad F_{i,j} = -f_1, \quad \Delta_{i,j} = \delta \psi_{i,j} \tag{2-47abcdefg}
\]

**Hole Continuity**

\[
A_{i,j} = \frac{\partial f_2}{\partial p_{i-1,j}}, \quad B_{i,j} = \frac{\partial f_2}{\partial p_{i,j}}, \quad C_{i,j} = \frac{\partial f_2}{\partial p_{i+1,j}}, \quad D_{i,j} = \frac{\partial f_2}{\partial p_{i,j-1}}
\]
\[ E_{i,j} = \frac{\partial f_2}{\partial p_{i,j+1}}, \quad F_{i,j} = -f_2, \quad \Delta_{i,j} = \delta p_{i,j} \tag{2-48} \]

**Electron Continuity**

\[ A_{i,j} = \frac{\partial f_3}{\partial n_{i-1,j}}, \quad B_{i,j} = \frac{\partial f_3}{\partial n_{i,j}}, \quad C_{i,j} = \frac{\partial f_3}{\partial n_{i+1,j}}, \quad D_{i,j} = \frac{\partial f_3}{\partial n_{i,j-1}} \]

\[ E_{i,j} = \frac{\partial f_3}{\partial n_{i,j+1}}, \quad F_{i,j} = -f_3, \quad \Delta_{i,j} = \delta n_{i,j} \tag{2-49} \]

In Gummel's method, the linear Poisson equation (2-10) is replaced by a nonlinear Poisson equation. This equation, as generalized to the heterogeneous problem in Appendix D, has the following form:

\[
\nabla^2 \psi^{g+1} + \frac{1}{\varepsilon} (\nabla \psi^{g+1} \cdot \nabla \varepsilon) + \frac{q}{\varepsilon} \left[ p \exp \left( \frac{\psi}{Vt} \right) - n \exp \left( \frac{\psi^{g+1}}{Vt} \right) - n \exp \left( \frac{\psi}{Vt} \right) + C \right] = 0
\tag{2-50}

Actually, in Gummel's original implementation only one Newton iteration was performed on the uniform composition analog to (2-50) for each Gummel iteration (i.e., for each cycle through the three equations).

A consequence of solving the semiconductor equations sequentially is that they are solved as a decoupled set. Therefore, when the equations are strongly coupled, such as in regions of high-level injection, the convergence of Gummel's method is adversely affected.
For $i = 1$ to $3$
(i.e., for Poisson's equation, hole continuity, and electron continuity)

Determine trial values for variables.

Solve $f_i$ system equation.

Self-Consistent Convergence Between Equations?

yes
Stop

no

Update variables

Equation Convergence?

yes

no

Simultaneous Method

The semiconductor equations can also be solved simultaneously (three equations and three unknowns), as shown in Fig. 2-5. When these equations are discretized using five point discretization, three nonlinear algebraic equations result for each point of the mesh; each with the same fifteen unknowns. Linearization yields equations of the form of (2-44) with the
following matrix definitions:

\[
A_{i,j} = \begin{bmatrix}
\delta f_1 & \delta f_1 & \delta f_1 \\
\delta p_{i-1,j} & \delta n_{i-1,j} & \delta \psi_{i-1,j} \\
\delta f_2 & \delta f_2 & \delta f_2 \\
\delta p_{i-1,j} & \delta n_{i-1,j} & \delta \psi_{i-1,j} \\
\delta f_3 & \delta f_3 & \delta f_3 \\
\delta p_{i-1,j} & \delta n_{i-1,j} & \delta \psi_{i-1,j}
\end{bmatrix}, \quad B_{i,j} = \begin{bmatrix}
\delta f_1 & \delta f_1 & \delta f_1 \\
\delta p_{i,j} & \delta n_{i,j} & \delta \psi_{i,j} \\
\delta f_2 & \delta f_2 & \delta f_2 \\
\delta p_{i,j} & \delta n_{i,j} & \delta \psi_{i,j} \\
\delta f_3 & \delta f_3 & \delta f_3 \\
\delta p_{i,j} & \delta n_{i,j} & \delta \psi_{i,j}
\end{bmatrix}
\]

\[
C_{i,j} = \begin{bmatrix}
\delta f_1 & \delta f_1 & \delta f_1 \\
\delta p_{i+1,j} & \delta n_{i+1,j} & \delta \psi_{i+1,j} \\
\delta f_2 & \delta f_2 & \delta f_2 \\
\delta p_{i+1,j} & \delta n_{i+1,j} & \delta \psi_{i+1,j} \\
\delta f_3 & \delta f_3 & \delta f_3 \\
\delta p_{i+1,j} & \delta n_{i+1,j} & \delta \psi_{i+1,j}
\end{bmatrix}, \quad D_{i,j} = \begin{bmatrix}
\delta f_1 & \delta f_1 & \delta f_1 \\
\delta p_{i,j+1} & \delta n_{i,j+1} & \delta \psi_{i,j+1} \\
\delta f_2 & \delta f_2 & \delta f_2 \\
\delta p_{i,j+1} & \delta n_{i,j+1} & \delta \psi_{i,j+1} \\
\delta f_3 & \delta f_3 & \delta f_3 \\
\delta p_{i,j+1} & \delta n_{i,j+1} & \delta \psi_{i,j+1}
\end{bmatrix}
\]

\[
E_{i,j} = \begin{bmatrix}
\delta f_1 & \delta f_1 & \delta f_1 \\
\delta p_{i,j+1} & \delta n_{i,j+1} & \delta \psi_{i,j+1} \\
\delta f_2 & \delta f_2 & \delta f_2 \\
\delta p_{i,j+1} & \delta n_{i,j+1} & \delta \psi_{i,j+1} \\
\delta f_3 & \delta f_3 & \delta f_3 \\
\delta p_{i,j+1} & \delta n_{i,j+1} & \delta \psi_{i,j+1}
\end{bmatrix}, \quad F_{i,j} = \begin{bmatrix}
-f_1 \\
-f_2 \\
-f_3
\end{bmatrix}
\]

\[
\Delta_{i,j} = \begin{bmatrix}
\delta p_{i,j} \\
\delta n_{i,j} \\
\delta \psi_{i,j}
\end{bmatrix}
\]
An advantage of using the simultaneous method is that the problem of high-level injection associated with Gummel's method is avoided. Disadvantages are a higher level of programming complexity (many matrix operations) and an increased memory requirement of at least nine times as compared to Gummel's method (compare coefficient definitions of Eqs (2-47) and (2-51)).

Fig. 2-5. Flow chart for the simultaneous method.
Chapter Three

SOLAR CELL SIMULATION PROGRAM

Solar Cell Simulator (SCS) is a simulation program for one- and two-dimensional numerical modeling of multi-layer Al$_x$Ga$_{1-x}$As /GaAs and (Al$_x$Ga$_{1-x}$)$_{0.47}$In$_{0.53}$As/InP solar cells. SCS simulates the following solar cell device characteristics:

* Efficiency
* Current vs Voltage Characteristics; including short circuit current density, $I_{sc}$, open circuit voltage, $V_{oc}$, maximum power, $P_{max}$, and fill factor, FF.
* Carrier Concentration Profiles; One- or two-dimensional electron and hole concentration profiles for all simulated bias points.
* Potential Profile; One- or two-dimensional potential profiles for all simulated bias points.
* Energy Band Profile
* Material Parameter Profiles; including generation rate, doping concentration, electron affinity, permittivity, and electron and hole mobilities.

How these simulated characteristics are achieved through parameter modeling and the application of numerical algorithms to the solution of the semiconductor equations is examined in this chapter. The simulator's architecture and interface are also discussed.
3.1 Material and Device Parameter Modeling

Device simulation parameters can be divided into two groups: input parameters that are defined by the user, and material parameters which are dependent on the input parameters. The members of each group as implemented in this work are now discussed.

3.1.1 Material and Device Input Parameters

A simulator attempts to model the behavior of a system. A useful simulator allows for the investigation of changes in system behavior in response to changes in variable system parameters. These variable parameters, called "input parameters," are entered by the user to define system variables, and thereby affect simulated system behavior. SCS allows the definition of the following input parameters:

* Material System -- defines which material system is simulated; $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ or $(\text{Al}_x\text{Ga}_{1-x})_{0.47}\text{In}_{0.53}\text{As}/\text{InP}$.

* Device Geometry -- group of parameters for the definition of solar cell geometry; including the number of layers, layer widths, and, for 2-D simulations, contact finger width and exposed area width.

* Doping Profile -- defines linear doping profile within layers.

* Composition Profile -- defines linear aluminum mole fraction profile within layers.

* Surface Recombination Velocity -- defines electron and hole recombination velocities.

* Minority Carrier Lifetime
* Surface Charge Density
* Solar Spectrum -- defines air mass.
* Number of Suns -- defines multiplication factor for solar spectrum data.

