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TWO-DIMENSIONAL NUMERICAL ANALYSIS OF
SEMICONDUCTOR DEVICES: APPLICATION
TO BIPOLAR TRANSISTORS

DISSERTATION

Presented in Partial Fulfillment of the Requirements
for the Degree Doctor of Philosophy in the Graduate
School of The Ohio State University

by

David D. Meyer, B.S.E.E., M.S.E.E.

* * * * * * * *

The Ohio State University
1972

Approved by

[Signature]
Adviser
Department of Electrical Engineering
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VITA

January 16, 1939. . . . . Born - Peoria, Illinois

1961. . . . . . . . . . . . B.S.E.E., Purdue University, Lafayette, Indiana

1963. . . . . . . . . . . . M.S.E.E., Purdue University, Lafayette, Indiana


1969-1972 . . . . . . . Graduate Student, The Ohio State University, Columbus, Ohio

FIELDS OF STUDY

Major Field: Electrical Engineering

(1) Studies in Solid State Design. Professor Arthur E. Middleton


(3) Studies in Network Synthesis. Professor William C. Davis
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<tr>
<td>$D_B$</td>
<td>impurity diffusion constant (base)</td>
<td>$DB$</td>
</tr>
<tr>
<td>$D_{BL}$</td>
<td>impurity diffusion constant (buried layer)</td>
<td>$DBL$</td>
</tr>
<tr>
<td>$D_E$</td>
<td>impurity diffusion constant (emitter)</td>
<td>$DE$</td>
</tr>
<tr>
<td>$D_{ISO}$</td>
<td>impurity diffusion constant (isolation)</td>
<td>$DISO$</td>
</tr>
<tr>
<td>$D_n$</td>
<td>electron diffusion constant</td>
<td></td>
</tr>
<tr>
<td>$D_p$</td>
<td>hole diffusion constant</td>
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</tr>
<tr>
<td>$E$</td>
<td>electric field intensity</td>
<td>$FIELDX, FIELDY$</td>
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<td>$J$</td>
<td>total current density</td>
<td>$TOCURX, TOCURY$</td>
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<td>$J_n$</td>
<td>electron current density</td>
<td>$CURNX, CURNY$</td>
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<td>$J_p$</td>
<td>hole current density</td>
<td>$CURPX, CURPY$</td>
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<td>normalization length</td>
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<td>electron concentration</td>
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<td>$n_i$</td>
<td>intrinsic carrier concentration</td>
<td>$CI$</td>
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<td>$n_1$</td>
<td>electron concentration for Fermi level at trap level</td>
<td>$CN1$</td>
</tr>
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<td>$N_A$</td>
<td>accepter concentration</td>
<td>$CA$</td>
</tr>
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<td>$N_D$</td>
<td>donor concentration</td>
<td>$CD$</td>
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<td>donor minus acceptor concentration</td>
<td>CDIFF</td>
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<tr>
<td>N_SUM</td>
<td>donor plus acceptor concentration</td>
<td>CSUM</td>
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<td>N_v</td>
<td>valence band effective density of states</td>
<td></td>
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<tr>
<td>N_c</td>
<td>conduction band effective density of states</td>
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<td>p</td>
<td>hole concentration</td>
<td>CP</td>
</tr>
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<td>P_0</td>
<td>thermal equilibrium hole concentration</td>
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<td>P_l</td>
<td>hole concentration for Fermi level at trap level</td>
<td>CPL</td>
</tr>
<tr>
<td>q</td>
<td>electronic charge</td>
<td>Q</td>
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<td>r_{n+1}</td>
<td>acceleration factors for iterative methods</td>
<td>ACC</td>
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<tr>
<td>R_n</td>
<td>electron recombination-generation rate</td>
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<td>R_p</td>
<td>hole recombination-generation rate</td>
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<td>R_{X(i)}</td>
<td>i^{th} spatial step in x-direction</td>
<td>RX(I)</td>
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<td>j^{th} spatial step in y-direction</td>
<td>RY(J)</td>
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<td>S_{X(i)}</td>
<td>i^{th} spatial step in x-direction</td>
<td>SX(I)</td>
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<td>j^{th} spatial step in y-direction</td>
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<td>i^{th} spatial step in x-direction</td>
<td>SSX(I)</td>
</tr>
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<td>S_{SY(j)}</td>
<td>j^{th} spatial step in y-direction</td>
<td>SSY(J)</td>
</tr>
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<td>V_D</td>
<td>diffusion potential</td>
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<td>V_T</td>
<td>normalization potential</td>
<td>VT</td>
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<tr>
<td>\alpha_p</td>
<td>generalized Einstein relation for holes</td>
<td>AP</td>
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<td>\alpha_n</td>
<td>generalized Einstein relation for electrons</td>
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<td>\xi_p</td>
<td>hole chemical potential</td>
<td>ZETAP</td>
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<td>\xi_n</td>
<td>electron chemical potential</td>
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</tr>
<tr>
<td>$\mu_P$</td>
<td>hole mobility</td>
<td>SMP</td>
</tr>
<tr>
<td>$\mu_n$</td>
<td>electron mobility</td>
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<td>$\Phi_G$</td>
<td>band gap potential</td>
<td>GAP</td>
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<td>$\Phi_P$</td>
<td>hole quasi-Fermi level</td>
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<td>electron quasi-Fermi level</td>
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<td>$\Psi_V$</td>
<td>valence band edge potential</td>
<td>PSI</td>
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INTRODUCTION

The importance of accurate computational performance evaluations of semiconductor devices has been recognized recently especially since the advent of high performance devices constructed by precise process control and technology. It has become evident that the standard assumptions used to achieve a linear set of equations do not characterize the high performance semiconductor devices with sufficient accuracy. In the past few years, several articles have been published which use numerical methods to solve the basic set of nonlinear equations which describe the semiconductor device. In this way, the following normal 'first-order' assumptions given below can be eliminated.

(a) Doping profiles are taken to be step or linear graded distributions or some combination of the two. The profiles are considered to be symmetric or highly asymmetric.

(b) The physical structure of the device is separated into regions with abrupt boundaries which are either fully depleted of mobile carriers or space-charge neutral.

(c) Carrier mobilities are considered to be constants and independent of electric field and doping.

(d) The carrier recombination laws are either neglected or restricted to low-level linear cases.

(e) External boundary conditions are considered to be ohmic
and explicit boundary conditions of the relevant quantities are given for the internal interfaces defined by the assumptions in (b).

(f) Minority carrier currents are considered to be totally diffusive in nature and the drift currents are neglected. These and other 'first-order' assumptions are not required if numerical methods are used to solve the basic set of nonlinear equations which include Poisson's equation, carrier continuity equations, and carrier transport equations.

Several articles have been published which consider the semiconductor device as a one-dimensional structure. One of the major early articles is by Gummel[1] which describes a self-consistent iterative scheme which solves the nonlinear one-dimensional equations but for certain boundary conditions converges very slowly or is unstable. Since then, many authors[2,3,4,5,6,7,8,9] have worked to improve the numerical methods and have succeeded to a great extent to develop efficient numerical techniques to solve the one-dimensional nonlinear equations. However, by the very nature of one-dimensional analysis, many effects which occur in high performance semiconductor devices can not be accurately determined. Effects such as emitter current crowding, lateral current flow, base resistance, oxide-semiconductor interface, etc. are very difficult if not impossible to determine accurately with a one-dimensional model of a semiconductor device.

In order to improve upon the semiconductor modeling techniques, Kennedy[10,11,12], Reiser[13], Collins[14], Vandorpe and Xuong[15],
Slotboom[16], and Heydemann[17] have extended the numerical methods to various two-dimensional models of junction field effect transistors and bipolar transistors. The semiconductor models of these authors are in general simplified and idealized versions of the actual physical device. For example, the isolation, buried layer, and usually the substrate regions have been neglected, and degenerate material effects have not been considered. The numerical methods which are used to solve the basic nonlinear semiconductor equations range from relaxation methods to more advanced alternating direction implicit methods. Kennedy is the only author who uses numerical methods to accurately determine the two-dimensional impurity atom concentrations.

It is the purpose of the present work to introduce a two-dimensional numerical method for the determination of the impurity atom distributions from the parabolic diffusion equation. The numerical diffusion method is shown to be extremely efficient and accurate and has the capabilities of considering spatial variations in the impurity diffusion constant. Also, the initial formulation of a two-dimensional numerical method for semiconductor device modeling which accurately considers degenerate materials is presented. Finally, the two numerical methods are applied to an integrated silicon N-P-N transistor model which includes the isolation region and a buried layer and to a diode model.

The two-dimensional numerical method for the solution of the diffusion equation utilizes the integral formulation of the finite difference approximations and the Peaceman-Rachford[24] alternating
direction implicit (ADI) method. The numerical diffusion algorithm is utilized in determining the emitter, base, and buried layer diffusions. To illustrate the capabilities of this method, the impurity diffusion constant of the emitter diffusion is assumed to be a function of the base acceptor concentration and thus varies with position. Also, the differences between the 'emitter push' effect (EPE) base diffusion and the idealized (planar) base diffusion are illustrated by using a spatially enhanced impurity diffusion constant for the base diffusion in the emitter region. The numerical diffusion method is shown to be an extremely efficient algorithm and is greater than 60 times more efficient than the analytical method of Kennedy and O'Brien[26]. As is shown in the diffusion computer program in the appendices, the ADI method is straight-forward and easy to program as compared to the rather random procedures of the simple relaxation methods of Kennedy and Murley[18]. Once the ADI method is understood, the modification of the diffusion computer program to simulate other semiconductor devices and structures is obvious. The accuracy of the ADI method seems to depend almost solely on the mesh structure selected for the semiconductor model. The mesh structure requirement is illustrated by the analysis of an integrated diode. Therefore, the numerical diffusion algorithm is shown to be a straight-forward and efficient method and is a significant advance in the area of diffusion modeling.

The formulation of the two-dimensional numerical method for the analysis of semiconductor devices is also given. To accurately characterize the degenerate material in the emitter and base regions, the
Fermi-Dirac integral evaluation for the carrier concentrations is used. Two different numerical algorithms are developed to solve the two-dimensional, nonlinear, elliptic equations which describe semiconductor materials. The nonlinear elements of the elliptic equations are shown to be quite involved. The two numerical algorithms presented in this work for the semiconductor device modeling have not fully achieved operational status due to numerical error problems associated with the insufficient density of nodes in the mesh structure. The problem areas are defined and discussed in detail, and the basic computer requirements for the numerical algorithms are stated. Thus, no computational results are obtained from the semiconductor device algorithms, and the computer programs in the appendices are presented as examples of the numerical methods and not as operational programs. The first numerical method given for the semiconductor device method is the simplest method for solving nonlinear elliptic equations and thus must function properly if the nonlinear equations of the formulation are to be solved. The numerical error which inhibits this numerical method is illustrated and shown to be a strong function of the node density of the mesh structure.

The presentation is divided into five chapters with Chapter I containing a general discussion of the formulation and the limitations of the basic equations which comprise the diffusion and the semiconductor device models. Also, the N-P-N transistor model's physical structure and its finite difference mesh structure are described. Chapter II contains the analytical formulation and numerical methods for the
diffusion and the semiconductor device models. For the semiconductor device model, the linearization, discretization, and iterative methods are discussed as well as the functional relationships which are used to represent the carrier density relations, the mobility variations, and the recombination-generation law in the model. The computational results for the diffusion processes and the thermal equilibrium values for the semiconductor device model are given in Chapter III. Numerical problems which occur in the semiconductor device model are discussed and analyzed. Chapter IV presents the discussion and conclusions of the diffusion and the semiconductor device models. Detailed discussions of the limitations, problem areas, and possible solutions to the problems of the semiconductor device model are also given. The recommendations in Chapter V describe the present state of the diffusion and the semiconductor device models and the possible improvements and future extensions to the models.

The appendices contain the detailed data concerning the physical properties of the simulated silicon N-P-N transistor and a discussion of the mesh structure selection. The various finite difference formulations used throughout the work are presented. A discussion of the accuracy of the numerical methods is also given in the appendices. The computer programs for the diffusion and the semiconductor device models are listed.
CHAPTER I

FORMULATION OF DIFFUSION AND SEMICONDUCTOR DEVICE
EQUATIONS AND BIPOLAR TRANSISTOR MODEL DESCRIPTION

The two-dimensional numerical simulation of semiconductor devices requires computational models to accurately represent the physical structure of the device and determine the electronic charge flow and variation of potential within the device. To achieve this, two computational methods are developed in this work. A diffusion model determines the impurity atom concentrations within the semiconductor device. A semiconductor device model then solves the nonlinear equations which govern the electron and hole concentrations and the potential throughout the device. The basic equations which constitute the diffusion model and the semiconductor device model are presented, and the assumptions and limitations involved in the models are discussed. The bipolar transistor model which is used to illustrate the capabilities of the diffusion and semiconductor device models is described in terms of its physical structure and its finite difference mesh structure which defines the transistor model for the numerical computations.

1.1 Diffusion Analysis

To simulate accurately semiconductor devices produced by diffusion of impurity atoms, it is necessary to define a diffusion model to
compute the impurity atom distribution. The diffusion model used in this work is a modification of the method described by Kennedy and Murley[18].

1.1.1 Physical Model

It is assumed that the impurity atom distributions produced by the diffusion processes are described accurately by the solution of the elementary diffusion equation. Certain assumptions are made in order to greatly simplify the boundary value problem. First, the surface of the device model is assumed to be stationary and planar. This assumption significantly simplifies the numerical development but does not correspond well to the nonstationary stair-step effect which occurs during a normal series of diffusion processes in the fabrication of bipolar transistors. The oxide layer is assumed to instantaneously form an impenetrable barrier to impurity atoms and is assumed to be neither a source nor sink of impurity atoms. The individual diffusion processes are assumed to be independent of each other except in the case where the diffusion constant is a function of the impurity atom concentration already existing in the device model. However, the temperature cycles which occur after the preceding diffusion process are taken into account by modifying the diffusion constant-time product. Finally, the path along the semiconductor-oxide interface is assumed to have the same diffusion constant as the bulk material so that enhanced diffusion does not occur along the interface.
1.1.2 Mathematical Formulation

The elementary diffusion equation,

\[ \frac{\partial}{\partial x} (D(x,y) \frac{\partial N}{\partial x}) + \frac{\partial}{\partial y} (D(x,y) \frac{\partial N}{\partial y}) = \frac{\partial N}{\partial t} \]  

(1.1)

where \( N(x,y,t) \) is the impurity atom concentration and \( D \) is the impurity diffusion constant, is assumed to describe the results of the various diffusion processes accurately. In order to simulate the actual process conditions occurring during the various diffusion cycles, two types of boundary conditions are used. First, a constant impurity atom concentration is assigned to the surface which is not covered by an oxide layer and thus is directly exposed to a constant source of impurity atoms during the diffusion cycle. The second type of boundary condition occurs when the surface is covered by an impenetrable oxide layer. Since no impurity atoms can cross the surface, the normal derivative of the impurity atom concentration is zero at the surface. See Figure 2.

\[
\begin{align*}
N(\text{surface}) &= C_0 \quad \text{for oxide-free surfaces} \\
N(\text{internal}) &= C_B \quad \text{for boundaries within the device} \\
\frac{\partial N}{\partial y}(\text{surface}) &= 0 \quad \text{for oxide-covered surfaces} \\
\frac{\partial N}{\partial y}(\text{symmetry}) &= 0 \quad \text{for boundaries between symmetrical regions}
\end{align*}
\]

1.2 Semiconductor Device Equations

The basic set of nonlinear semiconductor equations which describes the behavior of the semiconductor device is presented for the
two-dimensional steady state case. The set of nonlinear equations is normalized into dimensionless form in order to simplify the notation and to clarify the mathematical manipulations. These dimensionless equations are then rearranged into a set of three nonlinear, second-order, partial differential equations which are more conducive to an iterative procedure of solution. The set of three equations is designated in this work as the reduced semiconductor device equations. The boundary conditions for the carrier concentrations and potentials are given to complete the basic mathematical description of the semiconductor device model.

1.2.1 Physical and Mathematical Model

In formulating the basic set of semiconductor device equations, certain assumptions are made to greatly simplify the basic equations.

(a) constant temperature (T = 300°K in this work)

(b) time-independent impurity atom distribution

(c) complete ionization of the impurity atoms

(d) no applied magnetic fields

(e) steady state conditions

The following equations are assumed to accurately describe the behavior of semiconductor devices, particularly junction devices. Although more general and complete formulations of the problem may be devised, this set of equations is normally considered to be a fundamental set and is used since it can be manipulated to a form which is suitable for iterative techniques.

The first two equations are the hole and electron continuity
equations.

\[
\frac{\partial n}{\partial t} = 0 = \nabla \cdot \overrightarrow{J}_n - qR_n \tag{1.2}
\]

\[
\frac{\partial p}{\partial t} = 0 = -\nabla \cdot \overrightarrow{J}_p - qR_p \tag{1.3}
\]

where \(R_n\) and \(R_p\) represent the net rate of recombination over generation of electrons and holes, respectively. It is assumed that the recombination-generation process can be adequately defined by an additive term solely in the continuity equations. The next two equations are a conventional form of the solution to the Boltzmann transport equation. A conventional approximation of the solution treats the hole and electron current densities as a sum of a diffusion component proportional to the carrier density gradient and a drift component which is a form of Ohm's law.

\[
\overrightarrow{J}_n = qD_n \nabla n + qu_n n \overrightarrow{E} \tag{1.4}
\]

\[
\overrightarrow{J}_p = -qD_p \nabla p + qu_p p \overrightarrow{E} \tag{1.5}
\]

In employing this approximate solution to the Boltzmann equation, several significant assumptions are made which seriously limit the validity of the basic set of equations. The approximate solution assumes that the electric field is small. Thus, regions such as the transition of a P-N junction, the enhanced channel of a MOSFET, and ohmic contacts are not accurately described by these current density relations.