3.1.2 Dependent Material Parameters

Once input parameters have been defined, the dependence of any other parameters on the input parameters must be modeled. In semiconductor device modeling, many of these dependent parameters are material parameters that depend on the doping and composition. Since many of these dependencies are not accurately modeled analytically, good material parameter data is desired. However, for most ternary and quaternary alloy systems, complete material data is not available, and interpolation techniques, such as those given by Adachi [26][27], must be used.

Of the ternary Al$_x$Ga$_{1-x}$As and quaternary (Al$_x$Ga$_{1-x}$)$_{0.47}$In$_{0.53}$As systems modeled, the Al$_x$Ga$_{1-x}$As system has been extensively characterized, and much material data is available. However, when unavailable, ternary material parameters can be modeled by interpolation:

$$P(Al_xGa_{1-x}As) = P(GaAs) + x(P(AlAs) - P(GaAs)),$$

(3-1)

where $P(XxXx)$ is a material parameter for material XxXx. Material parameters for the quaternary (Al$_x$Ga$_{1-x}$)$_{0.47}$In$_{0.53}$As can be interpolated by

$$P((Al_xGa_{1-x})_{0.47}In_{0.53}As) = P(Ga_{0.47}In_{0.53}As)$$

$$+ x [P(Al_{0.47}In_{0.53}As) - P(Ga_{0.47}In_{0.53}As)],$$

(3-2)

when the ternary end-point data is available, or by
\[ P(\text{Al}_x \text{Ga}_{1-x})_{0.47}\text{In}_{0.53}\text{As}) = P(\text{InAs}) \]
\[ + \ 0.47 \ [P(\text{Al}_x \text{Ga}_{1-x}\text{As}) - P(\text{InAs})], \]
(3-3)

when only the binary, \( P(\text{InAs}) \), and ternary, \( P(\text{Al}_x \text{Ga}_{1-x}\text{As}) \), parameters are known. Both methods should be more accurate than pure binary interpolation. SCS models the following dependent material parameters:

**Bandgap**

For \( \text{Al}_x \text{Ga}_{1-x}\text{As} \), bandgaps are modeled by [27]
\[
E_g^\Gamma(x) = 1.424 + 1.247x \quad (0 \leq x \leq 0.45), \]
(3-4)
\[
E_g^X(x) = 1.424 + 1.247x + 1.147(x-0.45)^2 \quad (0.45 < x \leq 1.0), \]
(3-5)
\[
E_g^L(x) = 1.708 + 0.642x \]
(3-6)
\[
E_g(x) = \begin{cases} 
E_g^\Gamma(x) & (0 \leq x \leq 0.45), \\
E_g^X(x) & (0.45 < x \leq 1.0), 
\end{cases} \]
(3-7)

For \( \text{Al}_x \text{Ga}_{1-x})_{0.47}\text{In}_{0.53}\text{As} \), the bandgap is modeled by [28]
\[
E_g((\text{Al}_x \text{Ga}_{1-x})_{0.47}\text{In}_{0.53}\text{As}) = 0.76 + 0.49x + 0.20x^2. \]
(3-8)

For \( \text{InP} \) [26],
\[
E_g(\text{InP}) = 1.351 \]
(3-9)
Effective Mass

For Al$_x$Ga$_{1-x}$As

\begin{align*}
    m_e^\Gamma &= 0.067 + 0.083x, \quad (3-10) \\
    m_e^X &= 0.85 - 0.14x, \quad (3-11) \\
    m_e^L &= 0.56 + 0.1x, \quad (3-12) \\
    m_{lh} &= 0.087 + 0.063x, \quad (3-13) \\
    m_{hh} &= 0.62 + 0.14x, \quad (3-14)
\end{align*}

For (Al$_x$Ga$_{1-x}$)$_{0.47}$In$_{0.53}$As

\begin{align*}
    m_e^\Gamma &= 0.0427 + 0.0328x, \quad (3-15) \\
    m_{lh} &= 0.027 + 0.47(0.087 + 0.063x - 0.027), \quad (3-16) \\
    m_{hh} &= 0.60 + 0.47(0.62 + 0.14x - 0.60), \quad (3-17)
\end{align*}

where $m_e^\Gamma$ is from [28] and the effective masses for InAs in the $m_{lh}$ and $m_{hh}$ terms are from [26]. For InP [26]

\begin{align*}
    m_e^\Gamma &= 0.08, \quad m_{lh} = 0.089, \quad m_{hh} = 0.85. \quad (3-18abc)
\end{align*}

The electron effective mass used in the calculation of the effective density of states, $N_C$, must account for the distribution of electrons in the $\Gamma$, $X$, and $L$ conduction band minima:
For all the material systems modeled except $\text{Al}_x\text{Ga}_{1-x}\text{As}$, the differences between the gap energy and the X and L minima are assumed to be large enough that the $m_e^L$ and $m_e^X$ terms in (3-19) need not be modeled. In all cases, the hole density-of-states effective mass in the valence band is calculated as

$$m_{\text{dh}} = (m_{\text{lh}}^{3/2} + m_{\text{hh}}^{3/2})^{2/3}. \quad (3-20)$$

**Density-of-States**

The effective density of states are then given by

$$N_c = 2\left(2\pi m_{\text{de}} kT/h^2\right)^{3/2} \quad (3-21)$$

$$N_v = 2\left(2\pi m_{\text{dh}} kT/h^2\right)^{3/2} \quad (3-22)$$

**Intrinsic carrier concentration**

$$n_i = (N_c N_v)^{1/2} \exp(-E_g/2kT) \quad (3-23)$$

**Electron Affinity**

Electron affinity is modeled by

$$\chi(\text{Al}_x\text{Ga}_{1-x}\text{As}) = \begin{cases} 4.07 - 1.1x, & (0 \leq x \leq 0.45) \\ 3.64 - 0.14x, & (0.45 < x \leq 1.0) \end{cases} \quad (3-24)$$
\[ \chi((Al_xGa_{1-x})_{0.47}In_{0.53}As) = 4.54 \]
\[ + 0.47 (\chi(Al_xGa_{1-x}As) - 4.54) , \quad (3-25) \]
\[ \chi(InP) = 4.37 , \quad (3-26) \]

where \( \chi(Al_xGa_{1-x}As) \) is from [27] and \( \chi(InAs) = 4.54 \) is taken from [29].

**Dielectric Constant**

Dielectric constants are given by
\[ \epsilon(Al_xGa_{1-x}As) = 13.18 - 3.12x , \quad (3-27) \]
\[ \epsilon((Al_xGa_{1-x})_{0.47}In_{0.53}As) = 14.6 + 0.47(13.18 - 3.12x - 14.6) , \quad (3-28) \]
\[ \epsilon(InP) = 12.4 , \quad (3-29) \]

where \( \epsilon(Al_xGa_{1-x}As) \) is from [27], and \( \epsilon(InAs) = 14.6 \) and \( \epsilon(InP) \) are from [26].

**Mobility**

For \( Al_xGa_{1-x}As \), low field electron and hole mobilities are modeled by

the following equations [8]:
\[ \log_{10} \mu_e = [-1.5545 + 0.0106x + (0.735 + 0.0013x) \log_{10} N \]
\[ - (0.0253 + 0.0052x) (\log_{10} N)^2] , \quad (3-30) \]
\[ \log_{10} \mu_h = [-9.723 + 0.0095x + (1.576 + 0.0012x) \log_{10} N \]
\[ - (0.0507 + 0.0034x) (\log_{10} N)^2] , \quad (3-31) \]

where \( N \) is greater than \( 10^{15} \text{ cm}^{-3} \). For \( (Al_xGa_{1-x})_{0.47}In_{0.53}As \), low field electron mobility as a function of composition was modeled by fitting a curve to the
data given in [30] for \( N_{d,a} = 2 \times 10^{17} \text{ cm}^{-3} \):

\[
\mu_e[(\text{Al}_x\text{Ga}_{1-x})_{0.47}\text{In}_{0.53}\text{As}] = 5166 - 5072.5x - 7013.9x^2 + 7241.6x^3 \\
+ 447.8x^4 \tag{3-32}
\]

Equation (3-32) is then scaled to account for doping concentration based on data given in [31]. As the hole mobilities of \( \text{Al}_x\text{Ga}_{1-x}\text{As} \) and \( \text{InAs} \) are approximately equal, the hole mobility for \( \text{Al}_x\text{Ga}_{1-x}0.47\text{In}_{0.53}\text{As} \) is modeled the same as for \( \text{Al}_x\text{Ga}_{1-x}\text{As} \), using (3-31).

The mobility modeling described above is valid only in low field regions. In regions of compositional grading, the resulting changes in electron affinity, bandgap, and density of states can introduce large effective fields; requiring the modeling of carrier saturation velocity.

Neglecting velocity overshoot, carrier velocities can be modeled (to first order) so that they do not exceed their saturation velocities by having their effective mobilities modeled as follows [12]:

\[
\mu_{\text{eff}} = \frac{v}{E_{\text{eff}}} = \frac{\mu_0}{1 + \frac{\mu_0 E_{\text{eff}}}{v_{\text{sat}}}} \tag{3-33}
\]

SCS models mobility using (3-33), where \( \mu_0 \) is the low field value, and the saturation velocity \( v_{\text{sat}} \) is taken in all cases as the \( \text{GaAs} \) value of \( 6 \times 10^6 \text{ cm/sec} \) [12], and \( E_{\text{eff}} \) is given by
\[ E_{\text{eff (electrons)}} = |d\psi/dx + d\chi/dx + (V_t/N_c)(dN_c/dx)| \] (3-34)

\[ E_{\text{eff (holes)}} = |d\psi/dx + d\chi/dx + dE_g/dx - (V_t/N_v)(dN_v/dx)|. \] (3-35)

Absorption Coefficient

For \( \text{Al}_x\text{Ga}_{1-x}\text{As} \) the absorption coefficient is determined from data given by Aspnes [32]. This data gives the \( \alpha \) versus \( E \) profile for several values of composition \( x; \alpha(E, x_i) \). For values of \( x \) between \( x_i \) and \( x_{i+1} \), \( \alpha(E, x) \) is determined by taking a weighted average of the energy shifted \( \alpha(E, x_i) \) and \( \alpha(E, x_{i+1}) \) profiles:

\[
\alpha(E, x) = \frac{\alpha(E - (E_g(x) - E_g(x_i)), x_i)(E_g(x_{i+1}) - E_g(x)) + \alpha(E - (E_g(x) - E_g(x_{i+1})), x_{i+1})(E_g(x) - E_g(x_i))}{E_g(x_{i+1}) - E_g(x_i)}, \] (3-37)

Unfortunately, absorption coefficient data for the \( (\text{Al}_x\text{Ga}_{1-x})_{0.47}\text{In}_{0.53}\text{As} \) quaternary is unavailable for intermediate values of composition \( x \). However, using the approach of (3-36) and the end-point values for \( \alpha(\text{Al}_{0.47}\text{In}_{0.53}\text{As}) \) and \( \alpha(\text{Ga}_{0.47}\text{In}_{0.53}\text{As}) \), \( \alpha((\text{Al}_x\text{Ga}_{1-x})_{0.47}\text{In}_{0.53}\text{As}) \) was approximated by

\[
\alpha(E, x) = \frac{\alpha(E - (E_g(x) - E_g(0)), x=0)(E_g(1) - E_g(x)) + \alpha(E - (E_g(x) - E_g(1)), x=1)(E_g(x) - E_g(0))}{E_g(1) - E_g(0)}, \] (3-37)

where \( \alpha(E, x=1) = \alpha(\text{Al}_{0.47}\text{In}_{0.53}\text{As}) \) and \( \alpha(E, x=0) = \alpha(\text{Ga}_{0.47}\text{In}_{0.53}\text{As}) \).
\(\alpha(\text{Al}_{0.47}\text{In}_{0.53}\text{As})\) was similarly modeled as

\[
\alpha(E, 0.47) = \frac{\alpha(E - (E_g(0.47) - E_g(1)), x=0)(E_g(1) - E_g(0.47)) + \alpha(E - (E_g(0.47) - E_g(0)), x=1)(E_g(0.47) - E_g(0))}{E_g(1) - E_g(0)}, \quad (3-38)
\]

where \(\alpha(E, x=0) = \alpha(\text{InAs})\) is from tabulated data [33], and \(\alpha(E, x=1) = \alpha(\text{AlAs})\) is taken as \(\alpha(\text{Al}_x\text{Ga}_{1-x}\text{As})\) for \(x=1\) in (3-36). Although an absorption coefficient profile for \(\text{Ga}_{0.47}\text{In}_{0.53}\text{As}\) can be found in [34], reference was not made to the tabulated data. Therefore, \(\alpha(\text{Ga}_{0.47}\text{In}_{0.53}\text{As})\) was also modeled with (3-38), where \(\alpha(E, x=1) = \alpha(\text{GaAs})\) is taken as \(\alpha(\text{Al}_x\text{Ga}_{1-x}\text{As})\) for \(x=0\) in (3-36). Coefficients \(\alpha(\text{InP})\) are modeled from tabulated data [35].

Although interpolating the data for \(\alpha(\text{Al}_x\text{Ga}_{1-x}\text{As})\) should provide accurate absorption coefficient modeling for that system, the interpolation technique for \(\alpha((\text{Al}_x\text{Ga}_{1-x})_{0.47}\text{In}_{0.53}\text{As})\) is expected not to be very accurate. Both require extensive interpolation. Adachi has presented a method [36] for analytically determining optical dispersion relations that are continuous functions of energy and composition, and achieve excellent agreement between calculated and measured absorption coefficient data. This analytical method has not been implemented herein, but it should prove very useful in modeling the absorption characteristics of many ternary and quaternary alloy systems that have not been empirically studied.

3.2 Device Simulation

The Solar Cell Simulator uses Gummel's algorithm for the solution of
Poisson's equation and the current continuity equations. How SCS implements the major components of this algorithm is described in this section.

3.2.1 Device Equations

SCS uses Gummel's algorithm for the solution of Eqs. (2-29), (2-38), and (2-39). Boundary conditions at metal contacts, assumed ohmic, are calculated using Eqs. (2-13) to (2-16) for carrier concentrations, and are based on the discussion at the end of Appendix A for the potential. Neumann boundary conditions in the exposed areas between contact fingers are modeled with Eqs. (2-17) to (2-20). With reference to the coordinate system of Fig. 2-1, and using the interpolation technique of (2-40), the discretized current continuity equations at the surface become

\[
\frac{1}{q} \left( \frac{J_{p x}^{i+1/2, j} - J_{p x}^{i-1/2, j}}{h_i + h_{i-1}} \right) + \frac{1}{q} \left( \frac{J_{p y}^{i, j+1/2} - R_{SURF}}{k_j + k_{j-1}} \right) - R_{i,j} + G_{i,j} = 0 \quad (3-39)
\]

\[
\frac{1}{q} \left( \frac{J_{n x}^{i+1/2, j} - J_{n x}^{i-1/2, j}}{h_i + h_{i-1}} \right) + \frac{1}{q} \left( \frac{J_{n y}^{i, j+1/2} - R_{SURF}}{k_j + k_{j-1}} \right) - R_{i,j} + G_{i,j} = 0 \quad (3-40)
\]

where surface recombination is modeled by (2-19). This approach cannot be used to model surface recombination in one-dimensional simulations, since, in this case, terminal current can only be resolved with a surface contact.
Therefore, for one-dimensional simulations, majority carriers at the surface are modeled by the Dirichlet contact boundary condition, and minority carriers are modeled by the one-dimensional form of either (3-39) or (3-40), depending on the minority carrier type. Accordingly, the surface recombination rate modeled by (2-19) reduces to:

\[ R_{\text{SURF}} = S_p (p-p_0), \]  

(3-41)

and

\[ R_{\text{SURF}} = S_n (n-n_0), \]  

(3-42)

for the two minority carrier types; where, in (2-19), majority carrier recombination velocities have been taken as infinite, and majority carrier concentrations have been taken as their thermal equilibrium values.

Optical generation rates are determined by a method based on (2-10i), where the transmission coefficient is taken as unity, photon flux per wavelength interval is given by [37], and absorption coefficients are calculated as described in section 3-1. The author found that the direct implementation of (2-10i), with the integral in the exponent, is error prone. An accurate method, developed by the author, of implementing generation rate calculations based on (2-10i) is described in Appendix E.

Recombination rates are calculated using the SRH formula,

\[ R^\text{SRH} = \frac{n_p - n_i^2}{\tau_p(n+n_i) + \tau_n(p+n_i)}, \]  

(3-43)
where the trap energy is assumed to be at the intrinsic Fermi level, and \( \tau_p = \tau_n \) is a minority carrier lifetime input parameter.

### 3.2.2 Mesh Design

Mesh spacing is generated by a mapping function such that mesh spacing is smallest near interfaces. A graphical representation of the method, developed by the author, is shown in Fig. 3-1.

![Graphical representation of mesh generation technique](image)

**Fig. 3-1.** Graphical representation of mesh generation technique (N=8).

For a bounded region divided by \( N+1 \) mesh lines, the mapping function used is defined by
\[ x_i = \frac{\Delta x}{2} \left( \frac{i}{N/2} \right)^{\text{pow}}, \quad 0 \leq i \leq \frac{N}{2} \]  
\[ x_i = \frac{\Delta x}{2} + \frac{\Delta x}{2} \left( \frac{i - N/2}{N/2} \right)^{\text{pow}}, \quad \frac{N}{2} < i \leq N \]

where
\[ \Delta x = x_N - x_0. \]

As pow is increased, the mesh lines become more closely spaced near the boundaries and more sparse in the interior region (a uniform mesh results for pow = 1). Therefore, once the device geometry has been specified, mesh generation can be controlled with variables \( N \) and \( \text{pow} \) in all bounded regions.