This approximate solution of the Boltzmann transport equation is valid when the distribution function is relatively close to the equi-
librium distribution function so that the solution is only valid for situations which are close to the equilibrium conditions. In the derivation of the drift current density term, the assumption is made that the drift velocity is much less than the thermal velocity so that the lifetimes of the carriers are determined primarily by their equilibrium distribution of velocities after their last collision. Thus, when the drift velocity becomes comparable with the thermal velocity, the assumption breaks down, and the Ohm's law form of the drift current density is no longer valid.

While the conventional Boltzmann transport equation is written for each band separately if the interactions between different bands can be neglected, the Boltzmann transport equation can be modified (see, for example, Smith, Janak, and Adler[19]) to take into account the changes in the electron concentrations due to interband transitions. Assuming a simple relaxation-time approximation for the interband scattering transitions, the recombination time or lifetime is assumed to be large as compared to the intraband relaxation times. This assumption implies that if the equilibrium distribution is disturbed, the distribution function for the electrons in the conduction band will rapidly return to a quasi-equilibrium distribution, and then the conduction band quasi-equilibrium distribution will gradually relax to an equilibrium state with the valence band. Another assumption which is used in obtaining Equations (1.4) and (1.5) is that the semiconductor is nondegenerate so that the Boltzmann distribution function can be used. Thus, the small electric field and the nondegenerate material assumptions seriously limit the
validity of the basic set of semiconductor equations. Later, the restriction of degenerate material is diminished by a different solution to the Boltzmann transport equation which does not use the Boltzmann distribution function.

The final equation of the set of basic semiconductor equations is Poisson's equation.

\[ \nabla \cdot \mathbf{E} = \frac{q}{\varepsilon} (p - n + N_D - N_A) \quad (1.6) \]

Inherent in this equation is the assumption that all impurity atoms are ionized. At the temperature of 300°C, this is a valid assumption for the impurities considered in the various diffusions. However, at lower temperatures or for impurities with energy levels further from the band edges, this assumption would not be justified, and partial ionization should be considered.

Several subsidiary relations are used to relate the various variables. Since steady state conditions are assumed, the displacement current is zero so

\[ \mathbf{J} = J_n + J_p \quad (1.7) \]

In order to consider nonequilibrium conditions, quasi-Fermi potentials are defined as

\[ \phi_p \equiv \psi_v + \zeta_p (p) \quad (1.8) \]
\[ \phi_n \equiv \psi_v - \phi_v - \zeta_n (n) \quad (1.9) \]
where \( \Phi_p \) and \( \Phi_n \) are the hole and electron quasi-Fermi levels, \( \zeta_p \) and \( \zeta_n \) are the hole and electron chemical potentials, \( \phi_G \) is the band gap potential, and \( \Psi_v \) is the valence band edge potential. Figure 1 illustrates these potentials and indicates their polarities. The electric field is the negative gradient of the valence band edge potential.

\[
E = - \nabla \Psi_v
\]

(1.10)

In order to consider the effects of degenerate material, the current density equations (1.4) and (1.5) can be modified by solving the Boltzmann transport equation without the assumption of the Boltzmann distribution function. The current density equations can then be written as

\[
\begin{align*}
\vec{J}_p &= q \mu_p \left[ p \vec{E} - (kT/q) \alpha_p(p) \nabla p \right] \\
\vec{J}_n &= q \mu_n \left[ n \vec{E} + (kT/q) \alpha_n(n) \nabla n \right]
\end{align*}
\]

(1.11)

(1.12)

where

\[
\begin{align*}
\alpha_p(p) &= \left( q/kT \right) \left( D_p/\mu_p \right) = \left( q/kT \right) \left( \partial \zeta_p(p) / \partial \ln p \right) > 1 \\
\alpha_n(n) &= \left( q/kT \right) \left( D_n/\mu_n \right) = \left( q/kT \right) \left( \partial \zeta_n(n) / \partial \ln n \right) > 1
\end{align*}
\]

(1.13)

(1.14)

The relations (1.13) and (1.14) show that the diffusion constants are nonlinear, monotonically increasing functions of the carrier density and can be considered as generalized Einstein relations which are valid for degenerate and nondegenerate materials since the limits of the generalized Einstein relations are unity as the carrier concentrations decrease.
FIGURE 1. Potential Diagrams
to zero. A development of these equations and relations is given in Spenke[20].

1.2.2 Normalization of Basic Equations

It is convenient to normalize the relevant parameters to dimensionless form in order to considerably simplify and clarify the analysis. The list of normalization factors is given in Table 1. This normalization which is presented for silicon decreases the wide range of values for the various concentrations to smaller ranges which can be handled with more accuracy by the computer. The hole and electron diffusion constants are normalized in a symmetrical fashion with the use of an arbitrary diffusion constant $D_0$ which is equal to 1.0 cm$^2$/sec. It should be noted that the symbols adopted for the unnormalized quantities will also be used for the normalized quantities in order to reduce the number of extra symbols and confusion. Thus, from this point, all quantities will be normalized unless specifically stated otherwise.

The basic set of equations may be written in normalized terms as

\begin{align}
\bar{J} &= \bar{J}_n + \bar{J}_p \\
\bar{J}_n &= \mu_n [nE + \alpha_n(n) \nabla n] \\
\bar{J}_p &= \mu_p [pE - \alpha_p(p) \nabla p] \\
\nabla \cdot \bar{F} &= p - n + N_D - N_A = - \nabla^2 \psi_v \\
\nabla \cdot \bar{J}_n &= R
\end{align}

(1.15)  (1.16)  (1.17)  (1.18)  (1.19)
<table>
<thead>
<tr>
<th>DESCRIPTION</th>
<th>NORMALIZED QUANTITY</th>
<th>SYMBOL</th>
<th>NORMALIZATION FACTOR</th>
</tr>
</thead>
<tbody>
<tr>
<td>position coordinates</td>
<td>$x, y$</td>
<td>$L_D = \sqrt{eV_T/qn_i}$</td>
<td>$3.396938 \times 10^{-3}$ cm</td>
</tr>
<tr>
<td>electrostatic potential</td>
<td>$\psi$</td>
<td>$V_T = kT/q$</td>
<td>$0.025875$ volts</td>
</tr>
<tr>
<td>quasi-Fermi potentials</td>
<td>$\phi_n, \phi_p$</td>
<td>$V_T$</td>
<td>$0.025875$ volts</td>
</tr>
<tr>
<td>chemical potentials</td>
<td>$\xi_n, \xi_p$</td>
<td>$V_T$</td>
<td>$0.025875$ volts</td>
</tr>
<tr>
<td>applied voltages</td>
<td>$V_{BE}, V_{CB}, V_{IC}$</td>
<td>$V_T$</td>
<td>$0.025875$ volts</td>
</tr>
<tr>
<td>diffusion voltage</td>
<td>$V_D$</td>
<td>$V_T$</td>
<td>$0.025875$ volts</td>
</tr>
<tr>
<td>electric field</td>
<td>$E$</td>
<td>$V_T/L_D$</td>
<td>$7.617154$ volts/cm</td>
</tr>
<tr>
<td>carrier densities</td>
<td>$n, p$</td>
<td>$n_i$</td>
<td>$1.45 \times 10^{10}$ cm$^{-3}$</td>
</tr>
<tr>
<td>impurity densities</td>
<td>$N_D, N_A$</td>
<td>$n_i$</td>
<td>$1.45 \times 10^{10}$ cm$^{-3}$</td>
</tr>
<tr>
<td>current densities</td>
<td>$J, J_n, J_p$</td>
<td>$qD_0 n_i/L_D$</td>
<td>$6.838217 \times 10^{-7}$ amp/cm$^2$</td>
</tr>
<tr>
<td>recombination rates</td>
<td>$R, R_n, R_p$</td>
<td>$D_0 n_i^2/L_D^2$</td>
<td>$1.256588 \times 10^{15}$ cm$^{-3}$sec$^{-1}$</td>
</tr>
<tr>
<td>carrier mobilities</td>
<td>$\mu_n, \mu_p$</td>
<td>$D_0/V_T$</td>
<td>$38.64734$ cm$^2$/volt-sec</td>
</tr>
<tr>
<td>carrier diffusion</td>
<td>$D_n, D_p$</td>
<td>$D_0$</td>
<td>$1.0$ cm$^2$/sec</td>
</tr>
</tbody>
</table>
\[ \nabla \cdot \mathbf{J}_p = -R \]  

(1.20)

In addition, the quasi-Fermi potential equations (1.8) and (1.9) are normalized and have the same form.

1.2.3 Boundary Conditions

The three independent variables of the basic set of semiconductor equations are chosen as the electron concentration \( n \), the hole concentration \( p \), and the valence band edge potential \( \psi_v \) from considerations of the simplicity of the normalized set of equations and of degenerate material. The reference level of the valence band edge potential is arbitrary so the base contact is defined to be at zero potential.

Figure 2 shows the basic cross-sectional view of the bipolar transistor model used in this work.

There are four different types of boundaries in the device model to be considered. Similar types of boundary conditions are required for any semiconductor device model. Boundary conditions on the electron and hole concentrations and the valence band edge potential are required for the contacts, the buried layer internal surface, the isolation and substrate surfaces, and the oxide-semiconductor interface. Ohmic contacts are assumed for the emitter, base, collector, and isolation contacts. If nonohmic contacts were desired, a contact potential could be created. The ohmic contact assumption requires that the electron and hole densities must be equal to the thermal equilibrium values of \( n_o \) and \( p_o \), respectively. However, it should be noted that the product of \( n_o \) and \( p_o \)
Figure 2. Cross-sectional View of Transistor Model
does not necessarily equal the square of the intrinsic carrier concentration when Fermi-Dirac statistics are utilized to describe degenerate material carrier concentrations (for example, see Blakemore[21]). This condition is equivalent to requiring that the quasi-Fermi levels $\phi_p$ and $\phi_n$ be equal at the contacts. Since the excess carrier densities are zero at the contacts, the assumption of space charge neutrality is valid. Thus, at the contacts

$$P_o - n_o + N_D - N_A = 0 \quad (1.21)$$

can be inserted into the definitions of the quasi-Fermi potentials to develop the condition that

$$\zeta_p(P_o) + \zeta_n(P_o + N_D - N_A) + \phi_C = 0 \quad (1.22)$$

at the ohmic contacts. This equation can be solved by iterative methods at each contact.

The boundary conditions for the buried layer are somewhat more restrictive since the buried layer internal surface is created by the finite dimensions of the device model and thus is artificial. It is normally assumed that the majority of the lateral collector current flows in the first few microns of the buried layer diffusion. It is assumed that the total perpendicular current density is zero at the buried layer surface. This assumption can be realized if the normal current densities for the holes and electrons are zero individually at the surface. One method of achieving this is to make the normal derivatives of the electron and hole concentrations and the valence band edge potential equal.
to zero, or

$$\frac{\partial n}{\partial y} = \frac{\partial p}{\partial y} = \frac{\partial n_y}{\partial y} = 0$$  \hspace{0.5cm} (1.23)$$

at the buried layer surface. This type of boundary condition is very convenient from a numerical viewpoint.

The boundary conditions for the oxide-semiconductor interface are difficult to generate without assuming rather unrealistic conditions to exist at the interface. In the literature\[13,15,16,17\], the boundary conditions are assumed to be of the form of Equation (1.23). This flat-band condition is rather restrictive. In order to investigate other possible boundary conditions for the oxide-semiconductor interface, the main requirement is that the normal total current density is zero at the interface. After investigating the possible boundary conditions, it was concluded that it is extremely difficult if not impossible to derive a set of simple boundary conditions from the assumption that the total normal current density is zero since the mobilities are functions of the electric field and the generalized Einstein relations are functions of the carrier concentrations. Thus, the boundary conditions of Equation (1.23) are assumed, but the lifetimes of the recombination-generation law and the mobilities can be altered near the interface to diminish the restrictive nature of these boundary conditions.

The boundary conditions for the isolation and substrate surfaces are also somewhat artificial mainly due to the limited amount of isolation and substrate regions contained in the device model. The isolation con-
tact regions are treated as the other contact areas. After consideration of many possible boundary conditions, two types of boundary conditions are used in this work for the isolation and substrate surfaces. First, the surfaces can be considered to be sufficiently far from the nonequilibrium regions that the surfaces can be considered in thermal equilibrium. Constant values of $n$, $p$, and $\psi_V$ can be determined at each surface point by Equation (1.22). The second type of boundary condition which is considered assumes that the total normal current density is zero at the surfaces. This condition implies that all of the isolation leakage current flows through the isolation contact which is not precisely true. In order to implement the second boundary condition, the boundary conditions of Equation (1.23) are used.

The relationships between the valence band edge potentials at the contacts are fixed by the external sources for which

\[
\psi_{VB} - \psi_{VB} = V_{BE} - V_{D(BE)}
\]

\[
\psi_{VC} - \psi_{VB} = V_{CB} + V_{D(CB)}
\]

\[
\psi_{VI} - \psi_{VC} = V_{IC} - V_{D(IC)}
\]

(1.24)

can be written where, for example, $\psi_{VI}$ is the valence band edge potential of the isolation contact, $V_{D(IC)}$ is the diffusion potential between the isolation and the collector contacts, and $V_{IC}$ is the applied potential between the isolation and collector contacts. In order to define the diffusion potentials, an assumption is made. The diffusion potentials are defined under the conditions of thermal equilibrium and
are assumed to remain constant for nonequilibrium conditions. From one-dimensional analysis[8], this assumption appears to be valid for forward and low-to-medium reverse bias. At high reverse bias, the actual applied potential may be slightly larger than the applied potential of the boundary condition.

With the valence band edge potential at the base contact fixed at zero reference, the following relations can be derived under the conditions of thermal equilibrium at the contacts. See Figure 1.

\[ \psi_{VC} = \xi_{PB} - \xi_{PC} \]  
\[ \psi_{VE} = \xi_{PB} - \xi_{PE} \]  
\[ \psi_{VI} = \xi_{PB} - \xi_{PI} \]  \hspace{1cm} (1.25) \hspace{1cm} (1.26) \hspace{1cm} (1.27)

If voltage bias is applied to the contacts, the following relations can be derived.

\[ V_{BE} = \phi_{PB} - \phi_{nE} \]  \hspace{1cm} (1.28)
\[ V_{CB} = \phi_{nC} - \phi_{PB} \]  \hspace{1cm} (1.29)
\[ V_{IC} = \phi_{PI} - \phi_{nC} \]  \hspace{1cm} (1.30)

where the normal polarity convention is used. Solving for the valence band edge potentials at the contacts,

\[ \psi_{VC} = V_{CB} - \xi_{PE} + \xi_{PB} \]  \hspace{1cm} (1.31)
\[ \psi_{VI} = V_{IC} + V_{CB} - \xi_{PI} + \xi_{PB} \]  \hspace{1cm} (1.32)
1.3 Bipolar Transistor Model

The physical device model which is used to illustrate the numerical methods in the diffusion model and the semiconductor device model is a bipolar N-P-N transistor in integrated circuit form. The bipolar transistor model has two different forms. The first form consists of an idealized transistor model which does not have an extended base region due to EPE. The second form consists of an EPE transistor which has a nonplanar base region. Figure 2 shows the cross-sectional view of the transistor, and Figure 3 shows the top view.

1.3.1 Device Structure

The N-P-N silicon transistor model which is used in this work is a basic integrated circuit transistor with diffused sidewall isolation regions and a diffused buried layer region. The transistor model, which is an idealized version of the D3 transistor developed by the Integrated Circuits Group at the Avionics Laboratory at Wright-Patterson Air Force Base, is an asymmetrical design with only one base stripe. The detailed data concerning this device is in Appendix A. From the numerical results of the diffusion model, Figures 4 and 5 show the approximate donor and acceptor impurity atom concentrations for the transistor model. The emitter-base junction is located 0.6 microns below the surface, and the base-collector junction without EPE is 1.2 microns deep. The change in

\[ \psi_{VE} = -V_{BE} - \zeta_{PE} + \zeta_{PB} \]
Figure 3. Top View of Transistor Model
Figure 4  Donor Impurity Atom Concentrations
Figure 5. Acceptor Impurity Atom Concentrations
the base-collector junction depth due to EPE is 0.2 microns. The final epitaxial layer thickness is 5.0 microns.

1.3.2 Mesh Structure

In order to use finite difference methods in the solution of the two-dimensional partial differential equations, it is necessary to represent the physical model of the semiconductor device by a two-dimensional array of nodes or mesh structure. The selection of the mesh structure is discussed in detail in Appendix B. For the N-P-N transistor model considered in this work, a region of 100 by 6 microns is taken as the model area and contains the complete emitter, base, and collector regions and part of the isolation, substrate, and buried layer areas. In order to decrease the truncation error due to the large gradients of various quantities, a nonuniform grid structure is selected which concentrates nodes in the junction and contact regions. Figure 6 shows the basic mesh structure which contains 52 horizontal lines and 100 vertical lines which creates 5200 nodes. The superposition of the transistor model structure on the mesh structure is shown in Figure 7 which shows the location of the junctions relative to the mesh structure. The heavy lines on the surface of the mesh structure in Figure 7 indicate the contact regions. For future reference, it should be noted that the x-direction is parallel to the surface of the transistor model, and the y-direction extends down into the model region.
Figure 6. Mesh Structure
Figure 7. Superposition of Transistor Model on Mesh Structure
CHAPTER II

ANALYTICAL FORMULATION AND NUMERICAL METHODS

The diffusion model and the semiconductor device model are defined by the equations in Chapter I. For the diffusion model, the linear parabolic two-dimensional diffusion equation (1.1) is solved by implicit numerical methods. The semiconductor device model can be clarified by combining the basic semiconductor equations (1.15) to (1.20) into three two-dimensional nonlinear elliptical equations which are called the reduced set of semiconductor equations. The reduced set of semiconductor equations are linearized and solved by iterative numerical methods. Table 2 contains a summary of the notation used in this chapter.

2.1 Diffusion Model

2.1.1 Numerical Methods

Several numerical methods which employ finite difference approximations can be used to solve the two-dimensional diffusion equation with mixed boundary conditions which are given in texts such as Forsythe and Wasow[22] and Ames[23]. Basically, the numerical methods can be generally classified into two broad categories, explicit and implicit. In general, explicit methods are stable and converge
### TABLE 2. NOTATION FOR NUMERICAL METHODS

- **X(i)** = value of x-coordinate at line i
- **Y(j)** = value of y-coordinate at line j
- **SX(i)** = \(X(i+1) - X(i)\) = forward x-step magnitude at line i
- **SY(j)** = \(Y(j+1) - Y(j)\) = forward y-step magnitude at line j
- **SSX(i)** = **SX(i)** + **SX(i-1)** = sum of consecutive x-steps at line i
- **SSY(j)** = **SY(j)** + **SY(j-1)** = sum of consecutive y-steps at line j
- **RX(i)** = **SX(i)**/**SX(i-1)** = ratio of consecutive x-steps at line i
- **RY(j)** = **SY(j)**/**SY(j-1)** = ratio of consecutive y-steps at line j
- **U(i,j)** = value of continuous function \(U(x,y)\) at node \((i,j)\)
- **U(i,j,t)** = value of continuous function \(U(x,y)\) at node \((i,j)\) and time \(t\)
- **U_x(i,j)** = \(\partial U(i,j)/\partial x\) = first partial derivative in x-direction evaluated at node \((i,j)\)
- **U_y(i,j)** = \(\partial U(i,j)/\partial y\) = first partial derivative in y-direction evaluated at node \((i,j)\)
- **U_{xx}(i,j)** = \(\partial^2 U(i,j)/\partial x^2\) = second partial derivative in x-direction evaluated at node \((i,j)\)
- **U_{yy}(i,j)** = \(\partial^2 U(i,j)/\partial y^2\) = second partial derivative in y-direction evaluated at node \((i,j)\)
- **U^m(i,j)** = value of \(U(i,j)\) at the \(m^{th}\) inner iteration cycle and the \(m^{th}\) outer iteration cycle
to the solution of the diffusion equation only if

\[ D\Delta t \left[ \frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} \right] \leq \frac{1}{2} \]

where \( D \) is the impurity diffusion constant, \( \Delta t \) is the maximum time step, \( \Delta x \) and \( \Delta y \) are the minimum spatial steps. Thus for small mesh spatial steps and large diffusion constants as in the emitter diffusion, the time step must be extremely small, for example, less than ten seconds for the emitter diffusion, and this condition would require excessive computation time. To alleviate the diffusion constant-time step-mesh spacing limiting condition, various implicit methods have been devised. In this work, the Peaceman and Rachford implicit method [24] which is an 'alternating-direction implicit method' or ADI method is used since it decreases the number of simultaneous linear equations which must be solved at each time step. It should be noted that there are other ADI methods than this one, but the Peaceman and Rachford method seems to be the best suited for the solution of the two-dimensional parabolic diffusion equation. In the ADI method, the process of passing from the time \( t \) to \( t+\Delta t \) is carried out in two steps. Advancing to \( t+\Delta t/2 \) in the first step, the ADI method uses implicit difference approximations in the \( x \)-direction and explicit differences in the \( y \)-direction. Then advancing to \( t+\Delta t \) in the second step, the explicit differences are used in the \( x \)-direction and implicit differences in the \( y \)-direction.

For the parabolic diffusion equation, the integral formulation of the finite difference approximations is utilized. A discussion of
the integral formulation is given in Appendix C and other texts such as Varga[25]. The general form of the two sets of equations for each time step can be written for a nonuniform mesh structure as follows where the implicit terms are grouped on the left side of the equations and the explicit terms are on the right side.

\[
- \frac{N(i-1,j,t+1/2)D(i-1/2,j)SSY(j)}{2SX(i-1)} + \frac{N(i,j,t+1/2)SSY(j)}{2} \left\{ \right.
\]
\[
\frac{D(i-1/2,j)}{SX(i-1)} + \frac{D(i+1/2,j)}{SX(i)} + \frac{SSX(i)SSY(j)}{2\Delta t} \left. \right\} - 
\]
\[
\frac{N(i+1,j,t+1/2)D(i+1/2,j)SSY(j)}{2SX(i)} - \frac{N(i,j-1,t)D(i,j-1/2)SSX(i)}{2SY(j-1)}
\]
\[
N(i,j,t) \left[ \frac{SSX(i)}{2} \left( \frac{D(i,j-1/2)}{SY(j-1)} + \frac{D(i,j+1/2)}{SY(j)} \right) \right] - \frac{SSX(i)SSY(j)}{2\Delta t} \left. \right\} + 
\]
\[
\frac{N(i,j+1,t)D(i,j+1/2)SSX(i)}{2SY(j)} \ 
\]
(2.1)

\[
- \frac{N(i,j-1,t+1)D(i,j-1/2)SSX(i)}{2SY(j-1)} + \frac{N(i,j,t+1)SSX(i)}{2} \left[ \frac{D(i,j-1/2)}{SY(j-1)} \right.
\]
\[
+ \frac{D(i,j+1/2)}{SY(j)} \right] + \frac{SSX(i)SSY(j)}{2\Delta t} \left. \right\} - \frac{N(i,j+1,t+1)D(i,j+1/2)SSX(i)}{2SY(j)}
\]
\[
= \frac{N(i-1,j,t+1/2)D(i-1/2,j)SSY(j)}{2SX(i-1)} - \frac{N(i,j,t+1/2)SSY(j)}{2} \left\{ \right.
\]
\[
\frac{D(i-1/2,j)}{SX(i-1)} + \frac{D(i+1/2,j)}{SX(i)} \right\} - \frac{SSX(i)SSY(j)}{2\Delta t} \left. \right\} + 
\]
\[
\frac{N(i+1,j,t+1/2)D(i+1/2,j)SSY(j)}{2SX(i)} \ 
\]
(2.2)
where $N$ is the impurity concentration which is donor type or acceptor type depending on the particular diffusion, $D$ is the impurity diffusion constant, and $\Delta t$ is the time step. The notation $D(i+1/2,j)$ represents the average value of the diffusion constants at node $(i+1,j)$ and node $(i,j)$ or $[D(i+1,j) + D(i,j)]/2$, for example. The sets of equations can be written in matrix notation as

$$[H + \frac{1}{\Delta t} I]N(t+1/2) = [\frac{1}{\Delta t} I - V]N(t) \quad (2.3)$$

$$[V + \frac{1}{\Delta t} I]N(t+1) = [\frac{1}{\Delta t} I - H]N(t+1/2) \quad (2.4)$$

where $H$ is the matrix representation of the finite difference approximation of $-\frac{\partial}{\partial x}(D \frac{\partial}{\partial x})$ in rectangular coordinates, $V$ is the matrix representation of the finite difference approximation of $-\frac{\partial}{\partial y}(D \frac{\partial}{\partial y})$, and $I$ is the identity matrix. Both matrices $H$ and $V$ can be made tridiagonal (but not simultaneously) by ordering the nodes horizontally for $H$ and vertically for $V$. Since the matrices are tridiagonal, a modified Gaussian elimination routine can be used to efficiently solve the algebraic equations for the unknown impurity atom concentrations. The choice of the time step is arbitrary except that smaller time steps increase the accuracy of the solution.

2.1.2 Direct Solution Techniques

Since the $H$ and $V$ matrices are tridiagonal, a modified Gaussian elimination routine which is often called the Thomas algorithm[23] is used to solve directly the simultaneous algebraic equations. The system of simultaneous linear equations can be written in matrix form as
Ax = d \tag{2.5}

where

\begin{align*}
A &= H + \frac{1}{\Delta t} I \\
x &= N(t+1/2) \\
d &= \left[ \frac{1}{\Delta t} I - V \right] N(t)
\end{align*}

in the case of Equation (2.3). Since the matrix is irreducible and diagonally dominant, pivoting is not used.

Illustrating the algorithm which is contained in the subroutine TRIDT, let A be a matrix with the subdiagonal elements $a_2$ to $a_m$, the diagonal elements $b_1$ to $b_m$, and the superdiagonal elements $c_1$ to $c_{m-1}$. All other elements of the A matrix are zero when horizontal ordering of the nodes is used. Transforming the system into a simpler one of upper bidiagonal form, the elements are changed so

\begin{align*}
a_i &= 0 \quad \text{for } i = 2, m \\
b_i &= 1 \quad \text{for } i = 1, m
\end{align*}

and

\begin{align*}
c_1 &= c_1/b_1 \\
d_1 &= d_1/b_1 \tag{2.6}
\end{align*}

Thus, in general,

\begin{align*}
c_i &= c_i/(b_i - a_i c_{i-1}) \tag{2.7} \\
&\quad \text{for } i = 2, m \\
d_i &= (d_i - a_i d_{i-1})/(b_i - a_i c_{i-1}) \tag{2.8}
\end{align*}

Solving for the unknown concentrations in the reverse order,
The isolation diffusion presents significant numerical problems since only a small portion of the diffusion window is located within the diffusion model region. The basic problem occurs because the isolation diffusion concentration is still changing in the x-direction at the y-axis boundary. Thus, boundary conditions for the y-axis are extremely difficult if not impossible to describe accurately with either a constant concentration or a normal derivative. Taking this into consideration, the isolation diffusion is calculated using an analytical method described by Kennedy and O'Brien[26]. The concentrations at the various nodes can be given as

\[
 N(r,\theta,t) = N_0 \left[ 1 - \sum_{n=0}^{\infty} \frac{\sin((n + 1/2)\phi)}{\pi} \frac{[r/(2\sqrt{DE})]^{n+1/2} \Gamma((n+1/2)/2)}{2\Gamma(n+3/2)} \times M[1/2(n+1/2); n+3/2; - \frac{r^2}{4DE}] \right] 
\]

where

\[
 M(a;b;z) = \sum_{k=0}^{\infty} \frac{a_k z^k}{b_k} = \text{Kummer function}
\]

\[
 a_k = a(a+1)(a+2) \cdots (a+k+1), \quad a_0 = 1
\]

\[
 b_k = b(b+1)(b+2) \cdots (b+k+1), \quad b_0 = 1
\]

Figure 8 shows the structure diagram for this analytical method which defines the variables. It should be noted that the terms in the Kummer function and the gamma functions become quite large as n and k increase.
Plane Source
of Impurity Atoms
Diffusion Mask

Silicon Substrate

where
\[ \phi = \theta + \pi \]
\[ 0 < \theta < \pi \]

Figure 8. Structure Diagram For Analytical Diffusion Method
for small values of \( r \). Considering the upper limit of the real constant of \( 10^{78} \) due to computer limitations, the maximum values of \( n \) and \( k \) are limited by the magnitude of the radius \( r \).

The epitaxial-substrate redistribution is basically a one-dimensional diffusion. The assumption is made that the epitaxial growth rate \( \nu \) is much larger than the diffusion constant \( D \) so \( \nu t \gg \sqrt{D} \). The redistribution can then be considered in two parts as described by Grove, et al[27]. First, the substrate impurities diffuse into the epitaxial layer as

\[
N_1(y,t) = \frac{1}{2} N_{\text{sub}} \text{erfc} \left( \frac{y}{2\sqrt{D_1t}} \right) \quad (2.11)
\]

Then, the epitaxial impurity atoms diffuse into the substrate as

\[
N_2(y,t) = \frac{1}{2} N_{\text{epi}} \left[ 1 + \text{erf} \left( \frac{y}{2\sqrt{D_2t}} \right) \right] \quad (2.12)
\]

2.1.3 Applications

The emitter diffusion is numerically determined by the ADI methods discussed in Section 2.1.1. The emitter diffusion is basically a 14 minute, 1050°C, phosphorus diffusion, and the diffusion constant is determined to be \( 3 \times 10^{-13} \text{cm}^2/\text{sec} \) as obtained from Burger and Donovan[28]. Accuracy is maintained by using a constant time step of 15 seconds which is approximately twice the explicit method limit. A variable time step has also been used which had short time steps occurring early in the diffusion cycle when the second partial derivatives are varying rapidly with time. However, the improvement in accuracy
was insignificant as compared to the additional computation time so a constant 15 second time step is selected. The effect of the high base concentration on the emitter diffusion constant is taken into consideration by using data presented by Wolf [29]. The phosphorus emitter diffusion constant is assumed to be constant for boron base concentrations below $10^{14}$ cm$^{-3}$ and increases with increasing base concentration as

\[ D_E = D_E^{14} \left[ 1.0 + 0.016 \log \left( \frac{N_A}{10^{14}} \right) + 0.008 \left( \log \left( \frac{N_A}{10^{14}} \right) \right)^2 + 0.004 \left( \log \left( \frac{N_A}{10^{14}} \right) \right)^3 \right]^2 \]  

(2.13)

which is a least squares fit of the data by Wolf. For example, the phosphorus emitter diffusion constant is increased by a factor of five when the base impurity concentration is $1.0 \times 10^{20}$ cm$^{-3}$ which is equal to the base source concentration. The controlling parameter of the iteration cycle is the desired junction depth. Thus, when the donor concentration is equal to or exceeds the base acceptor concentration at a point which is 0.6 microns below the surface, the iteration cycle is terminated. Therefore, the accuracy of the junction location is a function of the time step size and increases as the time step size decreases.

The base diffusions are numerically more complicated since the boundary conditions are time-dependent. In the idealized model of the transistor, the diffusion constants for both the deposition and drive-in diffusions are constants which are independent of position. However, in the EPE transistor model, the diffusion constant of the drive-in diffusion is enhanced in the region under the emitter region in order
to exhibit the nonplanar diffusion associated with the 'emitter push' effect. The deposition diffusion process is basically an 18 minute, 950°C, boron diffusion. The deposition diffusion constant is determined to be $3 \times 10^{-15}$ cm$^2$/sec. The drive-in diffusion is a three-step diffusion process which is considered to be approximately described by a diffusion process which has a combined diffusion constant of

$$(D t)_{\text{ave}} = \sum D t$$

The summation includes the diffusion constant-time product of the three-step drive-in diffusion plus all temperature cycles which occur later in the processing. By this method, the drive-in diffusion constant is calculated to be $6 \times 10^{-14}$ cm$^2$/sec. For the enhanced drive-in diffusion constant, the computer is given the desired final boundary conditions and generates the necessary diffusion constant. For the EPE transistor model, the enhanced diffusion constant for the drive-in base diffusion is calculated to be $8.5 \times 10^{-14}$ cm$^2$/sec. Other possible methods for obtaining the enhanced diffusion could be used such as using an enhanced drive-in diffusion constant during only the emitter diffusion temperature cycle time. This method may be more accurate but creates a much larger diffusion constant which may in turn create numerical accuracy problems. The controlling parameter of the deposition diffusion is time which terminates the iterations when the time steps sum to 18 minutes. Time is used since the experimental determination of the very shallow deposition junction depth is not sufficiently accurate. The drive-in diffusion iterations are controlled by the desired junction depth.
The buried layer diffusion is used to determine the expansion of the buried layer into the epitaxial layer due to the various temperature cycles such as epitaxial growth, isolation diffusion, base diffusion, and emitter diffusion. Due to the finite size constraints of the model, the buried layer diffusion into the substrate which is a very deep diffusion can not be simulated exactly. It is assumed that the buried layer region is a constant source of impurity atoms for the epitaxial layer. However, the constant source of impurity atoms is considered to be located arbitrarily two microns below the original epitaxial-substrate interface in order to exhibit some portion of the diffusion tail extending into the buried layer region. The diffusion constant for the buried layer diffusion is determined by Equation (2.14) and is calculated to be $4 \times 10^{-14}$ cm$^2$/sec for the arsenic impurities. The iteration process of the ADI method for the buried layer diffusion is controlled by the desired junction depth.

The isolation diffusion and the epitaxial-substrate redistribution are calculated using the direct methods which are described in Section 2.1.2. The isolation diffusion is basically a 4 hour, 1150°C boron diffusion process. Considering all of the temperature cycles which occur after the isolation diffusion, the impurity diffusion constant-time product is determined by Equation (2.14) and is calculated to be $1.60786 \times 10^{-8}$ cm$^2$. The two impurity diffusion constant-time products for the epitaxial-substrate redistribution are also determined by Equation (2.14) and are calculated to be

$$D_1 t = 0.090 \times 10^{-8} \text{ cm}^2 \text{ and } D_2 t = 0.300 \times 10^{-8} \text{ cm}^2$$
The diffusion model computer programs are located in Appendix E.

2.2 Semiconductor Device Model

From the normalized basic set of semiconductor device equations given in Section 1.2.2, it is possible to combine the various equations into a reduced set of semiconductor device equations. Additional relationships concerning the carrier densities, mobilities, and the recombination-generation mechanism are given to complete the reduced set of semiconductor device equations. The nonlinear, elliptic equations are then linearized by a method which is conceptually similar to Newton's method, and the linearized equations are solved by iterative methods.

2.2.1 Reduced Set of Semiconductor Equations

Of the five equations of the basic set of normalized semiconductor equations (1.16) to (1.20), two equations can be eliminated if the normalized current density equations (1.16) and (1.17) are inserted into the appropriate current continuity equation (1.19) and (1.20), respectively. Thus,

$$\nabla \cdot \mathbf{J}_n = \nabla \cdot [\mu_n (-n\nabla \psi_v + \alpha_n \nabla n)] = R \tag{2.15}$$

$$\nabla \cdot \mathbf{J}_p = - \nabla \cdot [\mu_p (p\nabla \psi_v + \alpha_p \nabla p)] = - R \tag{2.16}$$

The third equation of the reduced set of semiconductor equations is Poisson's equation.
\( \nabla^2 \psi_V = n - p + N_A - N_D \) \hspace{1cm} (2.17)

These three equations combined with the carrier density relationships, the mobility relations, and the recombination-generation law constitute the reduced set of semiconductor equations. It should be noted that these three equations are coupled elliptical equations. With the particular choice of variables, \( n, p, \) and \( \psi_V, \) Poisson's equation is linear while the combined current density-continuity equations are nonlinear.