### 3.2.3 Trial Values

For one-dimensional simulations, majority carrier trial values are taken as the doping concentration, and minority carrier trial values are then determined from the thermal equilibrium condition \( n_p = n_1^2 \). Using these carrier trial values, potential trial values are determined from Eqs. (A-11) and (A-12). For two-dimensional simulations, trial values are determined by interpolating the results of two separate one-dimensional simulations: one with a surface contact at zero bias, and one with Neumann boundary conditions at the surface.
3.2.4  Linearization

For one-dimensional simulations, linearization is performed by (2-42) and the resulting linear system is solved by direct tri-diagonal Gaussian elimination and back substitution [25]. For two-dimensional simulations, linearization is performed so that the resulting matrix-vector equation is solved directly for updated unknown variables, \( \Theta \), rather than for incremental correction terms \( \Delta \). This matrix-vector equation is derived as follows:

If the equation in Fig. 2-3 is represented as

\[
[J] \Delta^{k+1} = [F],
\]  \hfill (3-46)

where

\[
\Delta^{k+1} = \Theta^{k+1} - \Theta^k,
\]  \hfill (3-47)

then

\[
[J] \Theta^{k+1} = [F] + [J] \Theta^k.
\]  \hfill (3-48)

For two-dimensional simulations, (3-48) is solved by the successive line overrelaxation method [19]. Note that the Jacobian coefficient matrix for both methods (Eqs. (3-46) and (3-48)) is the same. One advantage of using (3-48) for two-dimensional simulations is that the number of terms in the "known" right-hand vector is reduced by cancellation. Another is that extra memory for correction terms need not be allocated; the \( \Theta^{k+1} \) simply replace the \( \Theta^k \).
3.3 Program Architecture and Interface

The Solar Cell Simulator is written in C and was developed on an IBM PC/AT. It is a collection of programs that are coordinated by a batch execution file (SCS.BAT). A flow chart of the SCS.BAT program is shown in Fig. 3-2. SCS has a friendly user interface for the entering of input parameters, tracking of run-time information, and the displaying and storing of simulation results.
Fig. 3-2: Flow chart showing the simulator’s SCS.BAT master program flow. Each rectangle represents a separate sub-program.
When the simulator is first entered, a menu is displayed, shown in Fig. 3-3, which shows the titles of stored solar cell structures, the dimension of the simulation, and whether or not a simulation has been performed for the structure. This menu allows the user to exit the program, invoke the graphics program, select the creation of a new cell structure, or select a stored structure.

![Menu Display](image)

Fig. 3-3. Top level simulator interface menu. Allows selection of a new or stored solar cell structure.

If a stored structure is selected, a menu, shown in Fig. 3-4, is displayed that allows for the selection of modifying the cell's structure and parameters, initiating a simulation of the selected cell structure, or performing the deletion of the cell structure and its associated simulation results from storage.
Choose Desired Task

Modify Cell Structure.
Modify Cell Parameters.
Modify Control Parameters.
Simulate This Solar Cell.
Delete This Solar Cell.
Return To Cell List.

Fig. 3-4. Modify, Simulate, or Delete solar cell simulator interface menu.

If "Modify Cell Structure" is selected from the menu of Fig. 3-4, an interactive input form is displayed, an example of which is shown in Fig. 3-5 for the cell selection "window", which shows the physical structure parameters of the selected solar cell. The user can move around this form and edit the different parameter fields. The "MATERIAL SYSTEM" field allows toggling between the AlGaAs/GaAs and (AlGa)InAs/InP structure types.
If "Modify Cell Parameters" is selected from the menu of Fig. 3-4, the interactive input form of Fig. 3-6 is displayed. This form allows the user to set various material and solar irradiation parameters. And, if "Modify Control Parameters" is selected, the interactive input form of Fig. 3-7 is displayed. This form allows the user to set simulator control variables.
When "Simulate This Solar Cell" is selected from the menu of Fig. 3-4, the input program is exited and a simulation of the selected solar cell is initiated. First, initializations such as mesh design, material parameter calculations, generation rate calculations, and 1-D initial trial value calculations are performed in the INITIAL program. Then, the 1-D simulation program is entered and a 1-D simulation is performed. This includes separate simulations for as many bias points necessary to define the current-voltage characteristic (from zero bias to Voc). During a solar cell simulation a run-time display, an example of which is shown in Fig. 3-8, provides information on the simulator's progress.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum Gummel Iterations:</td>
<td>30</td>
</tr>
<tr>
<td>Maximum Newton Iterations:</td>
<td>5</td>
</tr>
<tr>
<td>Maximum SOR Iterations:</td>
<td>20</td>
</tr>
<tr>
<td>Relative Error:</td>
<td>1.8e-07</td>
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<tr>
<td>Divisions Per Layer:</td>
<td>50</td>
</tr>
<tr>
<td>Divisions Per Finger Contact:</td>
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</tr>
<tr>
<td>Divisions Between Contacts:</td>
<td>10</td>
</tr>
</tbody>
</table>

Fig. 3-7. Simulator control variable, interactive input form.
<table>
<thead>
<tr>
<th>BIAS VOLTAGE:</th>
<th>0.00</th>
<th>ELAPSED TIME:</th>
</tr>
</thead>
<tbody>
<tr>
<td>GUMMEL ITERATION:</td>
<td>4</td>
<td></td>
</tr>
</tbody>
</table>

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<tr>
<td>HOLE CONTINUITY:</td>
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**Numerical Solution in Progress.**

Fig. 3-8. Simulator 1-D run-time display.

The simulator interface menus of Figs. 3-3 to 3-8 are all invoked from the INPUT program. However, when "GRAPHICS" is selected from the top level simulator menu of Fig. 3-3, the input program is exited and the graphics program is entered. When this occurs, the top level graphics menu shown in Fig. 3-9 is displayed. From here, SCS.BAT can be exited, the INPUT program can be invoked, or simulation results can be viewed.
When a cell is selected from the menu of Fig. 3-9, a menu, shown in Fig. 3-10, is displayed which allows the selection of a variety of simulation results.
for the selected solar cell.

The selections "Electron Concentration", "Hole Concentration", "Potential", and "Energy Bands" all are dependent on the applied bias. Therefore, for these selections an additional menu, shown in Fig. 3-11, is displayed. This menu allows the selection of the desired bias point from a list of all the bias points performed during the simulation.

![Possible choices:]

0.050 0.100 0.150 0.200
0.250 0.300 0.350 0.400 0.450
0.500 0.550 0.600 0.650 0.700
0.750 0.800 0.850 0.900 0.950
0.880 0.900 0.910 0.920
0.930 0.940 0.950 0.960

Fig. 3-11. Simulation results, bias point selection menu.

For the four bias point dependent selections mentioned, multiple curves for different bias points can be displayed on the same graph. A zoom feature is also available for discerning detailed regions of a graph. Examples of these graphs will be seen in the next chapter where simulation results are discussed.
Chapter Four

SIMULATION RESULTS AND DISCUSSION

Simulation results for AlGaAs/GaAs and (AlGa)InAs/InP solar cells are presented in this chapter. In the first, and main, section, results for one-dimensional simulations are given. Preliminary two-dimensional results are given in the second section. Simulation results are discussed throughout.

4.1 One-Dimensional Simulations

A presentation and discussion of the results of one-dimensional simulations is given in this section. First, the inner and terminal characteristics of individual variable composition AlGaAs/GaAs and (AlGa)InAs/InP solar cells are investigated. It is shown how varying the geometrical and material structure of a cell affects the carrier and potential profiles internal to the device, and how these profiles can then be used to explain the resultant terminal characteristics. Second, trends in terminal characteristics, when structural parameters are varied, are investigated.

4.1.1 Internal Device Investigations

Internal device operation is investigated for four cells:

Cell 1. A four layer, n-p AlGaAs/GaAs solar cell.

Cell 2. A two layer, p-n (AlGa)InAs/InP solar cell.

Cell 3. A two layer, n-p (AlGa)InAs/InP solar cell with low emitter doping.

Cell 1.

First, the AlGaAs/GaAs solar cell, cell1, defined by Table 4-1 is investigated. Since simulation results exist for AlGaAs/GaAs solar cells, this simulation, although interesting in its own right, doubles as a simulator verification check. Simulation results for this cell are shown in Figs. 4-1 to 4-9.