2.2.2 Carrier Density Relations

Close inspection of the semiconductor device model reveals that the regions of the emitter and base diffusions have sufficiently high impurity atom concentrations to be considered as degenerate material. In these regions, the normal assumption of Boltzmann statistics is not sufficiently accurate to be valid. Thus, in order to accurately describe the degenerate regions, parabolic distributions for the density of states function and Fermi statistics are assumed. The relationship between the carrier densities and the chemical potentials are given in terms of the Fermi-Dirac integral[20].

\[
\frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{\epsilon}}{\exp(\epsilon - \xi_p) + 1} \, d\epsilon = \frac{p}{N_V} = F_{1/2}(\xi_p) \tag{2.18}
\]

\[
\frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{\epsilon}}{\exp(\epsilon - \xi_n) + 1} \, d\epsilon = \frac{n}{N_C} = F_{1/2}(\xi_n) \tag{2.19}
\]
where \( N_v \) and \( N_c \) are the effective density of states for the valence and conduction bands, respectively, and in normalized form are equal to

\[
N_v = 1.72986 \times 10^9 \left( \frac{m^*_n}{m} \right)^{3/2} (T/300^\circ K)^{3/2} \quad (2.20)
\]
\[
N_c = 1.72986 \times 10^9 \left( \frac{m^*_e}{m} \right)^{3/2} (T/300^\circ K)^{3/2} \quad (2.21)
\]

The evaluation of the Fermi-Dirac integral has been tabulated by McDougall and Stoner[30]. The Fermi-Dirac integral can be approximated for nondegenerate material by Boltzmann statistics

\[
n = N_c \exp(\zeta_n) \quad \text{for } n \ll N_c \quad (2.22)
\]
\[
p = N_v \exp(\zeta_p) \quad \text{for } p \ll N_v \quad (2.23)
\]

and for strongly degenerate material by

\[
n = N_c \left( \frac{4}{3\sqrt{\pi}} \right) \left( \zeta_n \right)^{3/2} \quad \text{for } n \gg N_c \quad (2.24)
\]
\[
p = N_v \left( \frac{4}{3\sqrt{\pi}} \right) \left( \zeta_p \right)^{3/2} \quad \text{for } p \gg N_v \quad (2.25)
\]

Solving for the chemical potentials,

\[
\zeta_n = \ln(n/N_c) \quad \text{for } n \ll N_c \quad (2.26)
\]
\[
\zeta_p = \ln(p/N_v) \quad \text{for } p \ll N_v \quad (2.27)
\]
\[
\zeta_n = \left( \frac{3\sqrt{\pi}n}{4N_c} \right)^{2/3} \quad \text{for } n \gg N_c \quad (2.28)
\]
\[
\zeta_p = \left( \frac{3\sqrt{\pi}p}{4N_v} \right)^{2/3} \quad \text{for } p \gg N_v \quad (2.29)
\]

In Figure 9, the approximations are plotted along with the actual Fermi-
Figure 9. Fermi-Dirac integral valuation and approximations.

Strongly Degenerate Approximation
\[ \zeta = \left( \frac{3n^2}{\Omega^2} \right)^{2/3} \]
\[ = 1.209 \left( \frac{n}{N} \right)^{2/3} \]

Nondegenerate Approximation
\[ \zeta = \ln \left( \frac{n}{N} \right) \]

Chemical Potential volts
Dirac integral values. Assuming a maximum error between the approximations and the actual integral values of 0.625%, the nondegenerate approximation is valid for values of chemical potentials up to -4.0. The degenerate approximation with a maximum error of 0.38% is valid for values of chemical potentials down to +20.0. The generalized Einstein relations $\alpha_p(p)$ and $\alpha_n(n)$ require that numerically determined derivatives be calculated from the tabulated values of the Fermi-Dirac integral for the range of $-4.0 < \zeta_n, \zeta_p < +20.0$. For the nondegenerate approximation

$$\alpha_n = 1 \text{ and } \alpha_p = 1$$

(2.30)

For strongly degenerate material

$$\alpha_n = 2/3(3\sqrt{\pi}n/4N_C)^{2/3}$$

(2.31)

$$\alpha_p = 2/3(3\sqrt{\pi}p/4N_V)^{2/3}$$

(2.32)

2.2.3 Mobility Variations

In this work, the carrier mobilities are considered to be functions of the electric field and the impurity atom concentrations. Extensive experimental data is available in the literature[31-35], for example, and empirical relationships which agree relatively well with most of the experimental data have been developed by Caughey and Thomas [36], Gwyn, Scharfetter, and Wirth[6], Hachtel, Joy, and Cooley[4], and Scharfetter and Gummel[5]. Comparing the four empirical methods, the method by Hachtel et al is very accurate in the low field range since
the data of Prince[33] for minority carriers and Irvin[35] for the majority carriers is used directly. However, the mobility variations with electric field appear to decrease too slowly with the electric field in the low impurity concentration region. The method by Gwyn et al agrees well with experimental data for zero electric field but varies much too rapidly with increasing electric field. The method by Caughey et al is less accurate in the regions of high electric field and of high impurity concentration. Scharfetter and Gummel's model agrees reasonably well with the published data for all ranges of impurity concentrations and electric field. The mobility relationship of Scharfetter and Gummel is used in this work and is

\[
(\mu_0/\mu)^2 = 1 + \left[ \frac{N}{N/D + C} \right] + \left[ \frac{(E/A)^2}{E/A + F} \right] + \left( \frac{E}{B} \right)^2
\]  

(2.33)

where

<table>
<thead>
<tr>
<th></th>
<th>Holes</th>
<th>Electrons</th>
</tr>
</thead>
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<tr>
<td></td>
<td>unnormalized</td>
<td>normalized</td>
</tr>
<tr>
<td>A</td>
<td>6.1x10^3</td>
<td>8.01x10^2</td>
</tr>
<tr>
<td>B</td>
<td>2.5x10^4</td>
<td>3.28x10^3</td>
</tr>
<tr>
<td>C</td>
<td>4.0x10^16</td>
<td>2.76x10^6</td>
</tr>
<tr>
<td>D</td>
<td>81</td>
<td>81</td>
</tr>
<tr>
<td>F</td>
<td>1.6</td>
<td>1.6</td>
</tr>
<tr>
<td>(\mu_0)</td>
<td>480</td>
<td>12.42</td>
</tr>
</tbody>
</table>
2.2.4 Recombination-Generation Law

In this work, trapping is neglected. The effects of recombination are represented by the Shockley-Read-Hall recombination model[37] due to its simplicity and general agreement with experimental evidence.

\[ R_n = R_p = \frac{p_0 n_0 - p_0 p_1}{\tau_n (p + p_1) + \tau_p (n + n_1)} \]  \hspace{1cm} (2.34)

where \( p_0 \) and \( n_0 \) are the thermal equilibrium values of the hole and electron densities, respectively. As noted previously, the product of \( n_0 \) and \( p_0 \) does not necessarily equal \( n_1^2 \) for Fermi-Dirac statistics. \( \tau_n \) and \( \tau_p \) are the carrier lifetimes, and \( p_1 \) and \( n_1 \) are the hole and electron concentrations that would exist if the Fermi level were at the trap level. The trap level is assumed to be at the center of the energy gap so in this case

\[ n_1 = p_1 = n_1 \] \hspace{1cm} (unnormalized)
\[ = 1 \] \hspace{1cm} (normalized)

There are however several conditions involved in using the Shockley-Read-Hall recombination model which should be noted. Several assumptions are used to derive the model which makes its use of questionable validity in certain cases. Two minor assumptions which are made are steady-state conditions and thermal equilibrium among carriers in a band. However, for small perturbations in carrier densities, these assumptions do not unnecessarily restrict the semiconductor model. The main assumption which causes concern is the assumption of nondegenerate
material. In the development of Equation (2.34), it is assumed that the probability function of finding electrons in the conduction band is nearly zero. This condition is violated for degenerate material, and significant changes are required in the simple band model with discrete impurity levels to describe degenerate material accurately. However, for the lack of any better theory, it is assumed that the Shockley-Read-Hall recombination model is sufficiently accurate for all levels of impurity atom concentration found in the semiconductor model.

2.2.5 Numerical Methods

There are many numerical methods which could be employed to obtain an approximate solution for the electron concentration, hole concentration, and valence band edge potential from the reduced set of semiconductor equations (2.15 - 2.17) at each node in the mesh. The various numerical methods are described, for example, by Ortega and Rheinbold[38] and Ames[23]. In solving nonlinear elliptic equations, a commonly used technique is to employ a form of Newton's method to linearize the system of equations followed by some iterative technique such as alternating-direction methods or successive over-relaxation method. This process is repeated, thus constructing a cascade of outer linearizing iterations alternating with a large sequence of inner linear iterations. However, the complexity of these techniques suggests that alternatives would be highly desirable. One direct and simple method which is particularly well adapted for solving algebraic systems of equations associated with nonlinear elliptic equations is
called nonlinear over-relaxation (NLOR) as described by Lieberstein [39,40].

To develop the algebraic systems of equations from the three elliptic equations of the reduced set of semiconductor equations, the integral formulation of the finite difference approximations is used which is described in Appendix C. Writing Poisson's equation in the form used in Appendix C,

\[- \nabla^2 \psi_v - p + n - N_{\text{DIFF}} = 0 = H_1(x,y,\psi_{vxxx},\psi_{vyy}) \quad (2.36)\]

The electron current continuity equation is

\[- \nabla \cdot (\mu_n \nabla n) + \frac{1}{\alpha_n}(R + \mu_n n_x (\psi_{vx} - \alpha_{nx}) + \mu_n n_y (\psi_{vy} - \alpha_{ny})) + n[\mu_{nx} \psi_{vx} + \mu_{ny} \psi_{vy} + \mu_n (n - p - N_{\text{DIFF}})] = 0 = H_2(x,y,n,n_x,n_y,n_{xx},n_{yy}) \quad (2.37)\]

where Poisson's equation is used to eliminate the second partial derivatives of the valence band edge potential. Similarly, the hole current continuity equation is

\[- \nabla \cdot (\mu_p \nabla p) + \frac{1}{\alpha_p}(R - \mu_p p_x (\psi_{vx} + \alpha_{px}) - \mu_p p_y (\psi_{vy} + \alpha_{py})) - p[\mu_{px} \psi_{vx} + \mu_{py} \psi_{vy} + \mu_p (n - p - N_{\text{DIFF}})] = 0 = H_3(x,y,p,p_x,p_y,p_{xx},p_{yy}) \quad (2.38)\]

Using Poisson's equation as an example, the discretized equation for an interior point is
\[- \psi_v(i-1,j) \left[ \frac{SSY(j)RX(i)}{SSX(i)} \right] - \psi_v(i,j-1) \left[ \frac{SSX(i)RY(j)}{2SY(j)} \right] + \psi_v(i,j) \left[ \frac{SSY(j)(RX(i) + 1.0)}{2SSX(i)} + \frac{SSX(i)(RY(j) + 1.0)}{2SY(j)} \right] - \psi_v(i+1,j) \left[ \frac{SSY(j)}{2SSX(i)} \right] - \psi_v(i,j+1) \left[ \frac{SSX(i)}{2SY(j)} \right] + \left[ \frac{SSX(i)SSY(j)}{4} \right] \left[ n(i,j) - p(i,j) - N_{DIFF}(i,j) \right] = 0 = G_1 \] (2.39)

where \( G_1 \) is the discretized form of \( H_1 \). Similar but more involved expressions can be generated for the electron current continuity equation and the hole current continuity equation. \( G_2 \) is then the discretized form of \( H_2 \), and \( G_3 \) is the discretized form of \( H_3 \).

The nonlinear over-relaxation method used to solve the three systems of 5200 algebraic equations reduces to the successive over-relaxation method for linear equations such as the Poisson's equation. The general form of the NLOR method for the three systems of equations with an outer iteration loop which solves first for hole concentrations, then electron concentrations, and finally the valence band edge potential is

\[
p^{n+1}(i,j) = p(i,j) - \omega_p [G_3(p^n,n^n,\psi_v^n)/\partial G_3(p^n,n^n,\psi_v^n)/\partial p] \] (2.40)

\[
n^{n+1}(i,j) = n(i,j) - \omega_n [G_2(p^{n+1},n^n,\psi_v^n)/\partial G_2(p^{n+1},n^n,\psi_v^n)/\partial n] \] (2.41)

\[
\psi_v^{n+1}(i,j) = \omega_{\psi_v} [G_1(p^{n+1},n^{n+1},\psi_v^{n+1}),/\partial G_1(p^{n+1},n^{n+1},\psi_v^n)/\partial \psi_v] \] (2.42)

where \( \omega_p \), \( \omega_n \), \( \omega_{\psi_v} \) are the relaxation factors which can have any value
between 1.0 and 2.0. To make the process most efficient, the optimum value of \( \omega \) should be calculated at each iteration by minimizing the spectral radius of the lower triangular matrix formed from the Jacobian of the coefficient matrix \( A \) when the system is written as \( Ax = b \).

However, this procedure is extremely time-consuming and may not be rewarding since it is better to overestimate \( \omega_{\text{opt}} \) than to underestimate it. Due to the size of the three systems of equations, \( \omega_{\text{opt}} \) is approximately determined by comparing the rates of convergence of a series of calculations utilizing a series of \( \omega \)'s.

The nonlinear over-relaxation method is about the simplest method which could be used to solve the elliptic equations. However, it is probably not the most efficient method since in general line-SOR or block-SOR methods are more efficient than a point-SOR method which is the linear version of NLOR. Also, alternating direction (ADI) methods are sometimes more efficient than line-SOR methods depending on the type of equation and the size of the system of equations. In order to explore the more efficient methods than the NLOR method, a quasi-linear-ADI method which is conceptionally similar to a Newton-ADI method is formulated. Looking at Equations (2.36-2.38), the equations can be written as

\[
\nabla \cdot (\mu_n \nabla n) = \frac{1}{\alpha_n} \left[ R + \mu_n n_x (\psi_{nx} - \alpha_{nx}) + \mu_n n_y (\psi_{ny} - \alpha_{ny}) + n [\mu_{nx} \psi_{nx} + \mu_{ny} \psi_{ny} + \mu_n (n - p - N_{\text{DIFF}})] \right]
= F_1(n, p, n_x, n_y, \psi_{nx}, \psi_{ny})
\]

(2.39)
\[ \nabla \cdot (\mu_p \nabla \psi) = \frac{1}{\alpha_p} (n - \mu_p n_x (\psi) + \alpha_p n_x) - \mu_p n_y (\psi, \alpha_p n_y) \]

\[ - p [\mu_p n_x \psi_x + \mu_p n_y \psi_y + \mu_p (n - p - N_{DIFF})] \]

\[ = F_2 (p, n, n_x, n_y, \psi_x, \psi_y) \quad (2.40) \]

\[ \nabla^2 \psi = n - p - N_{DIFF} = F_3 (n, p) \quad (2.41) \]

Now using a quasi-linearization described by Lee [41] and Bellman and Kalaba [42], the equations can be linearized as

\[ \nabla \cdot (\mu_n \nabla m^{+1}) = F_1 |_{m} + (n^{m+1} - n) \frac{\partial F_1}{\partial n} |_{m} + (p^{m+1} - p) \frac{\partial F_1}{\partial p} |_{m} \]

\[ + \left( n_{x}^{m+1} - n_x \right) \frac{\partial F_1}{\partial n_x} |_{m} + \left( n_{y}^{m+1} - n_y \right) \frac{\partial F_1}{\partial n_y} |_{m} \]

\[ + \left( \psi_{x}^{m+1} - \psi_x \right) \frac{\partial F_1}{\partial \psi_x} |_{m} + \left( \psi_{y}^{m+1} - \psi_y \right) \frac{\partial F_1}{\partial \psi_y} |_{m} \]

\[ (2.42) \]

\[ \nabla \cdot (\mu_p \nabla m^{+1}) = F_2 |_{m} + (p^{m+1} - p) \frac{\partial F_2}{\partial p} |_{m} + (n^{m+1} - n_m) \frac{\partial F_2}{\partial n} |_{m} \]

\[ + \left( p_{x}^{m+1} - p_x \right) \frac{\partial F_2}{\partial p_x} |_{m} + \left( p_{y}^{m+1} - p_y \right) \frac{\partial F_2}{\partial p_y} |_{m} \]

\[ + \left( \psi_{x}^{m+1} - \psi_x \right) \frac{\partial F_2}{\partial \psi_x} |_{m} + \left( \psi_{y}^{m+1} - \psi_y \right) \frac{\partial F_2}{\partial \psi_y} |_{m} \]

\[ (2.43) \]

where the partial derivatives of \( F_1 \) and \( F_2 \) are given in Tables 3 and 4. A similar procedure can be performed for the linear Poisson's equation so

\[ \nabla^2 \psi^{m+1} = F_3 |_{m} + (n^{m+1} - n) - (p^{m+1} - p) \]

\[ (2.44) \]
TABLE 3. PARTIAL DERIVATIVES OF $F_1$

\[ \frac{\delta F_1}{\delta n} = \frac{1}{\alpha_n} \left( \frac{[\tau_n(p + p_1) + \tau_p(n + n_1)]n - (pn - p_o^2)\tau_p}{[\tau_n(p + p_1) + \tau_p(n + n_1)]^2} \right) \]

\[ + \mu_n x \psi_v_x + \mu_n y \psi_v_y + \nu_n(2n - p - N_{DIFF}) - \frac{F_1}{\alpha_n} \frac{\partial \alpha_n}{\partial n} \]

\[ \frac{\delta F_1}{\delta p} = \frac{1}{\alpha_n} \left( \frac{[\tau_n(p + p_1) + \tau_p(n + n_1)]n - (pn - p_o^2)\tau_n}{[\tau_n(p + p_1) + \tau_p(n + n_1)]^2} \right) \]

\[ - \nu_n \right) \]

\[ \frac{\delta F_1}{\delta n_x} = \frac{1}{\alpha_n} (\mu_n \psi_v_x - \alpha_n) \]

\[ \frac{\delta F_1}{\delta n_y} = \frac{1}{\alpha_n} (\mu_n \psi_v_y - \alpha_n) \]

\[ \frac{\delta F_1}{\delta \psi_v_x} = \frac{1}{\alpha_n} (\nu_n n_x + \mu_n n_x) \]

\[ \frac{\delta F_1}{\delta \psi_v_y} = \frac{1}{\alpha_n} (\nu_n n_y + \mu_n n_y) \]
TABLE 4. PARTIAL DERIVATIVES OF \( F_2 \)

\[
\frac{\partial F_2}{\partial p} = \frac{1}{\alpha_p} \left( \frac{[\tau_n(p + p_1) + \tau_n(n + n_1)]n - (p_n - P_n n_o) \tau n}{[\tau_n(p + p_1) + \tau_p(n + n_1)]^2} \right)
- \mu_p \psi_v_x - \mu_p \psi_v_y - \mu_p (n - 2p - N_{DIFF}) - \frac{F_2}{a_n} \frac{\partial a_p}{\partial p}
\]

\[
\frac{\partial F_2}{\partial n} = \frac{1}{\alpha_p} \left( \frac{[\tau_n(p + p_1) + \tau_n(n + n_1)]p - (p_n - P_n n_o) \tau p}{[\tau_n(p + p_1) + \tau_p(n + n_1)]^2} \right)
- \mu_p \phi
\]

\[
\frac{\partial F_2}{\partial \psi_v_x} = -\frac{1}{\alpha_p} (\mu_p \psi_v_x + \alpha_p \psi_v_x)
\]

\[
\frac{\partial F_2}{\partial \psi_v_y} = -\frac{1}{\alpha_p} (\mu_p \psi_v_y + \alpha_p \psi_v_y)
\]

\[
\frac{\partial F_2}{\partial \psi_v_x} = -\frac{1}{\alpha_p} (p \mu_p \psi_x + \mu_p \psi_x)
\]

\[
\frac{\partial F_2}{\partial \psi_v_y} = -\frac{1}{\alpha_p} (p \mu_p \psi_y + \mu_p \psi_y)
\]
The integral formulation of the finite difference approximations is used for the discretization of the quasi-linearized elliptic equations (2.42-2.44) into three sets of algebraic equations. A discussion of the integral formulation is given in Appendix C. The three sets of algebraic equations are then solved by ADI methods which, in this case, the equations of the form \( Ax = k \) have the general form for the \( n+1 \) inner iteration of

\[
(H + r_{n+1}I)x_{n+1/2} = (r_{n+1} - \nu)x_n + k
\]

\[
(V + r_{n+1}I)x_{n+1} = (r_{n+1} - H)x_{n+1/2} + k
\]

where \( r_{n+1} \)'s are the acceleration parameters which increase the rate of convergence if properly chosen. The identification of the various matrices can be made for Equations (2.42-2.44). For the electron current continuity equation (2.42),

\[
H = - \frac{\partial}{\partial x} (\mu \frac{\partial F}{\partial x}) + \frac{1}{2} \frac{\partial F_1}{\partial n} |_m + \frac{\partial F_1}{\partial n_x} \frac{\partial}{\partial x}
\]

\[
V = - \frac{\partial}{\partial y} (\mu \frac{\partial F}{\partial y}) + \frac{1}{2} \frac{\partial F_1}{\partial n} |_m + \frac{\partial F_1}{\partial n_y} \frac{\partial}{\partial y}
\]

\[
k = - F_1 |_m + n \frac{m \partial F_1}{\partial n} |_m + n \frac{m \partial F_1}{\partial n_x} |_m + n \frac{m \partial F_1}{\partial n_y} |_m - (\mu^{m+1} - \mu) \frac{\partial F_1}{\partial p} |_m
\]

For the hole current continuity equation (2.43),

\[
H = - \frac{\partial}{\partial x} (\mu \frac{\partial \psi}{\partial x}) + \frac{1}{2} \frac{\partial F_2}{\partial p} |_m + \frac{\partial F_2}{\partial p_x} \frac{\partial}{\partial x}
\]

\[
V = - \frac{\partial}{\partial y} (\mu \frac{\partial \psi}{\partial y}) + \frac{1}{2} \frac{\partial F_2}{\partial p} |_m + \frac{\partial F_2}{\partial p_y} \frac{\partial}{\partial y}
\]
\[ k + - F_2 \bigg|_m + p \frac{\partial^2 F_2}{\partial p} \bigg|_m + p \frac{\partial^2 F_2}{\partial x} \bigg|_m + p \frac{\partial^2 F_2}{\partial y} \bigg|_m - (n^{m+1} - n) \frac{\partial F_2}{\partial n} \bigg|_m \\
- (\psi_{Vx}^{m+1} - \psi_{Vx}^{m}) \frac{\partial F_2}{\partial \psi_{Vx}} \bigg|_m - (\psi_{Vy}^{m+1} - \psi_{Vy}^{m}) \frac{\partial F_2}{\partial \psi_{Vy}} \bigg|_m \]

And for Poisson's equation (2.44),

\[ H \rightarrow - \frac{\partial^2}{\partial x^2} \]
\[ V \rightarrow - \frac{\partial^2}{\partial y^2} \]
\[ k \rightarrow - F_3 \bigg|_m - n^{m+1} + n^m + p^{m+1} - p^m \]

For example, Poisson's equation for an interior point in the form of Equation (2.45) becomes

\[ \left( \frac{m+1}{n+1/2} \right) \psi_{V(i-1,j)}^{(SSY(j))} + \left( \frac{m+1}{n+1/2} \right) \left( \frac{SSY(j)}{2SX(i)} - \frac{1}{2SX(i-1)} + \frac{1}{2SX(i+1)} \right) \]

\[ \left( \frac{m+1}{n+1/2} \right) \psi_{V(i+1,j)}^{(SSY(j))} = \psi_{V(i,j)}^{(SSX(i))} \left( \frac{SSX(i)}{2SX(j)} \right) \]

\[ \left( \frac{m+1}{n} \right) \psi_{V(i,j)}^{(SSX(i))} \left( \frac{1}{2SX(j)} + \frac{1}{2SX(j-1)} - r_{n+1} \right) + \frac{m+1}{n} \psi_{V(i,j+1)}^{(SSX(i))} \left( \frac{SSX(i)}{2SX(j)} \right) \]

\[ + \frac{SSX(i)SSY(j)}{4} \left[ - F_3 \bigg|_m - n^{m+1} + n^m + p^{m+1} - p^m \right] \quad (2.46) \]
and
\[ \psi_{n+1}^{m+1} \frac{SSX(i)}{2SY(j-1)} + \psi_{n+1}^{m+1} \left( \frac{SSX(i)}{2} \left( \frac{1}{SY(j)} + \frac{1}{SY(j-1)} \right) + r_{n+1} \right) \]

\[ - \psi_{n+1}^{m+1} \frac{SSX(i)}{2SY(j)} = \psi_{n+1/2}^{m+1} \frac{SSY(j)}{2SX(i-1)} \]

\[ - \psi_{n+1/2}^{m+1} \left( \frac{SSY(j)}{2} \left( \frac{1}{SX(i)} + \frac{1}{SX(j-1)} \right) - r_{n+1} \right) + \psi_{n+1/2}^{m+1} \frac{SSY(j)}{2SX(i)} \]

\[ + \frac{SSY(j)SSX(i)}{4} \left[ - F_3 m - n^{m+1} + n^m + p^{m+1} - p^m \right] \]  

(2.47)

The algebraic equations for the electron current continuity and hole current continuity equations are generated in a similar manner but are more complicated.

An example of a flow diagram for the semiconductor device model computer program is given in Figure 10. In this case, the valence band edge potentials are computed first, then the hole concentrations, and finally the electron concentrations. This constitutes the outer iteration loop which can solve for the three sets of variables in any desired sequence.

2.2.6 Application of Numerical Methods

The two semiconductor device model computer programs are
FIGURE 10. FLOW DIAGRAM FOR STEADY-STATE DEVICE COMPUTER PROGRAM.
contained in Appendix F. The two computer programs share the same
subsidary subroutines and differ in the MAIN program and the solution
subroutines. The TRIAL subroutine generates the initial solution for
each variable at every mesh node. The values of the variables are
basically the thermal equilibrium values modified by first-order theory
in the depletion areas and the contact areas. The hole and electron
mobility as a function of the electric field and impurity concentration
is calculated by the MQAL subroutine which also determines the general-
ized Einstein relations for each outer iteration. The FERMI subroutine
calculates the electron or hole concentrations for a given chemical
potential or a chemical potential for a given concentration. The sub-
routine uses Boltzmann statistics for values of chemical potential
below - 4.0, tabulated values of the Fermi-Dirac integral for chemical
potentials between - 4.0 and 20.0, and a 2/3 power-law for chemical
potentials above 20.0. The OUTPUT subroutine computes from the final
values of the hole and electron concentrations and the valence band
dge potentials the various current densities, the terminal currents,
and the electric field.

The NLOR computer program uses the RELAX subroutine to calcu-
late by iteration the values of the hole and electron concentrations
and the valence band edge potentials. Both the outer and inner iter-
ation loops are contained within this subroutine. The subroutine is
blocked in that the new values of one variable are obtained at all mesh
nodes before continuing to the next variable. The quasi-linearization-
ADI method uses three separate subroutines to solve for the three sets
of variables. The PSIV subroutine solves for the new values of the valence band edge potential, the ELECTC subroutine calculates the new electron concentrations, and the HOLECO subroutine determines new hole concentrations. Each of these subroutines contains the inner iteration loop, and the outer iteration loop is in the MAIN program. The TRIDT subroutine is a modified Gaussian elimination program which solves the tridiagonal matrix equations. The MAIN program for both computer programs reads in and normalizes the input data, sets up the outer iteration loop, calls the subroutines, and determines the termination point of the iterative process.
CHAPTER III

COMPUTATIONAL RESULTS

The numerical results of the diffusion model computer program and the semiconductor device model computer program for the idealized and the EPE transistor models are presented in this chapter. The semiconductor device model results are limited to thermal equilibrium values and studies of the numerical methods due to circumstances which are discussed in Section 4.2. Additional numerical results for a diffused diode in integrated form are presented in Section 3.1.5.

3.1 Diffusion Analysis

The numerical output of the diffusion program which determines the emitter, base, extended base, buried layer, and isolation impurity atom concentrations is displayed in this section. When the semiconductor model is viewed as a whole entity, it is difficult to exhibit the detail structure of the various diffusions. Figures 4 and 5 show the approximate variations of the donor and of the acceptor impurity concentration distributions for the whole idealized transistor model, respectively. Each diffusion is discussed separately in the following sections so that the detailed structure can be given.

3.1.1 Emitter Diffusion

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The emitter diffusion is a 14 minute, 1050°C phosphorus diffusion from a constant impurity surface source which is functioning at or near the solid solubility limit. The emitter diffusion constant is considered in two ways in this work. First, the diffusion constant is assumed to be independent of the background impurity concentration. Then, the diffusion constant is assumed to increase for high background acceptor concentrations and varies as a function of the acceptor concentration as given in Equation (2.13). In this case, the emitter diffusion constant decreases as a function of the distance from the surface since the base acceptor concentration is a decreasing function of the distance from the surface. It should be noted that, in the region of the emitter diffusion, the base acceptor concentration does not vary in the x-direction.

For a constant source diffusion, a complementary error function diffusion is to be expected in one-dimensional analysis. In the two-dimensional model, it is reasonable to expect an approximate complementary error function distribution in the y-direction at the center of the emitter diffusion since the center is sufficiently removed from the effects of the emitter edges. Figure 11 shows the center profile of the emitter diffusion for the fixed diffusion constant, and Figure 12 exhibits the center profile for the concentration-dependent diffusion constant. The fixed diffusion constant distribution approximates the complementary error function relatively well. For the concentration-dependent diffusion constant distribution, the impurity concentrations are larger near the surface and smaller deeper in the
FIGURE 11. CENTER PROFILE OF EMITTER DIFFUSION WITH INDEPENDENT DIFFUSION CONSTANT
FIGURE 12. CENTER PROFILE OF EMITTER DIFFUSION WITH CONCENTRATION-DEPENDENT DIFFUSION CONSTANT
device than the complementary error function diffusion. These effects are caused by the strongly varying emitter diffusion constant which increases by a factor of almost five near the surface. One point to be noted is that the numerical emitter diffusion is terminated when the donor concentration equals the acceptor concentration at a point 0.6 microns below the surface. Thus, the time of the diffusion with the concentration-dependent diffusion constant is less than the fixed diffusion constant, due to the enhanced diffusion constant. Therefore, the 'tail' of the diffusion with the concentration-dependent diffusion constant should be less than for the diffusion with the fixed diffusion constant. This effect can be seen in Figure 13 which compares the two center distribution profiles.

The lateral diffusion or the diffusion along the Si-SiO₂ interface is shown in Figures 14, 15, and 16. Figure 14 exhibits the lateral diffusion for the fixed diffusion constant case and compares it to the center diffusion and the calculations by Kennedy and O'Brien[26]. The lateral diffusion is somewhat less than the center diffusion at high concentration levels but actually surpasses the center profile at lower concentrations. However, the numerically determined lateral profile is at least a factor of two greater than the analytically derived data of Kennedy and O'Brien. (See Section 2.1.2). Figure 15 shows the center and lateral diffusion profiles for the concentration-dependent diffusion constant which also exhibits the lateral diffusion exceeding the center profile at low concentrations. Figure 16 compares the lateral diffusions. In Section 3.1.5, the possible reasons for the disagreement
FIGURE 13. COMPARISON OF CENTER PROFILES
EMITTER DIFFUSIONS
FIGURE 14. LATERAL AND CENTER PROFILES OF Emitter DIFFUSION WITH INDEPENDENT DIFFUSION CONSTANT
FIGURE 15. LATERAL AND CENTER PROFILES OF EMITTER DIFFUSION WITH CONCENTRATION-DEPENDENT DIFFUSION CONSTANT
FIGURE 16. COMPARISON OF LATERAL PROFILES OF_EMITTER DIFFUSION
are investigated. The location of the boundaries are varied by an order of magnitude and the constant boundary impurity concentrations are changed between 0.0 and the intrinsic concentration without any effect. As long as the boundary locations are greater than five times the junction depth from the source, the boundary conditions do not seem to have any effect on the diffusion. However, when the lateral spatial step size is decreased, the lateral diffusion profile moves toward the analytical data. Thus, the lateral diffusion is inaccurate as it is numerically determined with the present mesh structure, but, as explained in Section 3.1.5, the size of the available main memory storage of the computer prevents the addition of more closely spaced lines in the junction region. It is therefore necessary to use the somewhat inaccurate lateral diffusion profile for the emitter diffusion due to computer considerations. It is interesting to note that both the Taylor's series formulation and the integral formulation (see Appendix C) computer programs for the diffusion equation achieve the exact same results within the accuracy of the numerical calculations.

3.1.2 Base Diffusions

The base diffusions are basically two-step diffusions. The constant source predeposition diffusion which operates close to the solid solubility limit is an 18 minute, 950°C boron diffusion which is followed by a constant total impurity concentration drive-in diffusion at approximately 1100°C for about 60 minutes when all of the remaining temperature cycles are considered. The center of the base diffusions
should be a combination of a complementary error function distribution and a Gaussian profile and should more strongly resemble the corresponding Gaussian diffusion on the basis of the comparative magnitudes of the Dt products of the predeposition and drive-in diffusions. The extended base diffusion is numerically approximated by increasing the boron diffusion constant in the region directly under the emitter for the total drive-in cycle. While this method of numerically determining the extended base diffusion profile is rather arbitrary from an actual process standpoint, this method is numerically easy to accomplish and generates a diffusion profile which compares favorably with experimental data. The current confusion concerning the actual mechanism which produces the EPE diffusion variation and the point in the process at which the EPE occurs conceals any more accurate or realistic method of modeling the EPE diffusion.

Figure 17 shows the diffusion profiles of the center of the idealized base diffusion and the corresponding complementary error function and Gaussian diffusions for comparison. The center idealized base diffusion is extremely close to the Gaussian diffusion profile as expected. Slight deviation in the profiles between the concentrations of $10^{17}$ cm$^{-3}$ and $10^{19}$ cm$^{-3}$ is due to the short constant source predeposition diffusion since the impurity atom profile is not the normal theoretically assumed delta function at the start of the drive-in diffusion but is approximately a complementary error function distribution with a finite junction depth. Figure 18 exhibits the same information for the EPE base diffusion. Again, the EPE base diffusion strongly
FIGURE 17. CENTER PROFILE OF BASE DIFFUSION
FIGURE 18. CENTER PROFILE OF EPE BASE DIFFUSION
resembles the corresponding Gaussian diffusion. The EPE base diffusion actually approximates the Gaussian diffusion more closely than the idealized base diffusion. This is to be expected on the basis of the comparison of the Dt products for the predeposition and drive-in diffusions for both the EPE and idealized base diffusions.

As in the emitter diffusion case, the lateral diffusion along the Si-SiO₂ interface does not closely resemble either a Gaussian or complementary error function diffusion. The lateral base diffusion actually surpasses the center base diffusion concentration of the idealized base as shown in Figure 19 for depths greater than 0.7 microns from the surface. Similarly as in the emitter diffusion case, there is little correlation with the theoretical data of Kennedy and O'Brien, and the same considerations of this difference are valid here also. Thus, the numerically determined lateral diffusion profile is inaccurate. However, it should be noted that the analytical diffusion by Kennedy and O'Brien basically assumes a delta function impurity profile at the start of the drive-in diffusion which is not completely valid. The center profiles of the idealized and EPE base diffusions can also be compared in Figure 19. As expected, the surface concentration of the EPE diffusion is slightly less than the idealized diffusion, and the EPE impurity atom concentration surpasses the idealized diffusion concentration for depths greater than 0.3 microns. In the regions of the base diffusion outside of the emitter area, the EPE base diffusion almost exactly corresponds to the idealized base diffusion.
FIGURE 19. LATERAL AND CENTER PROFILES OF BASE DIFFUSIONS
3.1.3 Buried Layer Diffusion

An accurate Dt product for the buried layer diffusion is difficult to determine due to the numerous temperature cycles and the changing boundary conditions which occur during and after the buried layer diffusion cycle. Since the buried layer is diffused about 5.3 microns into the substrate, the artificial surface condition which is used in the numerical formulation is a constant source of impurity atoms. However, the location of the constant source is displaced 2.0 microns into the substrate so that some decrease in the concentration of the buried layer near the actual epitaxial-substrate interface can occur. It should be noted that due to the finite size limitations of the semiconductor device model, only part of the buried layer diffusion is modeled, and the rest of the diffusion deep in the substrate is neglected. This condition should create a slightly higher collector resistance but is reasonable since most of the collector current penetrates only the first few microns of the buried layer. Due to the constant source conditions, a complementary error function impurity atom profile should occur near the center of the buried layer diffusion. Figure 20 shows the center and lateral diffusion profiles and the corresponding complementary error function distribution using 2.25 microns as the junction depth. The center profile of the buried layer diffusion is slightly below the corresponding complementary error function profile.