<table>
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<th>DOPING TYPE</th>
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<th>CONC BOTTOM</th>
<th>MOLE FRAC TOP</th>
<th>MOLE FRAC BOTTOM</th>
<th>LAYER THICKNESS</th>
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SURFACE RECOMBINATION VELOCITY | 1.0e4 cm/sec
MINORITY CARRIER LIFETIME     | 1.0e-9 /cm^2
SOLAR SPECTRUM                | AM1.5
INTENSITY                     | 1 SUNS

Table 4-1. Input parameters of four layer n-p AlGaAs/GaAs solar cell.

The current-voltage characteristics are shown in Fig. 4-1, with the area defined by the fill-factor as a frame for displaying the important cell output parameters. The values of these parameters are seen to be in their expected ranges [7].
Efficiency = 22.58 x
Maximum Power Out = 18.81 mW
Power In = 83.28 mW
Jsc = 23.71 mA / sq cm
Voc = 0.955 V
FF = 83.01 x

Fig. 4-1. Current-voltage characteristic with output parameters for cell 1.

Fig. 4-2. Energy band diagram of cell 1 zoomed to top 4.83 microns.
Fig. 4-3. Energy band diagram of cell 1 zoomed to top 0.78 microns.

Fig. 4-4. Generation rate profile for cell 1.
Fig. 4-5. Electron concentration profile for cell 1 at zero bias.

Fig. 4-6. Electron concentration profile for cell 1 zoomed to top 4.83 microns, for applied biases of 0.0, 0.9, and 0.96 volts, from bottom to top.
Fig. 4-7. Hole concentration profile of cell 1 at zero bias, and zoomed to top 4.45 microns.

Fig. 4-8. Hole concentration profile of cell 1 for applied biases of 0.0, 0.6, and 0.96 volts, bottom to top, and zoomed to top 0.81 microns.
Fig. 4-9. Potential profiles of cell 1 for applied biases of 0.0, 0.2, 0.4, 0.6, and 0.8 volts.

The energy band diagram near the surface of cell 1 is shown in Figs 4-2 and 4-3. A back-surface-field at 3.6 microns is seen in Fig. 4-2. Conduction and valence band discontinuities are seen at the interface between the window and the emitter in Fig. 4-3. This is expected as the aluminum mole fraction transitions from 0.9 to 0.35 at this point.

The desired effect of the window layer is apparent from the generation rate profile shown in Fig. 4-4. It is seen that generation in the window layer is relatively low, but abruptly increases upon transition into the lower gap emitter region. In this way, more of the generated carriers experience the built-in field of the graded gap emitter region which draws them toward the collection junction. In the uniform composition GaAs substrate, the
generation rate is seen to decay exponentially.

Electron concentration profiles are shown in Figs. 4-5 to 4-6. From Fig. 4-6, it can be deduced that as the applied bias is increased, the dark current approaches the photo-generated current, since the diffusion gradient from base to emitter of the photo-generated electrons in the base goes to zero as the applied bias goes to the open-circuit voltage. The effect of the conduction band spike between window and emitter on the electron concentration is also evident.

Hole concentration profiles are shown in Figs. 4-7 and 4-8. By comparing Fig. 4-8 to 4-3 and 4-6 to 4-2 it is seen that the valence band discontinuity between window and emitter has a similar effect on the photo-generated holes as the back surface field has on the photo-generated electrons; that is, to act as a barrier from one side and a sink from the other.

Potential profiles for various applied biases are shown in Fig. 4-9.

Cell 2.

Input parameters used for the simulation of cell 2 are listed in Table 4-2. Simulation results for cell 2 are given in Figs. 4-10 to 4-17. From the current-voltage characteristic of Fig. 4-10, the open-circuit voltage of the p-n (AlGa)InAs/InP cell, cell 2, is seen to be much smaller than that of the AlGaAs/GaAs cell, and the short-circuit current to be larger. This is expected due to the smaller bandgaps inherent in the (AlGa)InAs/InP material system. Less expected is the relatively high efficiency of 17.11 percent.

Energy band diagrams for the cell are shown in Figs. 4-11 and 4-12. The
Table 4-2. Input parameters for two layer p-n (AlGa)InAs/InP solar cell.

<table>
<thead>
<tr>
<th>LAYER NAME</th>
<th>DOPING TYPE</th>
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<th>CONC BOTTOM</th>
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<tr>
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<td>1.0e18</td>
<td>0.00</td>
<td>0.00</td>
<td>2.5e-3</td>
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</tbody>
</table>

SURFACE RECOMBINATION VELOCITY  1.0e4 cm/sec
MINORITY CARRIER LIFETIME       1.0e-8 /cm^2
SOLAR SPECTRUM                  AM1.5
INTENSITY                       1 SUNS

Efficiency = 17.11 %
Maximum Power Out = 14.25 mW
Power In = 83.28 mW
Jsc = 30.84 mA / sq cm
Voc = 0.569 V
FF = 81.27 %

Fig. 4-10. Current-voltage characteristic with output parameters for cell 2.
Fig. 4-11. Energy band diagram of cell 2 zoomed to top 1.10 microns.

Fig. 4-12. Energy band diagram of cell 2 zoomed about junction so that the conduction band spike is visible.
Fig. 4-13. Generation rate profile for cell 2, 3, and 4 (generation modeling is not doping dependent).

Fig. 4-14. Electron concentration profile for cell 2 at zero bias and zoomed to top 0.92 microns.
Fig. 4-15. Electron concentration profile for cell 2 at an applied bias of 0.55 volts and zoomed to the top 0.93 microns.

Fig. 4-16. Hole concentration profile of cell 2 at applied biases of 0.0 and 0.55 volts.
built-in field in the emitter region is seen in Fig. 4-11, as evidenced by the conduction band gradient. A conduction band spike at the emitter-base junction is revealed in Fig. 4-12.

The generation rate in the cell is shown in Fig. 4-13. Whereas the generation rate in cell 1 is seen to increase in going from a large gap region to a small gap region, for this cell it is seen that the generation rate drops in going from the smaller gap GaInAs to the large gap InP regions.

Electron concentration profiles are shown in Figs. 4-14 and 4-15. The accumulation of electrons in the valley before the conduction band spike barrier is evident. The expected diffusion gradient of photo-generated electrons toward the junction is not seen. This is caused by the conduction band spike barrier. However, the large gradient in the opposite direction,
seen in Fig. 4-15, for an applied bias approaching Voc, is curious (it is a wonder there is any calculated power output from the cell at all).

Hole concentration profiles at zero and high bias are shown in Fig. 4-16. The two curves appear to be superimposed, although a small variation at the junction is seen under zoom. The large variations for different biases seen in Fig. 4-6 for cell 1, however, are not seen here.

Cells 3 and 4.

Cells 3 and 4 are the same configuration, but with different emitter doping levels. Cell 3 has a lowly doped emitter and cell 4 has a highly doped emitter.

Input parameters used for the simulation of cell 3 are listed in Table 4-3. Simulation results for cell 3 are given in Figs. 4-18 to 4-22.

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Table 4-3. Input parameters for two layer n-p (AlGa)InAs/InP solar cell with low emitter doping.
Fig. 4-18. Current-voltage characteristic with output parameters for cell 3.

Efficiency = 10.97 %
Maximum Power Out = 9.14 mW
Power In = 83.28 mW
Jsc = 31.13 mA / sq cm
Voc = 0.433 V
FF = 67.73 %

Fig. 4-19. Energy band diagram of cell 3 zoomed to top 1.28 microns. The valence band spike is visible.
Fig. 4-20. Electron concentration profile for cell 3 at applied biases of 0.0 and 0.44 volts.

Fig. 4-21. Hole concentration profile of cell 3 at applied biases of 0.0 and 0.44 volts.
Fig. 4-22. Potential profiles of cell 3 for applied biases of 0.0, 0.20, and 0.40 volts.

Input parameters used for the simulation of cell 4 are listed in Table 4-4.

Simulation results for cell 4 are given in Figs. 4-23 to 4-27.

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<tr>
<th>LAYER NAME</th>
<th>DOPING TYPE</th>
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<th>CONC BOTTOM</th>
<th>MOLE FRAC TOP</th>
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<td>8.0e-5</td>
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<tr>
<td>base</td>
<td>p</td>
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<td>1.0e18</td>
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</tr>
</tbody>
</table>

Table 4-4. Input parameters for two layer n-p (AlGa)InAs/InP solar cell with high emitter doping.
Fig. 4-23. Current-voltage characteristic with output parameters for cell 4.

Fig. 4-24. Energy band diagram of cell 4 zoomed to top 1.15 microns. The valence band spike is visible.
Fig. 4-25. Electron concentration profile for cell 4 at applied biases of 0.0 and 0.68 volts.

Fig. 4-26. Hole concentration profile of cell 4 at applied biases of 0.0 and 0.68 volts.
Fig. 4-27. Potential profiles of cell 4 for applied biases of 0.0, 0.20, 0.40, and 0.60 volts.