The lateral buried layer diffusion does not surpass the center
FIGURE 20. CENTER AND LATERAL PROFILES OF BURIED LAYER DIFFUSION
of the buried layer diffusion as has been noted in the emitter and idealized base diffusions. In the case of the buried layer diffusion profiles, it should be noted that now the y-direction spatial step size is also very large (either 0.25 or 0.50 microns). In addition, the lateral spatial step size increases significantly at about 1.5 microns removed from the impurity source. Thus, it appears that the apparent difference between the center of the buried layer diffusion and the corresponding complementary error function diffusion is due to the significant increase in the y-direction spatial step size in the buried layer region. The significant change in the slope of the decreasing concentration of the lateral diffusion can be explained by the numerical error which can occur when the spatial step size changes by a factor of eight. If the lateral data of Kennedy and O'Brien were plotted, the numerically determined lateral profile would be slightly above the analytical data except at the low concentration levels.

3.1.4 Isolation Diffusion

The isolation diffusion is analytically determined by use of the method described by Kennedy and O'Brien[26]. This method is used instead of the ADI method since the boundary conditions for the side of the model region are difficult to formulate accurately. Thus, the center of the isolation diffusion is a complementary error function diffusion, and the lateral isolation diffusion corresponds with the data of Kennedy and O'Brien. Figure 21 shows the center and lateral diffusion profiles of the isolation diffusion. It should be noted
FIGURE 21. CENTER AND LATERAL PROFILES OF ISOLATION DIFFUSION
that the isolation diffusion could be modeled by the ADI method if the model region is slightly enlarged. The normal derivatives of the impurity concentration in the y-direction are almost zero at the model boundaries. Thus, the zero normal derivative boundary condition could be used for the sidewalls of the isolation diffusion. The savings in computational time would be significant since almost one-half of the run-time for the entire diffusion model computer program is used for the isolation diffusion calculations.

3.1.5 Diffusion Investigation

In Sections 3.1.1 and 3.1.2, the numerically derived diffusion is shown to be in disagreement with the analytically determined data of Kennedy and O'Brien[26]. The reason for the disagreement is not clear. This disagreement is investigated in more detail in this section. In order to simplify the analysis, a diode in integrated form is utilized which is constructed from a constant donor impurity source of $1.0 \times 10^{21}$ cm$^{-3}$ into a constant acceptor background concentration with a junction depth of 0.3 microns. The mesh structure is designed to concentrate its nodes in the junction region. The x-direction (along the surface) spatial step size is 0.01 microns, and the y-direction spatial step size is 0.002 microns in the junction region. The side boundaries are located 9.7 microns from the lateral junction which gives a boundary location-to-junction depth ratio of about 32. The horizontal boundary is varied to determine its effect on the diffusion.

Numerically, there are three possible problem areas which can
cause the disagreement. First, the constant concentration boundary condition on the side and bottom boundaries of the mesh structure may be critical. Second, the base and emitter center diffusions may be artificially constrained by the bottom boundary condition which is located close to the junction (6.0 microns from the surface) while the lateral diffusion boundary conditions are at least 10.0 microns removed from the source. Finally, the significant difference in the spatial step size between the lateral and center diffusions may indicate that the accuracy of the lateral diffusion is poor. It should be noted that the numerically derived and the analytically determined lateral diffusions differ by approximately a factor of two.

The dependence of the lateral and center diffusions on the magnitude of the constant concentration boundary condition for the side and bottom boundaries is investigated for concentrations ranging from 0.0 to the intrinsic concentration. No dependence is found as all calculations are within 2% of each other which is within the error limits of the numerical calculations. To investigate the effect of the location of the boundary conditions, the location of the bottom boundary condition is varied from 1.5 microns to 6.0 microns or a ratio of boundary location-to-junction depth of 5 to 20. The results of these diffusions are identical so the center diffusion is not constrained as long as the boundary location-to-junction depth is equal to or greater than five.

The dependence of the numerical accuracy on the lateral spatial step size is investigated by varying the lateral spatial step size an
order of magnitude from 0.01 to 0.1 microns. It should be noted that the lateral spatial step size in the emitter and base diffusion regions of the transistor model is 0.125 microns. Figures 22 and 23 show the variation of lateral diffusions as a function of lateral spatial step size and give the center profile and the data of Kennedy and O'Brien for comparison. Figure 22 has a constant acceptor background concentration of \(1.0 \times 10^{16}\) cm\(^{-3}\), and Figure 23 has a background concentration of \(1.0 \times 10^{18}\) cm\(^{-3}\). It is seen that for 0.1 micron spatial step size the lateral diffusion does surpass the center profile at low concentration levels as is shown in the emitter and base diffusions of the transistor model. However, as the lateral spatial steps are decreased, the numerically derived profiles approach quite close to the analytical data of Kennedy and O'Brien. Thus, the lateral diffusions of the emitter and base are apparently inaccurate due to large lateral spatial step sizes.

Figures 22 and 23 also give an idea of the density of mesh nodes which are necessary to obtain an accurate lateral diffusion profile. For the simple integrated diode model, the minimum lateral spatial step size is 0.01 microns which is determined by the maximum main memory size (630K) of the IBM 370 Model 165 computer available. The results using the 0.01 micron spatial step size are relatively accurate except at high concentration levels. In order to exhibit the sharp decrease in concentration near the lateral edge of the impurity source as shown by Kennedy and O'Brien, significantly more nodes are required in this region. Translating these mesh structure requirements into the emitter, base, and isolation junctions of the transistor model,
FIGURE 22. CONSTANT SOURCE DIFFUSION WITH $C_B = 10^{16}$ cm$^{-3}$
FIGURE 23. CONSTANT SOURCE DIFFUSION WITH $C_B = 10^{18} \text{ cm}^{-3}$
an additional 350K main memory storage is required or a total of about 600K main memory storage is necessary for the diffusion model alone. If the semiconductor device model is now considered, the improved transistor model needs 850K additional main memory storage or a total of about 1330K main memory storage. That requirement which only improves the lateral diffusion situation is more than twice the currently available storage so that the inaccurate lateral diffusions are used in this analysis.

3.2 Semiconductor Device Analysis

The numerical results of the semiconductor device model are limited to analysis of the numerical methods and the thermal equilibrium values. Section 4.2 discusses in detail the problem areas in the semiconductor device model and methods of eliminating these problems.

3.2.1 Numerical Method Analysis

The numerical results from both the nonlinear over-relaxation (NLOR) computer program and the quasi-linearization-ADI computer program can be summarized in general as follows. The values of the electron concentration, hole concentration, and valence band edge potential converge to the correct solution in regions of the model which are removed from the junctions. In the junction regions, the electron and hole concentrations often have physically unrealizable negative values and frequently diverge. The valence band edge potentials occasionally take on values which are orders of magnitude too large. The areas of
greatest error are the lateral junction regions of the base and emitter junctions. Numerous numerical methods have been utilized in attempts to decrease the errors, but none have had more than limited success. Methods such as constraining the concentrations to be positive after each iteration, limiting the parameter variation per iteration, utilizing the geometric mean in cases of diverging or slowly converging concentrations, etc, have not completely eliminated the errors. Numerous modifications to the thermal equilibrium trial solution have been used. Using one-dimensional numerical results such as Arandjelovic[43], changes in the minority carrier densities, potential and concentration variations in the depletion regions, etc, have been employed to closely match the applied terminal voltage conditions with limited success. Attempts to iterate to a more correct solution with zero voltage conditions have been unsuccessful.

The two computer programs are significantly different so each program is discussed separately. The NLOR program is a point method in that only the equation of a single variable at one point is solved at a time. There are then two general approaches for solving for the three sets of variables. The three variables at each point can be solved by iterative methods before moving on to the next point. Or, the first set of variables can be solved at all points before going on to the next set of variables. The second method has proved to be the more resistant to divergence since the first method does not obtain a consistent set of variable values before solving for variables in the other sets. Thus, variables tend to drift and cause the next set of
variables to drift further from the solution. It is extremely important that each variable in a set be resolved quite accurately which requires numerous iterations (as many as 1000 for the concentrations) before going on to the next set of variables. The nonlinear current continuity equations seem to be extremely sensitive to small errors in relationships between the three sets of variables. Divergence has been almost completely eliminated by requiring basically three place accuracy for the concentrations and six place accuracy for the potentials. The linear Poisson's equation converges rapidly to the correct potential solution. The nonlinear current continuity equations occasionally oscillate and converge very slowly. The optimum relaxation parameter for the current continuity equations is in the range of 1.15 to 1.24.

The quasi-linearization-ADI program is a block method in that all values of a set of variables are solved for at the same time. It is, however, difficult to guarantee the accuracy of each individual variable, but the set of variables are usually more consistent than after one iteration of the NLOR method. The potential variables converge rapidly with an acceleration parameter of $4 \times 10^4$. The number of negative concentrations after each iteration decreases for increasing values of the acceleration parameter.

3.2.2 Thermal Equilibrium Analysis

The TRIAL subroutine generates an initial trial solution which consists of the thermal equilibrium value of each variable at every point with some 'first-order theory' modifications. To show the
extreme gradients in the three sets of variables, the thermal equilibrium values of electron and hole concentrations and the valence band edge potentials are plotted in Figures 24 and 25, respectively, along a line from the center of the emitter to the buried layer, or along the line i=55. Figures 26 and 27 exhibit the variation of the same variables along the surface, or along line j=1. The effects of the degenerate material considerations can be seen in the base and emitter regions where the product of the electron and hole concentrations are greater than the square of the intrinsic concentration. It should be noted that there are only two or three nodes in the sharp gradient regions with the transistor mesh structure.
FIGURE 24. CENTER VARIATION OF ELECTRON AND HOLE CONCENTRATIONS AT THERMAL EQUILIBRIUM
FIGURE 25. CENTER VARIATION OF VALENCE BAND EDGE POTENTIAL AT THERMAL EQUILIBRIUM
FIGURE 26. SURFACE VARIATION OF ELECTRON AND HOLE CONCENTRATIONS AT THERMAL EQUILIBRIUM
FIGURE 27. SURFACE VARIATION OF VALENCE BAND EDGE POTENTIAL AT THERMAL EQUILIBRIUM
CHAPTER IV

DISCUSSION AND CONCLUSIONS

Two numerical methods are presented in this work. First, the diffusion model is introduced which employs alternating direction implicit numerical methods to efficiently solve for the various two-dimensional diffusions. The semiconductor device model is then presented which calculates the electron and hole concentrations and the valence band edge potentials for the two-dimensional model of the bipolar transistor. Two different numerical methods are given for the semiconductor device model which differ in complexity and efficiency. The capabilities and limitations of the numerical methods as described in Chapter III are discussed in detail in this chapter, and possible solutions to the remaining problem areas are outlined.

4.1 Diffusion Method and Results

The impurity atom concentrations must be accurately determined at each node of the two-dimensional mesh structure before the semiconductor device model can produce accurate solutions. The numerical method which is presented in this work is the Peaceman-Rachford alternating direction implicit method[24] which solves the algebraic equations which are generated by the integral formulation of the finite difference approximations. This numerical method is extremely effic-
ient and accurate and can consider impurity diffusion constants which vary with position. The ADI method is a straight-forward process which eliminates the somewhat arbitrary procedures of the simple relaxation method of Kennedy and Murley [18]. The ADI method can be as accurate as the analytical method of Kennedy and O'Brien [26] if the proper mesh structure is utilized and is greater than 60 times more efficient than the analytical method whose accuracy depends only on the computational determination of the Kummer function. It should be noted that the Kummer function becomes inaccurate at points close to the source and for concentrations which are six or more orders of magnitude below the source concentrations due to computer limitations on the size of real constants. The ADI diffusion method can be used for any sequence of diffusion processes with various boundary conditions. The analytical method, however, is limited to a constant source condition or a two-step diffusion process where the predeposition diffusion is assumed to result in a delta function distribution which is a poor approximation for long predeposition processes.

The ADI diffusion method has one problem area which is computational accuracy. If the time step is too large or the spatial step size is too large or extremely nonuniform, the accuracy of the numerical methods decrease significantly. The simplest method to check the numerical accuracy for a constant source diffusion is to compare the results with the analytical results. The main problem of the bipolar transistor model in terms of the numerical solution of the diffusion equation is the lack of nodes in the lateral junction regions of the
emitter and base diffusions. Section 3.1.5 defines the lateral profile problem which is discussed in Sections 3.1.1 and 3.1.2. If the density of nodes could be increased in these regions by an order of magnitude, the accuracy of the lateral diffusion profile would be increased by an order of magnitude which would reduce the error from 200\% to 20\%. However, as calculated in Section 3.1.5, the semiconductor device model would then require roughly twice the available main memory storage of the IBM 370 Model 165 computer. Thus, the error in the lateral diffusion is allowed to remain at about 200\% in order to keep the semiconductor device model within the computational constraints. It should be noted that the real constants in this program are generally double precision (approximately 16 digit numbers) since extremely large errors, mainly round-off errors in the Gaussian elimination routine, are encountered with single precision numbers (approximately 7 digit numbers). Another example of numerical error due to large spatial step sizes is in the center profile of the emitter diffusion. The center diffusion of the emitter tends to flatten out and drop below the expected analytical profile between 0.2 and 0.4 microns below the surface. In this region, the spatial step size in the y-direction is increased from 0.025 to 0.1 microns in order to keep within the maximum number of nodes allowed.

The ability of the ADI method to handle positional dependent impurity diffusion constants is important in the emitter and EPE base regions. As expected, the center emitter distribution for the concentration-dependent diffusion constant is above the complementary error.
function profile near the surface where the emitter diffusion constant is maximum. The spatial dependent impurity diffusion constants have been varied up to two orders of magnitude without any significant error or instability occurring.

4.2 Semiconductor Device Method and Results

The two numerical methods which are designed to solve the three coupled elliptic equations of the semiconductor device model have not been completely successful. The problem areas and the possible solutions are discussed in this chapter. Only the nonlinear over-relaxation method (NLOR) is analyzed since it is the more elementary of the two methods and yields clear observations concerning the problem areas. Also, the NLOR method must function successfully if the quasi-linearization-ADI method is to succeed due to the more restrictive conditions in the quasi-linearization-ADI method. Comparisons with two-dimensional Boltzmann statistical methods are made to illustrate the more involved nature of the Fermi-Dirac statistical method.

In Section 3.2.1, the general problem areas which have been encountered are mentioned. The basic difficulty concerns the transition from the trial solution to the first iterative solution, mainly in the junction regions. The trial solution consists of the thermal equilibrium values for all three sets of variables as modified by 'first-order' theory. The depletion areas are inserted on the low concentration side of the junction, and the carrier concentrations are decreased and the potential is given a linear gradient in these regions.
Also, since the transistor model is roughly similar to that used in a one-dimensional numerical analysis by Arandjelovic[43], minority and majority carrier concentration levels are modified in accordance with this reference to agree with the applied terminal voltages. The voltage conditions for the first solution are 0.1 volts from the thermal equilibrium terminal conditions in order to minimize potential discontinuities. The terminal voltages of the first solution have also been set to zero in order to see if the trial solution would improve itself before making the transition to a nonzero applied voltage case.

The first disturbing factor which is encountered in the analysis of the two-dimensional numerical methods is that for similar density of nodes the Boltzmann statistical methods in the literature [10,11,12,13,15,16,17,48] seem to function correctly while the Fermi-Dirac statistical method presented here is only partially successful. It is true, however, that the other methods analyze much less involved device structures such as MOS transistors which have only two relatively unimportant junction regions. Also, statements such as 'smoothing functions are used for the potential and concentrations to obtain consistent final results' indicate that Boltzmann statistical methods may have numerical problems due to limited node density. Almost all authors comment on the lack of computer storage as being the limiting factor on the node density. However, there is a more fundamental difference which accounts for the success of Boltzmann methods and partial failure of the Fermi-Dirac method. To show this difference, it is necessary to analyze the Boltzmann methods.
The Boltzmann statistical methods basically start with the same set of equations as the Fermi-Dirac statistical method which are given in (2.15-2.17) with the exception that the generalized Einstein relations $\alpha_p$ and $\alpha_n$ are unity. Then, the simplicity of Boltzmann statistics can be used by inserting

$$n = \exp(\psi - \phi_n) = \lambda(x,y)\exp(\psi) \quad (4.1)$$

$$p = \exp(\psi - \phi_p) = \gamma(x,y)\exp(-\psi) \quad (4.2)$$

where $\psi$ is the electrostatic potential and $\phi_n$ and $\phi_p$ are the electron and hole quasi-Fermi levels, respectively. Thus, the set of equations become

$$\nabla \cdot (\mu_n \exp(\psi) \nabla \lambda) = R \quad (4.3)$$

$$\nabla \cdot (\mu_p \exp(-\psi) \nabla \gamma) = R \quad (4.4)$$

$$\nabla^2 \psi = \lambda \exp(\psi) - \gamma \exp(-\psi) - N_{DIFF} \quad (4.5)$$

At this point, the set of three equations are elliptic and nonlinear depending on the choice of the recombination law chosen. All authors neglect to define the recombination law used but state that Equations (4.3-4.4) are linear which implies that $R$ is of the form $(n-n_0)/\tau_n$ or $A(np-1)$. Thus, the Shockley-Read-Hall recombination law is not used in Boltzmann methods. To linearize the nonlinear Poisson's equation (4.5), the Gunnell[1] linearization method is used which defines

$$\psi^{m+1} = \psi^m + \delta \quad (4.6)$$
so

\[ \nabla^2 \delta - \delta \left[ \lambda \exp(\psi^n) + \gamma \exp(-\psi^n) \right] = \lambda \exp(\psi^n) - \gamma \exp(-\psi^n) \]

\[ - N_{\text{DIFF}} - \nabla^2 \psi^n \]  

(4.7)

Now since Equations (4.3,4.4,4.7) form a linear set of equations in \( \lambda, \gamma, \) and \( \psi, \) these equations can be solved efficiently by a number of numerical methods. The most recent method \[48\] uses ADI methods with Taylor's series formulation of the finite difference approximations.

This method is relatively efficient but could be greatly improved by using quasi-linearization techniques instead of the Gummel linearization and the integral formulation instead of the Taylor's series formulation.

The basic point to be illustrated by the formulation of the Boltzmann statistical method is the comparison between the simple set of equations (4.3,4.4,4.7) with very weak nonlinear terms for the Boltzmann statistics and the complex set of equations (2.36-2.38) with rather involved nonlinear terms for the Fermi-Dirac statistics.

It should be noted that there are spatial derivatives of the concentrations, potential, mobilities, and generalized Einstein relations along with a much more involved recombination law in the nonlinear terms of the Fermi-Dirac method which are not present in the Boltzmann method. The second consideration concerning the differences between the Boltzmann method and the Fermi-Dirac method is that the Fermi-Dirac integral can not be represented by an analytical expression for chemical potential values from -4.0 to 20.0. Thus, numerical derivatives must be employed in the determination of the generalized Einstein
relations for this range of chemical potentials and are therefore subject to common numerical errors. This problem does not exist in the Boltzmann method.

To show the actual numerical problems with the bipolar transistor model, it is convenient to look at one node which illustrates the problems. Looking at Figures 22-25, it is noticed that the potential and concentration gradients are extremely large in the junction regions. The 'first-order' theory and other numerical results which are used to modify the trial solution do decrease the gradients slightly but not significantly. A node (55,25) which clearly illustrates the numerical problems is located at the base-collector junction and is the first node on the collector side of the metallurgical junction. The terminal voltage conditions are set which applies reverse bias to the base-collector junction of 0.1 volt and forward bias of 0.1 volt to the emitter-base junction. At these voltages, one-dimensional numerical analysis[43] would indicate a large decrease in the electron concentration and a slight decrease in the hole concentration on the collector side of the base-collector junction. In normalized values, the hole concentration of node (55,25) is $4.78 \times 10^5$ cm$^{-3}$. The node (55,24) which is located directly across the metallurgical junction on the base side and is 0.0125 microns from node (55,25) has a hole concentration of $1.22 \times 10^{15}$ cm$^{-3}$.

Now, the $y$-direction first partial derivative (see Section C.1) of the hole concentration at node (55,25) is controlled by the hole concentration of node (55,24) since the hole concentration at node
(55,26) is also small and is calculated to be \(-1.47\times10^{17} \text{ cm}^{-4}\). Since the concentration gradient is so sharp, the accuracy of the numerical partial derivative is extremely poor. Now considering Equation (2.40) which is the hole concentration equation of the NLOR method, the equation is written in a partially discretized form for clarity and uses the notation of Table 2.

\[
p_{m+1}(i,j) = p^m(i,j) - \omega_p \left[0.5[p^m(i,j) - p^m(i-1,j)]SSY(j)ight.\]
\[
\times \mu_p(i-1/2,j)/SX(i-1) + 0.5[p^m(i,j) - p^m(i+1,j)]\]
\[
\times SSY(j) [\mu_p(i+1/2,j)/SX(i) + 0.5[p^m(i,j) - p^m(i,j-1)]\]
\[
\times SSX(i) [\mu_p(i,j-1/2)/SY(j-1) + 0.5[p^m(i,j) - p^m(i+1,j)] SSX(i)\]
\[
\times SY(i) [\mu_p(i,j+1/2)/SY(j) + 0.25SSY(i)\]
\[
\times SY(j)L_2/(0.5SSY(j) [\mu_p(i-1/2,j)/SX(i-1) + \mu_p(i+1/2,j)/SX(i)] + 0.5SSX(i) [\mu_p(i,j-1/2)/SY(j-1) + \mu_p(i,j+1/2)/SY(j)] + 0.25SSY(i) SSY(j)\]
\[
\times \frac{\partial^2 R}{\partial p^2} - \mu_p \psi_x v_x - \mu_p \psi_y v_y - \mu_p (n^m(i,j) - p^m(i,j) - N_{DIFF}(i,j)) - \frac{\partial^2 \alpha_p L_2}{\partial p \alpha_p} \alpha_p \right)
\]

where

\[
L_2 = [R - \mu_p Px(\psi_x + \alpha_p x) - \mu_p Py[\psi_y + \alpha_p y] - p[\mu_p \psi_x v_x + \mu_p \psi_y + \mu_p (n - p - N_{DIFF})] \]
and, for example,

$$\mu_p(i,j-1/2) = 0.5[\mu_p(i,j) + \mu_p(i,j-1)]$$

Now from the standpoint of the new hole concentration at node (55,25), there are two main factors which are important. It should be noted that the x-direction variation in all three variables is essentially zero so only the y-direction variations are important. The first term which is important is the $p^m(i,j) - p^m(i,j-1)$ since, in this case, $p^m(i,j-1)$ is ten orders of magnitude greater than $p^m(i,j)$. The second important term is in $L_2$ and is $p_y$ which is given above as $-1.47 \times 10^{-17}$ cm$^{-4}$. Both of these terms are in the numerator of Equation (4.8).

Condensing the numerator down to these important terms, the following expression is obtained.

$$-0.5SSX(i)\mu_p(i,j-1/2)p^m(i,j-1)/SY(j) - 0.25SSX(i)SSY(j)$$

The order of magnitude of these two terms is $10^{14}$ and the denominator of Equation (4.8) is approximately $10^{1}$. Now, in order for the new hole concentration at node (55,25) to be slightly less than the trial solution at that node, these two terms must be equivalent in magnitude for the first nine digits so that the two $10^{14}$ terms can yield a $10^5$ difference. This situation is the basis of the entire numerical problem with the Fermi-Dirac method. With such inaccuracy in the $p_y$ term, the difference is very likely to be equal to $\pm 10^{13}$. For example,
the solution of the first iteration for the hole concentration at node (55,25) is 1.96×10^{13} as compared to the trial solution of 4.78×10^{5}. The p_{v} term is slightly larger than the p^{n}(i,j-1) term and strongly predominates the whole equation.

The possible solution to the numerical problem is a significant increase in the density of the nodes in exactly the metallurgical junction region coupled with possibly a five-point finite difference derivative expression for the partial derivatives of the concentrations. Now the computer limitation must be considered. To be able to maintain the accuracy, double precision real numbers are absolutely necessary. For the NLOR method, a minimum of eight double precision numbers are required for each node. Each double precision number uses eight storage locations or bytes. Thus, for each node, 64 bytes of main memory storage are required. Considering the 630K of storage available on the IBM 370 Model 165 computer and allowing 80K for the program and buffers, a maximum number of nodes which can be used is about 8600. Since the present mesh structure uses 5200 nodes to model the three junction regions, 3400 extra nodes are insufficient to achieve anywhere near the required accuracy. Off-line storage could be considered if the significant decrease in access time can be tolerated. Note that all eight arrays of numbers and the five values around the node (i,j) for each variable must be simultaneously available so it is difficult to conceive of a system of mixing the storage arrangement of the eight arrays so that the right values can come off the disk serially. This would be a significant programming task and thus main storage is only con-
sidered in this work.

The conclusions concerning the semiconductor device model are simply that the numerical formulation with Fermi-Dirac statistics is very sensitive to numerical error and requires numerous nodes exactly at the metallurgical junction. In two-dimensional analysis, this requirement is difficult to implement. Considering the available computer storage, only the most elementary device could possibly be analyzed. The obvious conclusion is that the Boltzmann statistical programs should be used except in extreme cases of very high degeneracy.
CHAPTER V

RECOMMENDATIONS

From the conclusions of Chapter IV, several basic recommendations can be made concerning the diffusion model and the semiconductor device model. The diffusion model is shown to be a significant method for the determination of impurity atoms concentrations resulting from diffusion processes. The Peaceman-Rachford alternating direction method applied to the diffusion equation as discretized by the integral formulation of the finite difference approximations is extremely stable for large variations of the time step (up to about 20 times the explicit limit) and for spatial variations in the impurity diffusion constant. The consideration of the spatial variation of the impurity diffusion constant is a feature of the integral formulation of the finite difference approximations which is not found in the Taylor's series formulation. It is interesting to note that no other author of two-dimensional semiconductor device and diffusion analysis has ever used the integral formulation before. All other authors have used the Taylor's series expansion which can have significant problems when the mesh structure is extremely nonuniform. A Taylor's series diffusion model has been generated and performed well except for slight errors in sections of extremely nonuniform mesh structure. The Taylor's series diffusion model could handle the block enhancement of the base impurity diffusion
constant for the EPE base diffusion but becomes unstable when the concentration-dependent emitter diffusion constant is used. The integral formulation is used in both the diffusion and the semiconductor device models. The spatial variations of the impurity diffusion constant have been as great as two orders of magnitude without significant error. Comparing the ADI diffusion model with other possible methods, the ADI diffusion method is greater than 60 times more efficient than the analytical method of Kennedy and O'Brien and is much easier to program than the arbitrary procedures of the simple relaxation of Kennedy and Murley. Depending on the spatial step size of the mesh structure, the ADI diffusion method approaches quite close to the accuracy of the analytical method. Thus, the ADI diffusion model has been shown to be significantly superior to any other published numerical or analytical method. Extensions to the diffusion model in the areas of oxide growth and oxide interaction with impurity atoms are considered in Section 5.1.

The inability to achieve a fully operational numerical algorithm for the semiconductor device model leaves this model in an uncertain position. From the experience of the author, both the NLOR and the quasi-linearization-ADI methods have performed correctly in all regions except areas of large concentration gradients. The failure of the numerical methods in the large concentration gradient regions is blamed on the numerical error in the partial derivatives of the concentrations. This reason for the failure is given more validity by the results of the NLOR method on the integrated diode of Section 3.1.5.
With step sizes of 0.002 and 0.01 microns in the y-direction and x-direction, respectively, the NLOR method gives significantly better results especially along the planar junction region with its maximum node density. However, in the lateral junction regions, the same problems which are discussed in Section 4.2 occur. The diode mesh structure can not be made more dense in the lateral direction since the diode model contains the maximum number of nodes allowed by the computer.

The numerical algorithms for the semiconductor device model give all indications of performing correctly if the required density of nodes in the junction region can be achieved. The available computer storage seriously limits the complexity of the device model so that Boltzmann statistical methods are strongly recommended unless extreme degeneracy exists and a computer with multi-million byte storage is available. Thus, the future of the Fermi-Dirac statistical method may hinge on the advances in computers such as virtual memories, etc or more sophisticated system programming. It should be mentioned that the formulation of the semiconductor device equations is correct, and the numerical methods have been correctly applied to the solution of the three coupled, nonlinear, elliptic equations. The computer programs in Appendix F contain these numerical methods as applied to the bipolar transistor model. The only question marks about the numerical methods are concerning the ability of the numerical methods to be to solve the highly nonlinear equations and the accuracy of the device model to which the numerical methods are applied. The latter situation is considered to be the main problem.
5.1 Extensions to Diffusion Model

The surface of the model region is assumed to be flat and stationary in the diffusion model. This assumption simplifies the numerical method but corresponds poorly to the nonstationary stair-step surface of normal bipolar transistor devices. Also the oxide layer is assumed to be neither a sink nor source of impurity atoms. To diminish the effect of these assumptions, changes could be made in the diffusion model. The growth rate of the oxide for the different process conditions can be determined from references such as [28]. If numerous horizontal mesh lines were located in the region near the surface, the lines near the surface of the diffusion area could be removed from the diffusion model as the product of the summation of the time steps and the growth rate exceeds the horizontal line spacing. This method would result in a series of segmented horizontal lines, and the computer programs would have to be structured in a more general fashion in order to be able to handle this situation. Boundary conditions, lengths of mesh lines, and termination conditions would now be time-dependent.

To model the oxide layer's rejection or absorption of impurity atoms during thermal oxidation, the rate of rejection (such as for phosphorus) and absorption (such as for boron) would have to be determined. If these rates can be determined, then the boundary condition at the surface of a zero normal derivative of impurity concentration could be changed to a time-dependent impurity concentration source condition, and the magnitude of the surface concentration would be the instan-
taneous concentration at the surface as determined by the rate of re-
jection or absorption by the oxide.

5.2 Extensions to Semiconductor Device Model

As discussed in Section 4.2, the number of mesh nodes in the
metallurgical junction and other regions of significant concentration
variation is critical if the numerically determined partial derivatives
of the electron and hole concentrations are sufficiently accurate to
guarantee convergence to the correct solution in a finite computation
time. An algorithm to determine the density of mesh nodes which are
required to maintain a specified maximum error has not been generated.
The algorithm would be a function of the impurity concentrations and
their gradients and the electron and hole concentrations and their
gradients. As is discussed in Appendix D, a node-locating algorithm
based on the computational error in the various concentrations would
be time consuming for a method with numerically determined impurity
profiles, but may be necessary.

The quasi-linearization-ADI numerical method is an extremely
efficient method for solving large sets of nonlinear equations. How-
ever, more work could be done on the determination of the optimum accel-
eration parameters. Currently, the optimum parameters are approximately
determined by trial and error. References such as [25] and Wachspress
[44-47] give sufficient detail to more accurately determine the accel-
eration parameters. It should be mentioned that the theory of ADI
indicates that a series of a single acceleration parameter value will
guarantee convergence, but a series of parameter values may or may not converge. A properly selected series of descending acceleration parameter values, if they do converge, should converge more rapidly than a series of a single parameter value. Another numerical method which may be more efficient than the quasi-linearization-ADI method is the quasi-linearization-line successive over-relaxation method (LSOR). The LSOR method requires less programming than the ADI method.

If the degenerate material requirement is not present, simpler programs such as the recent article on two-dimensional modelling by Vandorpe et al [48] can be used. The method which is used in the Vandorpe article is the Gummel linearization of Poisson's equation and ADI or LSOR methods. It is straight-forward to replace the Gummel linearization procedure with the quasi-linearization technique which is used in this work to increase the efficiency of the modelling procedure significantly. Also, it is easy to reformulate the method to replace the Taylor's series formulation of the finite difference approximations with the integral formulation.
APPENDIX A

N-P-N TRANSISTOR MODEL DATA

The N-P-N silicon transistor model used in this work was designed around the D3 transistor which was developed by the Integrated Circuits Group at the Avionics Laboratory at Wright-Patterson Air Force Base. The D3 transistor is a basic integrated circuit transistor and thus is somewhat larger than the current high frequency devices. The asymmetrical design with one base stripe requires twice the number of mesh nodes to analyze than symmetrical devices but exhibits more interesting effects such as asymmetrical emitter current crowding. The N-P-N transistor model is investigated in two different configurations. First, an idealized transistor with no EPE is studied. Finally, a more realistic model of the transistor with EPE is analyzed. The two models are constrained to be as similar as possible so that the effects of EPE can be accurately observed. However, in the emitter-base region, some minor differences in the diffusions do occur even outside the main EPE region.

The approximate impurity atom profile drawing is shown in Figure 2, and the top view of the transistor model is given in Figure 3. The basic numerical data for the transistor model is presented in Table 5.
### TABLE 5. N-P-N TRANSISTOR MODEL DATA

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Emitter Surface Concentration</td>
<td>$1.0 \times 10^{21}$ cm$^{-3}$</td>
</tr>
<tr>
<td>Emitter-Base Junction Depth</td>
<td>$0.6 \times 10^{-4}$ cm</td>
</tr>
<tr>
<td>Base Surface Concentration (after deposition)</td>
<td>$5.0 \times 10^{20}$ cm$^{-3}$</td>
</tr>
<tr>
<td>Base Surface Concentration (after drive-in)</td>
<td>$3.2 \times 10^{19}$ cm$^{-3}$</td>
</tr>
<tr>
<td>Base-Collector Junction Depth</td>
<td>$1.2 \times 10^{-4}$ cm</td>
</tr>
<tr>
<td>Extended Base-Collector Junction Depth</td>
<td>$1.4 \times 10^{-4}$ cm</td>
</tr>
<tr>
<td>Buried Layer Surface Concentration (at substrate surface)</td>
<td>$1.0 \times 10^{19}$ cm$^{-3}$</td>
</tr>
<tr>
<td>Buried Layer Junction Depth (into substrate)</td>
<td>$5.3 \times 10^{-4}$ cm</td>
</tr>
<tr>
<td>Buried Layer Out-Diffusion (into epitaxy)</td>
<td>$1.25 \times 10^{-4}$ cm</td>
</tr>
<tr>
<td>Epitaxial Layer Concentration</td>
<td>$1.0 \times 10^{16}$ cm$^{-3}$</td>
</tr>
<tr>
<td>Epitaxial Layer Thickness (as deposited)</td>
<td>$4.0 \times 10^{-4}$ cm</td>
</tr>
<tr>
<td>Epitaxial Layer Thickness (after temperature cycles)</td>
<td>$5.0 \times 10^{-4}$ cm</td>
</tr>
<tr>
<td>Isolation Surface Concentration</td>
<td>$1.0 \times 10^{19}$ cm$^{-3}$</td>
</tr>
<tr>
<td>Isolation-Substrate Junction Depth</td>
<td>$7.0 \times 10^{-4}$ cm</td>
</tr>
<tr>
<td>Substrate Concentration</td>
<td>$1.0 \times 10^{15}$ cm$^{-3}$</td>
</tr>
</tbody>
</table>
APPENDIX B

MESH STRUCTURE

The primary considerations in the determination of the mesh structure for modeling a semiconductor device are the computational complexity and the desired accuracy of the results. A rectangular cell structure is selected since the semiconductor device model is conveniently conceived in a rectangular form and since the rectangular structure is more easily programmed and decreases the number of iterations necessary for convergence due to its simplicity. To decrease the truncation or discretization error of the finite difference approximations, the nodes of the mesh must be concentrated in the regions of significant parameter variation. Similarly, regions of minimum parameter variation can be represented by fewer nodes for the same truncation error which decreases the total number of nodes and thus equations to be solved. Thus, a highly non-uniform rectangular mesh is selected to maintain accuracy while minimizing computation time.