The discrepancy in efficiency between cell 3 and cell 4, as seen in Figs. 4-18 and 4-23, is explained by the position of the valence band spike barrier, as seen in Figs. 4-19 and 4-24. The relatively small depletion region on the emitter side of the junction of cell 4 positions the valence band spike such that it represents a large barrier to the collection of photo-generated holes; whereas in cell 3 the spike is within the limits of the potential change across the junction. Actual efficiencies of n-p (AlGa)InAs/InP solar cells should be greater than suggested by these simulations, since the tunneling of carriers through potential barriers has not been included in the simulator's carrier transport model.

Electron and hole concentration profiles of cells 3 and 4, shown in Figs.
4-20, 4-21, 4-25, and 4-26, exhibit similar characteristics to those of cell 2.

4.1.2 Trends in Terminal Characteristics

In addition to the detailed results for the four selected individual solar cells, trends in efficiency, open-circuit voltage, and short-circuit current are obtained for variations in simple cell structures for both the AlGaAs/GaAs and (AlGa)InAs/InP material systems. For both systems, the varied structure parameters are emitter width and emitter doping, where emitter doping is varied from 1e17 to 1e19 for each of several emitter widths between 1 and 0.4 microns. In each case, n-p cells are compared to their p-n counterparts. These results are shown in Figs. 4-28 to 4-33.

For the AlGaAs/GaAs system, the basic cell structure investigated is similar to that defined in Table 4-1, but without the window layer, and with an aluminum mole fraction of 0.9 at the top of the emitter. Trends in efficiency are shown in Fig. 4-28. It is seen that the efficiency increases as the emitter width is decreased. This is due to the finite lifetime of the photo-generated minority carriers in the graded emitter region. For a fixed minority carrier lifetime, as the emitter width is decreased, fewer of the carriers can recombine before being collected at the junction, and the efficiency increases. It was found the this trend could only be realized by the modeling of carrier saturation velocity. Without the modeling of saturation velocity, all generated carriers in the emitter region were found to be accelerated by the effective field to such exaggerated velocities that essentially all of them could make it to the collection junction before recombining.
Fig. 4-28. Efficiency vs emitter doping for graded emitter, three layer AlGaAs/GaAs solar cell. Solid lines are for n-p cells with emitter widths of 0.8, 0.6, and 0.4 microns (bottom to top). Dashed lines are for p-n cells with emitter widths of 1.0, 0.8, 0.6, and 0.4 microns.
Fig. 4-29. Open-circuit voltage vs emitter doping for graded emitter, three layer AlGaAs/GaAs solar cell. Solid lines are for n-p cells with emitter widths of 0.8, 0.6, and 0.4 microns. Dashed lines are for p-n cells with emitter widths of 1.0, 0.8, 0.6, and 0.4 microns.
Fig. 4-30. Short-circuit current vs emitter doping for graded emitter, three layer AlGaAs/GaAs solar cell. Solid lines are for n-p cells with emitter widths of 0.8, 0.6, and 0.4 microns. Dashed lines are for p-n cells with emitter widths of 1.0, 0.8, 0.6, and 0.4 microns.
Fig. 4-31. Efficiency vs emitter doping for graded emitter, two layer (AlGa)InAs/InP solar cell. Solid lines are for n-p cells with emitter widths of 1.0, 0.8, 0.6, and 0.4 microns. Dashed lines are for p-n cells with emitter widths of 1.0, 0.8, 0.6, and 0.4 microns.
Fig. 4-32. Open-circuit voltage vs emitter doping for graded emitter, two layer (AlGa)InAs/InP solar cell. Solid lines are for n-p cells with emitter widths of 1.0, 0.8, 0.6, and 0.4 microns. Dashed lines are for p-n cells with emitter widths of 1.0, 0.8, 0.6, and 0.4 microns.
Fig. 4-33. Short-circuit current vs emitter doping for graded emitter, two layer (AlGa)InAs/InP solar cell. Solid lines are for n-p cells with emitter widths of 1.0, 0.8, 0.6, and 0.4 microns. Dashed lines are for p-n cells with emitter widths of 1.0, 0.8, 0.6, and 0.4 microns.
Since wider emitters have more generated carriers, the efficiency trend is actually reversed when saturation velocity is not modeled. The author wonders how other investigators have achieved the correct efficiency trend without the modeling of carrier saturation velocity in regions of high effective fields.

For the (AlGa)InAs/InP system, the varied solar cell has the same basic structure as that shown in Tables 4-2 to 4-4. It is seen in Fig. 4-31 that the efficiency of the n-p (AlGa)InAs/InP cell dramatically decreases as the emitter doping level increases beyond $10^{18}\text{cm}^{-3}$. This is the point where the valence band spike emerges from the bounds of the junction potential and begins to block minority carrier collection at the junction (see Figs. 4-19 and 4-24). This blocking of carrier flow is shown graphically in Fig. 4-33, where the short-circuit current density is seen to experience the same trend. For the p-n (AlGa)InAs/InP cell, the small conduction band spike, seen in Fig. 4-12, does not, as modeled, affect carrier flow; as evidenced by the lack of variation in the short-circuit current density shown in Fig. 4-33. Also, the open-circuit voltage of the p-n cell, shown in Fig. 4-32, increases enough with increasing emitter doping that the efficiency attains respectable high teen values for high emitter dopings.
4.2 Two-Dimensional Simulations

Electrical contact to the top surface of a solar cell can be made with a series of uniformly separated parallel "finger" contacts. If the distance between contacts is small compared to the contact length, a true two-dimensional analysis results, with carrier concentrations and the electric potential varying periodically with contact spacing, in the direction perpendicular to the length of the contacts. Due to the periodicity, a complete analysis can be performed using a simulation domain defined by a half period. The artificial boundaries defining such a domain are shown in Fig. 4-34. The symmetry at the boundaries allows the application of the artificial boundary conditions given in Eqs. 2-21abc.

![Diagram of Finger Contacts and Artificial Boundaries](image)

**Fig. 4-34.** The positioning of artificial boundaries at symmetry points for definition of the two-dimensional simulation domain is shown.

Two-dimensional simulation results for the electron and hole
Fig. 4-35. Hole concentration profile for two-dimensional n-p GaAs solar cell simulation. The profile is limited to the top three microns of the cell so that the detailed structure in the emitter region can be seen.
Fig. 4-36. Electron concentration profile for a two-dimensional n-p GaAs solar cell simulation. The profile encompasses the entire cell width.
concentration profiles of an n-p GaAs solar cell are shown in Figs. 4-35 and 4-36, respectively.

The system of nonlinear two-dimensional partial differential equations was solved using the block SOR (SLOR) method [19], where line iterations were alternated in direction (successively iterating through all vertical lines, and then through all horizontal lines) until convergence was reached. Even with the use of strict convergence criteria, it was found that the total current calculated at the top surface was 10% greater than the total current at the back surface. Since the total current through any cross section of the device must be equal to any other, the results cannot be accurate. The error in the numerical solution routines that caused this discrepancy was not determined, and further investigation by two-dimensional simulation could not be pursued. Possible explanations for the error are the disproportionate mesh spacings in the vertical and horizontal directions, a short-fall in Gummel's algorithm for two-dimensional solutions, or a programming error in the implementation of the numerical routines. The probability of a programming error is low, since the results of Figs. 4-36 and 4-37 appear as expected, and it is the author's experience that programming errors in numerical routines are catastrophic.
Chapter Five

CONCLUSIONS AND RECOMMENDATIONS FOR FURTHER WORK

Simulation results, believed to be the first of their kind, indicate that p-n (AlGa)InAs/InP solar cells with heavily doped emitters are capable of efficiencies approaching 18 percent, and that n-p (AlGa)InAs/InP solar cells may only be capable of very low efficiencies. It was found that the n-p solar cell's low simulated efficiency was due to a large valence band spike that acts to inhibit minority carrier collection. Since the modeling of tunneling was not included in the simulator's transport model, it is expected that n-p cells would have much higher efficiencies than predicted. In fact, since the spike barrier becomes narrower as the emitter doping is increased, its current blocking ability should become quite small for heavily doped emitters. Coupled with the fact that the open-circuit voltage was seen to be greater for n-p cells, it is possible that efficiencies of n-p cells could be as great, or even greater, than those of p-n cells. These results, together with the self annealing property of InP under high energy irradiation [38], warrant the fabrication and testing of (AlGa)InAs/InP solar cells for space applications.

It was also found that carrier saturation velocity must be modeled in regions of high effective electric field, regions that are inherent in variable composition devices, when calculating solar cell efficiencies. Not modeling saturation velocity amounts to greatly increasing excess carrier lifetimes in high field regions, and yields incorrectly high efficiencies. It also gives the wrong trend in efficiency with emitter width.
In addition, an extensive review of the numerical simulation of variable composition semiconductor devices is given in this work. Detailed derivations of the discretized form of the semiconductor equations applicable for variable composition modeling have been provided. An accurate method for the implementation of the generation rate equation has also been given.

Finally, it has been shown that variable composition device simulation can be performed in a convenient and user friendly manner on a personal computer, as a convenient, user friendly, and reusable variable composition solar cell simulator, as described herein, has resulted from this work.

It is suggested that this work be continued in the following ways:

* Investigate various multilayer AlGaAs/GaAs and (AlGa)InAs/InP solar cells using the simulator as it exists.

* Investigate various multilayer AlGaAs/GaAs and (AlGa)InAs/InP solar cells using an improved version of the simulator, by adding the modeling of
  - radiative and Auger recombination for high solar intensity simulations,
  - Fermi-Dirac statistics and bandgap narrowing for better modeling of heavily doped cells,
  - tunneling and thermionic emission, for better modeling of transport across (through or over) conduction and valence band spike barriers,
  - and by completing the two-dimensional simulator, for the modeling of surface recombination, surface resistivity, and other two-dimensional effects.


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APPENDICES
A discussion of energy band diagrams is aided by reference to Fig. A-1.

For an arbitrary energy reference, the conduction and valence band energies are given by

\[
E_c = q(\psi_0 - \psi) - \chi_c \tag{A-1}
\]

\[
E_v = q(\psi_0 - \psi) - \chi_c - E_g \tag{A-2}
\]
Assuming nondegeneracy, the carrier concentrations are given by

$$n = N_c \exp \left( \frac{E_{Fn} - E_c}{kT} \right)$$

(A-3)

$$p = N_v \exp \left( \frac{E_v - E_{Fp}}{kT} \right)$$

(A-4)

Rearranging yields

$$E_{Fn} = E_c + kT \ln \left( \frac{n}{N_c} \right)$$

(A-5)

$$E_{Fp} = E_v - kT \ln \left( \frac{p}{N_v} \right)$$

(A-6)

Substituting (A-1) and (A-2) into (A-5) and (A-6), respectively, gives the following equations for the quasi-Fermi levels:

$$E_{Fn} = q(\psi_0 - \psi) - \chi_c + kT \ln \left( \frac{n}{N_c} \right)$$

(A-7)

$$E_{Fp} = q(\psi_0 - \psi) - \chi_c - E_g - kT \ln \left( \frac{p}{N_v} \right)$$

(A-8)

After $n$, $p$, and $\psi$ have been determined by the numerical simulation, an energy band diagram can be constructed using the above equations.
These equations can also be used to determine the built-in voltage across a junction. The built-in voltage is the difference in electrostatic potential across the junction at thermal equilibrium. But at thermal equilibrium

$$E_{F_n} = E_{F_p} = E_F = \text{constant.} \quad (A-9)$$

If the assignment

$$E_{F_n} = E_{F_p} = E_F = q\psi_0 \quad (A-10)$$

is made, (A-7) and (A-8) become

$$\psi(x) = -\frac{\chi_c(x)}{q} + \frac{kT}{q} \ln\left(\frac{n(x)}{N_c(x)}\right) \quad (A-11)$$

$$\psi(x) = -\frac{\chi_c(x)}{q} - \frac{E_g(x)}{q} - \frac{kT}{q} \ln\left(\frac{p(x)}{N_v(x)}\right) \quad (A-12)$$

Since the right-hand sides of (A-11) and (A-12) are equivalent under thermal equilibrium, either equation can be used to describe the equilibrium potential distribution. However, prior to a numerical solution, only the carrier concentrations at contacts are known (assuming thermal equilibrium and space-charge neutrality at metal-semiconductor contacts). Therefore, (A-11) and (A-12) are really only useful in determining equilibrium boundary conditions for the potential at contacts, and approximate trial equilibrium
potential values within the device based on approximate trial values for \( n(x) \) and \( p(x) \) in that region. The built-in voltage between contacts on either side of a junction is just the difference in the equilibrium potentials calculated there.

Nonequilibrium boundary conditions for the potential are just the equilibrium values modified by the applied bias.
APPENDIX B

Generalized Poisson Equation

A generalized Poisson equation is derived which takes into account position-dependent permittivity and which is applicable to materials of nonuniform composition.

Starting from Gauss's law,

\[ \nabla \cdot \mathbf{D} = \nabla \cdot \varepsilon \mathbf{E} = \rho \]  \hspace{1cm} (B-1)

the application of a common vector identity (basically the chain rule) yields

\[ \varepsilon (\nabla \cdot \mathbf{E}) + \mathbf{E} \cdot \nabla \varepsilon = \rho \]  \hspace{1cm} (B-2)

Rearranging gives

\[ \nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon} - \frac{1}{\varepsilon} (\mathbf{E} \cdot \nabla \varepsilon) \]  \hspace{1cm} (B-3)

Since

\[ \mathbf{E} = -\nabla \psi \]  \hspace{1cm} (B-4)

(B-3) becomes

\[ -\nabla \cdot \nabla \psi = \frac{\rho}{\varepsilon} + \frac{1}{\varepsilon} (\nabla \psi \cdot \nabla \varepsilon) \]  \hspace{1cm} (B-5)

In terms of the Laplacian operator, (B-5) is written as
\[
\n\nabla^2 \psi = -\frac{\rho}{\varepsilon} - \frac{1}{\varepsilon} (\nabla \psi \cdot \nabla \varepsilon) \quad (B-6)
\]

Expanding the charge density term yields

\[
\nabla^2 \psi = -\frac{q}{\varepsilon} (p - n + N_d^+ - N_a^-) - \frac{1}{\varepsilon} (\nabla \psi \cdot \nabla \varepsilon) \quad (B-7)
\]

In terms of two-dimensional cartesian coordinates

\[
\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\frac{q}{\varepsilon} (p - n + N_d^+ - N_a^-) - \frac{1}{\varepsilon} (\frac{\partial \psi}{\partial x} \frac{\partial \varepsilon}{\partial x} + \frac{\partial \psi}{\partial y} \frac{\partial \varepsilon}{\partial y}). \quad (B-8)
\]

The substitution of difference equations for the derivatives in (B-8) gives the discretized form of (2-29). If permittivities are approximated as weighted averages of their surrounding values, it can be shown that the discretized form of (B-8) will reduce to

\[
\epsilon_{i+1/2,j} \frac{\psi_{i+1,j} - \psi_{i,j}}{h_i} - \epsilon_{i-1/2,j} \frac{\psi_{i,j} - \psi_{i-1,j}}{h_{i-1}} \frac{h_i + h_{i-1}}{2}
\]

\[
+ q \left[ p_{i,j} - n_{i,j} + C_{i,j} \right] = 0 \quad (B-9)
\]
APPENDIX C

Integral-Form of the Current Density Equations

Derivation of the discretized integral-form of the current density equations (one-dimensional) is presented below.

Hole current density

The standard drift-diffusion hole current density equation is

\[
J_p = -q \left( \mu_p p \frac{d\psi}{dx} + D_p \frac{dp}{dx} \right) \quad (C-1)
\]

or,

\[
J_p = -q D_p \left( \frac{\psi'}{V_t} p + \frac{dp}{dx} \right) \quad (C-2)
\]

Separating variables yields

\[
dx = \frac{-1}{J_p \frac{dp}{qD_p} + \frac{\psi'}{V_t} p} \quad (C-3)
\]

Integrating between two adjacent mesh points gives
\[ \int_{x_i}^{x_{i+1}} dx = \int_{p(x_i)}^{p(x_{i+1})} \frac{-1}{J_p \left( \frac{d}{qD_p} + \frac{\psi'}{V_t} \right)} dp \]  \hspace{1cm} (C-4)

Or, assuming that the current density, the diffusion coefficient, and the potential gradient are constant within the integration interval,

\[ x_{i+1} - x_i = -\frac{V_t}{\psi'} \left[ \ln \left( \frac{J_p}{qD_p} + \frac{\psi'}{V_t} p(x_{i+1}) \right) - \ln \left( \frac{J_p}{qD_p} + \frac{\psi'}{V_t} p(x_i) \right) \right] \]  \hspace{1cm} (C-5)

Using the notational conveniences

\[ h_i = x_{i+1} - x_i, \quad u_i = u(x_i), \quad \text{and} \quad u_{i+1/2} = u \left( \frac{x_i + x_{i+1}}{2} \right), \]  \hspace{1cm} (C-6, C-7, C-8)

(C-5) becomes

\[ h_i = -\frac{V_t}{\psi'} \left[ \ln \left( \frac{J_p}{qD_p} + \frac{\psi'}{V_t} p_{i+1} \right) - \ln \left( \frac{J_p}{qD_p} + \frac{\psi'}{V_t} p_i \right) \right] \]  \hspace{1cm} (C-9)

Solving for the current density yields

\[ J_{p_{i+1/2}} = \frac{qD_{p_{i+1/2}} \psi'}{V_t} \frac{1}{\exp \left( \frac{\psi' h_i}{V_t} \right) - 1} \left( p_i - \exp \left( \frac{\psi' h_i}{V_t} \right) p_{i+1} \right) \]  \hspace{1cm} (C-10)
Rearranging in terms of the Bernoulli function, 

\[ B(u) = \frac{u}{\exp(u) - 1}, \quad (C-11) \]

the hole current density equation (C-10) becomes

\[ J_{p, i+1/2} = \frac{qD_{p, i+1/2}}{h_i} \left[ B\left(\frac{\psi' h_i}{V_t}\right) p_i - B\left(\frac{-\psi' h_i}{V_t}\right) p_{i+1} - \exp\left(\frac{\psi' h_i}{V_t}\right) - 1 \right] \quad (C-12) \]

or

\[ J_{p, i+1/2} = \frac{qD_{p, i+1/2}}{h_i} \left[ B\left(\frac{\psi'_{i+1} - \psi'_i}{V_t}\right) p_i - B\left(\frac{\psi'_{i} - \psi'_{i+1}}{V_t}\right) p_{i+1} \right] \quad (C-13) \]

Equation (C-13) is the discretized integral-form of the hole current density equation. It is applicable to uniform composition materials. The hole current density in a nonuniform composition material is modeled by (see Eqn. (2-8))

\[ J_p = \mu_p p \left[ - q \frac{d\psi}{dx} - \frac{d\chi_c}{dx} - \frac{dE_g}{dx} - \frac{kT dp}{p dx} - \frac{kT dN_v}{N_v dx} \right] \quad (C-14) \]
Rearranging yields

\[
J_p = -qD_p \left[ \left( \frac{d\psi + dc}{dx} + \frac{1}{q} \frac{dE_g}{dx} - V_t \frac{1}{N_v} \frac{dN_v}{dx} \right) p + \frac{dp}{dx} \right]
\]  \hspace{1cm} (C-15)

Comparing (C-15) with (C-2), it is seen that the term in parentheses in (C-15) can be thought of as the negative of an effective field. If all of the terms in the effective field term are assumed constant between integration points, the derivation of the discretized integral-form hole current density equation for nonuniform composition materials proceeds in exactly the same manner as in the uniform composition case. The result is

\[
J_{p,i+1/2} = \frac{qD_{p,i+1/2}}{h_i} \left[ B(\arg)p_i - B(-\arg)p_{i+1} \right], \hspace{1cm} (C-16)
\]

where

\[
\arg = \frac{\psi_{i+1} - \psi_i + \chi_{c_{i+1}} - \chi_{c_i} + E_{g_{i+1}} - E_{g_i}}{V_\tau} - \frac{N_v_{i+1} - N_v_i}{N_{v_{i+1/2}}}; \hspace{1cm} (C-17)
\]
Electron Current Density

Using the electron current density equation for uniform composition materials,

\[ J_n = -q \left( \mu_n n \frac{d\psi}{dx} - D_n \frac{dn}{dx} \right), \quad \text{(C-18)} \]

and that for nonuniform composition materials,

\[ J_n = \mu_n n \left[ - q \frac{d\psi}{dx} - \frac{d\chi}{dx} + \frac{kTd}{n} \frac{dn}{dx} - \frac{kTdN_c}{N_c} \right], \quad \text{(C-19)} \]

and proceeding in an exactly analogous fashion as for the hole current density equation, the following result is obtained for the discretized integral-form of the electron current density equation for materials of nonuniform composition:

\[ J_{n_{i+1/2}} = \frac{qD_{n_{i+1/2}}}{h_i} \left[ B(\arg) n_{i+1} - B(\arg) n_i \right], \quad \text{(C-20)} \]

where

\[ \arg = \frac{\psi_{i+1} - \psi_i + \chi_{c_{i+1}} - \chi_{c_i}}{V_{\tau}} + \frac{N_{c_{i+1}} - N_{c_i}}{N_{c_{i+1/2}}}. \quad \text{(C-21)} \]
APPENDIX D

Nonlinear Poisson Equation

The derivation of the nonlinear Poisson equation used in Gummel's method begins with the substitution of (A-1) into (A-3) and (A-2) into (A-4). This yields

\[
n = N_c \exp \left( \frac{E_{Fn} - q(\psi_0 - \psi) + \chi_c}{kT} \right) \quad (D-1)
\]

\[
p = N_v \exp \left( \frac{q(\psi_0 - \psi) - \chi_c - E_g - E_{FP}}{kT} \right) \quad (D-2)
\]

Then, substitution of (D-1) and (D-2) into (B-7) gives the general nonlinear Poisson equation:

\[
\nabla^2 \psi^{g+1} + \frac{1}{\epsilon} (\nabla \psi^{g+1} \cdot \nabla \epsilon) + \frac{q}{\epsilon} \left[ N_v \exp \left( \frac{q(\psi_0 - \psi^{g+1}) + \chi_c - E_g - E_{FP}}{kT} \right) \right] = 0,
\]

\[
- N_c \exp \left( \frac{E_{Fn} - q(\psi_0 - \psi^{g+1}) + \chi_c)}{kT} \right) + C = 0, \quad (D-3)
\]

where \( g \) is an iteration number for the most recently completed Gummel
iteration. The substitution of expressions for $E_{Fn}$ and $E_{Pp}$ (rearrangement of (D-1) and (D-2)) into (D-3) yields the general nonlinear Poisson equation in terms of the desired set of unknowns:

$$
\nabla^2 \psi^{g+1} + \frac{1}{\varepsilon} (\nabla \psi^{g+1} \cdot \nabla \varepsilon) + \frac{q}{\varepsilon} \left[ p \exp \left( \frac{\psi^{g} - \psi^{g+1}}{V_t} \right) - n \exp \left( \frac{\psi^{g+1} - \psi^{g}}{V_t} \right) + C \right] = 0
$$

(D-4)
Accurate solar cell efficiency calculations depend on the accurate calculation of the generation rate within a cell. Not only must the generation rate at all depths be calculated as accurately as possible, but the integral of the calculated generation rate within a cell must not exceed the total photon flux, of energies great enough to be absorbed, transmitted into the cell. An algorithm for implementing the generation rate equation that meets these conditions is based on determining the generation rate, per photon energy, at each discretized depth as a function of the absorption coefficient and the photon flux at that depth, where the photon flux is the flux at the previous depth minus the generation at the previous depth, as depicted in Fig. E-1.

Fig. E-1. Graphical depiction of the implementation of the generation rate equation. Photon flux equals flux minus generation at previous point: $F_{n+1} = F_n - G_n$. 

\[
\begin{align*}
F_0 & \quad F_1 & \quad F_2 & \quad F_3 \\
\downarrow & \quad \downarrow & \quad \downarrow & \quad \downarrow \\
G_0 & \quad G_1 & \quad G_2
\end{align*}
\]
Specifically, the general generation rate equation is
\[
G(y) = \sum_{\lambda} T(\lambda) F(\lambda) \alpha(C(y),\lambda) \exp\left(-\int_{0}^{y} \alpha(C(y),\lambda) \, dy\right)
\] (E-1)

For total transmittance, a single photon energy, and using a simplified notation, (E-1) reduces to
\[
G(y) = F \alpha(y) \exp\left(-\int_{0}^{y} \alpha(y) \, dy\right)
\] (E-2)

If the absorption coefficient is taken as constant between half interval points, the generation rate becomes
\[
G_n(y) = F_n \alpha_n \exp\left(-\alpha_n \, y\right)
\] (E-3)

for depths in the region
\[
\frac{Y_n + Y_{n-1}}{2} \leq y \leq \frac{Y_n + Y_{n+1}}{2}.
\]

The total generation associated with the point \( n \) is then
\[
G_n = \int_{\frac{Y_n + Y_{n-1}}{2}}^{\frac{Y_n + Y_{n+1}}{2}} G_n(y) \, dy
\] (E-4)

If the distance between half interval points around point \( n \) is denoted as \( h_n' \),
then a change in limits and the substitution of (E-3) into (E-4) yields

\[ G_n = \int_0^{h'_n} G(y) \, dy = \int_0^{h'_n} F_n \alpha_n \exp(-\alpha_n y) \quad (E-5) \]

The total generation at mesh point \( n \) is then given by

\[ G_n = F_n \left( 1 - \exp\left(-\alpha_n h'_n\right) \right) \quad (E-6) \]

It follows that the average generation rate about point \( n \) is

\[ G_n(\text{avg}) = \frac{G_n}{h'_n}. \quad (E-7) \]

Now, since (see Fig. E-1)

\[ F_{n+1} = F_n - G_n \quad (E-8) \]

upon the substitution of (E-6), \( F_{n+1} \) becomes

\[ F_{n+1} = F_n \exp(-\alpha_n h'_n). \quad (E-9) \]

Using Eqs. (E-6) to (E-9), the generation rate at all depths can be determined iteratively. The extension of this technique to multiple photon energies is obvious.