B.1 Spatial Step Determination

The possible methods of determining the non-uniform spatial step distribution range from the educated guess technique to a fully computerized routine which is based on either maximum truncation error or maximum number of points acceptable are considered. DeMari[2] describes methods of automatically adjusting the spatial step size
in one-dimensional device models using the assumption of analytically derived impurity atom concentrations. Basically, the automatic methods determine the spatial step size from the analysis of the truncation error of the finite difference approximations involving the electrostatic potential. Since the electrostatic potential varies quite rapidly in the junction regions of semiconductor devices, in the channels of FET's and MOSFET's, and at the contact regions, a significant increase in the density of nodes must occur in these regions to maintain a maximum allowable truncation error.

In two-dimensional analyses with numerically determined impurity atom concentrations, automatic methods for adjusting the spatial step distribution are significantly more difficult to develop. If the spatial step size is controlled by the truncation error of the finite difference approximations involving the electrostatic potential, an iterative loop would be required which includes the numerical computation of the impurity atom concentration so that the impurity atom concentration would be calculated at the new nodes. Even if only one iteration is permitted, the computation time would be excessive. Another method of automatically adjusting the spatial step distribution involves the truncation error of the finite difference approximations concerning the impurity atom concentrations. This method would concentrate nodes in the junction regions where the concentrations and also the electrostatic potential vary significantly. This method, however, fails to concentrate nodes in the contact regions and near the surface of a MOSFET, for example.
The second consideration of automatic spatial step methods in two-dimensional analyses involves the requirement for rectangular cell structures. If all nodes were allowed unrestricted spatial variations in both directions as a function of truncation error, the result would be in general a non-rectangular mesh structure. Thus, to retain the rectangular mesh structure, each line of nodes must vary as the node on the line which has the largest truncation error. Finally, considering the numerical solution to the diffusion equation, both spatial and time sizes must be varied with respect to the truncation error for each time period. In the case of normal diffusions, there exists an extremely abrupt concentration gradient near the surface at time t=0+ and shortly afterwards, and then the concentration gradient moves into the device. Thus, the spatial step size would have to be extremely small near the surface initially, and the small spatial step sizes would have to follow the diffusion front into the device as time progressed. The computation time for such an involved step procedure would be excessive.

Considering the above mentioned problems of automatic spatial step methods in two-dimensional analyses, it is concluded that the trade-off of computation time and minimizing the truncation error indicates that the educated guess method with high concentrations of nodes throughout the emitter, base, and contact regions is the best possible solution for two-dimensional analyses with numerically determined impurity atom concentrations. Since most of the rapid parameter variations are in the direction perpendicular to the surface, the spatial steps in this direction are tightly compressed in the emitter and base
junction regions.

B.2 Final Mesh Structure

The final mesh structure selected is a highly non-uniform rectangular grid. In the x-direction or parallel to the surface, the spatial step sizes vary from 2.5 microns in the collector and isolation regions to 0.125 microns in the emitter and base junction areas. The transition, however, between these significantly different spatial step sizes is made as gradual as possible in order to reduce the possibilities of excessive errors from the numerical approximations. In the y-direction or perpendicular to the surface, the spatial step sizes range from 0.0125 microns in the emitter and base junction regions to 0.5 microns in the collector and substrate areas. The method used to select the mesh structure does not automatically eliminate convergence problems as the truncation error methods would, but engineering estimates can significantly reduce the possibilities of slow convergence. The final mesh structure has 100 nodes in the x-direction and 52 nodes in the y-direction which gives 5200 nodes in the entire mesh. Figure 6 shows the mesh structure which is used for the N-P-N transistor model.
There are three basic methods of deriving the finite difference approximations for second partial differential equations in two spatial variables. A commonly used method is based on finite Taylor's series expansions of the solution. The second method is the integration method which associates an area to each node. Finally, a variational formulation of the solution can be used in deriving the finite difference approximations. In this work, the integral formulation is used which occasionally involves Taylor's series expansions for some derivatives. A good reference text for the integral formulation is Varga [25]. The integral formulation is used due to its added resistance to divergence which sometimes occurs in highly nonuniform grid structure as compared to the Taylor's series formulation. The integral approximations which are used to compute the terminal parameters are also given. The notation used in this appendix is defined in Table 2.

C.1 Taylor's Series Expansions

In this work, only the first and second partial derivatives of the function $U(x,y)$ are required at the mesh node $(i,j)$. Two- and three-point formulae are given, and the three-point formulae are used in general throughout the work except for slowly varying functions such
as mobility and generalized Einstein relations. Five-point formulae are not used due to the greatly increased computational load and insignificant increase in accuracy as reported by DeMari[2].

Two-point Formulae:

\[ U_x(i,j) = \frac{U(i+1,j) - U(i,j)}{sx(i)} \equiv \text{forward derivative} \]

\[ U_x(i,j) = \frac{U(i,j) - U(i-1,j)}{sx(i-1)} \equiv \text{reverse derivative} \]

\[ U_x(i,j) = \frac{U(i+1,j) - U(i-1,j)}{sx(i) + sx(i-1)} \equiv \text{center derivative} \]

Similar formulae can be written for the y-direction partial derivatives.

Three-point Formulae:

\[ U_x(i,j) = \frac{U(i+1,j) + (rx(i) - 1)U(i,j) - rx(i)^2U(i-1,j)}{rx(i)sx(i)} \]

\[ U_{xx}(i,j) = \frac{\partial^2 U(i,j)}{\partial x^2} \]

\[ \approx \frac{2[U(i+1,j) - (rx(i) + 1)U(i,j) + rx(i)U(i-1,j)]}{sx(i)sx(i)} \]

Similar formulae can be written for the y-direction second partial derivatives.

C.2 Integration Formulation

To illustrate the use of the integration formulation, consider the second-order self-adjoint elliptic partial differential equation
\[-[P(x,y)U_x]_x - [P(x,y)U_y]_y + B(x,y)U(x,y) = F(x,y)\]

With each mesh node \((i, j)\), a closed mesh region \(R(i, j)\) is defined as shown in Figure 28. The closed mesh region \(R(i, j)\) is bounded by the lines \(x = x_i - SX(i-1)/2, x = x_i + SX(i)/2, y = y_j - SY(j-1)/2,\) and \(y = y_j + SY(j)/2\). Integrating over the corresponding mesh area \(R(i,j)\),

\[- \int \int_{R(i,j)} [(P_U)_x dx + (P_U)_y dy] + \int \int_{R(i,j)} B dx dy = \int \int_{R(i,j)} F dx dy \]

By Green's Theorem, the first double integral can be changed to a line integral where \(C(i, j)\) is the boundary of \(R(i, j)\) and the line integral is taken in the positive sense.

\[- \int_{C(i,j)} [(P_U)_x dx - (P_U)_y dy] + \int \int_{R(i,j)} B dx dy = \int \int_{R(i,j)} F dx dy \]

The double integrals can be simply approximated by means of

\[\int \int_{R(i,j)} B dx dy \approx B(i,j)U(i,j)A(i,j)\]

\[\int \int_{R(i,j)} F dx dy \approx F(i,j)A(i,j)\]

where \(A(i,j)\) is the area of \(R(i,j)\). This area is obviously equal to \(SSX(i)SSY(j)/4\). The line integral is approximated by means of central differences and the resulting finite difference approximation is

\[D(i,j)U(i,j) - E(i,j)U(i-1,j) - W(i,j)U(i+1,j) - N(i,j)U(i,j+1)\]

\[- S(i,j)U(i,j-1) = F(i,j)SSX(i)SSY(j)/4\]
FIGURE 28. MESH STRUCTURE NOTATION
\[ E(i,j) = [P(i-1,j) + P(i,j)]SSX(i)/4SX(i-1) \]

\[ W(i,j) = [P(i+1,j) + P(i,j)]SSX(i)/4SX(i) \]

\[ N(i,j) = [P(i,j+1) + P(i,j)]SSY(j)/4SY(j) \]

\[ S(i,j) = [P(i,j-1) + P(i,j)]SSY(j)/4SY(j-1) \]

### C.3 Integral Approximations

With the choice of unknown variables, numerical integration is limited in this work to final parameter evaluation, mainly, the terminal current densities. Two- and three-point formulae are given. The three-point formula is used throughout the work except where the boundaries require the two-point formula.

**Two-point Formula:**

\[
\int_{X(i)}^{X(i+1)} U(x) \, dx = \frac{[U(i) + U(i+1)]SX(i)}{2}
\]

**Three-point Formula:**

\[
\int_{X(i-1)}^{X(i+1)} U(x) \, dx = \left( [2 - RX(i)]U(i-1) + [RX(i) + 2 + 1/RX(i)]U(i) + [2 - 1/RX(i)]U(i+1) \right) SSX(i)/6
\]
APPENDIX D

ACCURACY OF NUMERICAL METHODS

Several types of errors occur when numerical methods are employed in the solution of partial differential equations. One of the more difficult tasks in dealing with numerical methods is the determination of the magnitude of the various errors and the total error. Two methods are generally used to develop a relative magnitude of these errors. First, the more desirable method is to determine the individual errors introduced by each elementary operation in order to achieve an estimation of the total error for the entire sequence of operations. The second and more easily implemented method is to use appropriate sets of relations to test the accuracy of the final solution. This is the approach which is employed in this work. The sources of error are analyzed to determine techniques suitable to control the magnitude of these errors.

D.1 Types and Sources of Errors

The types of errors most commonly found in numerical studies can be divided into basically two groups. Discretization errors are the errors which occur when a continuous system is represented by a finite number of nodes using finite difference techniques. Thus, an error is introduced whenever an operation is performed on a discretized function, and the magnitude of the error depends on the order of the finite
difference approximation used. In this work, the computation of the first and second spatial derivatives of the hole and electron concentrations, the valance band edge potential, and other functions introduces errors by their discretized form. Discretization errors will obviously decrease as the spatial intervals decrease in size and the number of nodes increase in density. Discretization errors are a function of the physical model since trade-offs have to be made between computation time and the size of the model, the number of nodes, and the density of the nodes. Many authors have followed the methods of DeMari[2] and use the truncation error as a guide for the relative location of the nodes. Appendix B describes in some detail the problems associated with extending this concept into two dimensions for numerically determined impurity atom profiles.

One method to minimize the discretization error is to use high-order finite difference approximations such as the three-point or five-point approximations. However, if higher-order approximations than the three-point approximation are used, the band matrices of the ADI methods changes from a tridiagonal matrix to a five band matrix for the case of a five-point approximation. It is found that an insignificant change occurred in the diffusion program accuracy while a significant change occurred in the computation time. Thus, the three-point finite difference approximation is used throughout this work. Since the truncation error is not maintained constant automatically by the placement of nodes, it is to be expected that the truncation error
may increase in the regions of steep rates of change of important parameters. This is observed to occur especially along the side edges of the emitter and base diffusion regions. Fortunately, the contribution to the total final result is less significant from these regions than from others so that the relative importance of the truncation error from these regions is less.

The second type of errors which occur in numerical methods can be classified under the heading of numerical errors. The type of errors which fit into this category are:

(a) round-off errors
(b) quantities exceeding allowed ranges
(c) small differences between nearly equal numbers
(d) interruption of the iterative cycle

Round-off errors occur, in general, in any elementary operation on parameters which are represented by a finite number of digits. This error also occurs with various physical constants whose significant digits are limited by experimental accuracy. Otherwise, the round-off errors are strictly a function of the storage allotment of the computer. In the present case, the choice is between either single-precision (approximately 7.2 decimal digits) and double-precision (approximately 16.8 decimal digits) real constants. Double-precision real constants are used throughout the diffusion program except for constants with significant digits less than seven. For the steady-state device program, computer memory limitations forced the use of single-precision real constants for the less important parameters such as mobilities and
and the generalized Einstein relations. Double precision real constants are used for all parameters which are involved in the modified Gaussian elimination routine. Gaussian elimination routines can cause serious round-off errors for certain combinations of coefficients which can normally be avoided by pivoting. As discussed in Chapter II, pivoting is not required in this case.

Various parameter values exceeded the allowed magnitude of the computer which extends approximately from $10^{-78}$ to $10^{+75}$. In the computation of the isolation diffusion by the method of Kennedy and O'Brien[26], the factorials and the Gamma functions increase beyond the $10^{+75}$ limit. The number of terms must be decreased in order to stay within the limits, and thus error is introduced. Another type of numerical error occurs when the difference is required between two nearly equal numbers. Again, in the computation of the isolation diffusion, the higher order terms are alternating in sign and are very close in magnitude. Beyond a certain diffusion radius, the impurity atom concentrations oscillate since the number of terms are restricted, and the numerical differences are extremely small. In the recombination term of the continuity equations, this effect occurs particularly in nondegenerate regions which are close to thermal equilibrium.

Finally, the iterative procedure used to solve the partial differential equations must be terminated at some point which is usually a function of the computation time and the acceptable level of accuracy. In the steady-state device program, the condition for termination is that all changes in the hole and electron concentrations and
the valence band edge potential must be less than $10^{-6}$ from the previous iteration values. This condition assumes that the trial solution is converging to the final solution and not some intermediate point. This assumption was always found to be valid.

D.2 Accuracy Testing Relations

The testing criteria of the accuracy of the final results can be accomplished by several relationships. The valence band edge potential can be summed over several different paths through the device model to check its consistency against the known boundary conditions. The electric field can be determined at points throughout the model region by the differentiation of the potential and the integration of Poisson's equation. Thus, the consistency of Poisson's equation offers a method of determining the relative magnitude of the errors in the hole and electron concentrations and the valence band edge potential. If the recombination-generation term was neglected, then the consistency of the current could be checked at various planes through the model region. These test relationships and others are used to determine the order of magnitude of the error in the final results which is a combination of all of the errors mentioned above and others.
APPENDIX E

COMPUTER PROGRAM FOR DIFFUSION MODEL

The diffusion model computer program for the idealized and EPE transistors determines the impurity atom concentrations at every node in the mesh structure. The donor and acceptor concentrations are used as input data for the semiconductor device model computer programs which solves for the hole and electron concentrations and the valence band edge potentials. The diffusion model program solves the parabolic diffusion equation (1.1) by the Peaceman-Rachford alternating direction implicit method and two direct solution techniques which are described in Sections 2.1.1 and 2.1.2. A modified Gaussian elimination routine is used to solve the tridiagonal matrix equations which result from the ADI method. The program has been written in a general form which can be easily modified for different device structures and is not optimized for the particular transistor model used in this work. The output routine which is given is a simple 10×52 map per standard page of computer print-out.

The diffusion computer program is broken up into one MAIN program and six subroutines. The MAIN program calls the subroutines, solves the one-dimensional epitaxial-substrate redistribution, combines the results of all subroutines, and outputs the final results. The EMIT subroutine solves for the donor concentrations of the emitter
diffusion. The BASE and BASEX subroutines calculate the acceptor concentrations in the idealized base and the EPE base diffusions, respectively. The BURL subroutine determines the donor concentrations of the buried layer in the epitaxial layer. The EMIT, BASE, BASEX, and BURL subroutines use the Peaceman-Rachford alternating direction method to solve the algebraic equations. The TRIDT subroutine is a modified Gaussian elimination routine which solves the resulting tridiagonal equations. The SISOL subroutine uses a direct solution method to solve for the sidewall isolation diffusions.
INTEGRAL FORMULATION AND SOLVES THE TWO-DIMENSIONAL DIFFUSION EQUATION WITH MIXED BOUNDARY CONDITIONS FOR THE P-TYPE BASE DIFFUSION. THE PEACOCK-RACHFORDE AND DUAL-TYPE BASE DIFFUSION.

CONTAINS:

- MAIN PROGRAM: CALLING PROGRAM FOR ALL SUBROUTINES AND SOLVES THE ONE-DIMENSIONAL PROBLEM OF THE SUBSTRATE-EPITAXY Redistribution, DETERMINES THE EFFECTIVE IMPURITY ATOM CONCENTRATION AND NAL FOR THE ENTIRE MESH TO BE USED IN POTT'S EQUATION.

- EMIT SUBROUTINE: SOLVES THE TWO-DIMENSIONAL DIFFUSION EQUATION WITH MIXED BOUNDARY CONDITIONS FOR THE N-TYPE EMITTED DIFFUSION.

- BASE SUBROUTINE: SOLVES THE TWO-DIMENSIONAL DIFFUSION EQUATION WITH MIXED BOUNDARY CONDITIONS FOR THE TWO-STEP P-TYPE BASE DIFFUSION WITH THE 'REVIEW PULL' EFFECT.

- BASEX SUBROUTINE: SOLVES THE TWO-DIMENSIONAL DIFFUSION EQUATION WITH MIXED BOUNDARY CONDITIONS FOR THE TWO-STEP P-TYPE BASE DIFFUSION USING ANALYTICAL TECHNIQUE FOR THE P-TYPE BASE DIFFUSION.

- BURL SUBROUTINE: SOLVES THE TWO-DIMENSIONAL DIFFUSION EQUATION WITH MIXED BOUNDARY CONDITIONS FOR THE N-TYPE BURIED LAYER DIFFUSION.

- SSL SUBROUTINE: SOLVES THE TWO-DIMENSIONAL DIFFUSION EQUATION WITH MIXED BOUNDARY CONDITIONS USING ANALYTICAL TECHNIQUE FOR THE P-TYPE BASE DIFFUSION.

- TRISOL SUBROUTINE: GAUSSIAN ELIMINATION SUBROUTINE FOR SOLVING TRIANGULAR EQUATIONS DIRECTLY.

- BASE SUBROUTINE: BASE DETERMINES THE EFFECTIVE IMPURITY ATOM CONCENTRATION OF THE SUBSTRATE-EPITAXY Redistribution, FOR THE N-TYPE EMITTED DIFFUSION.

- BASEX SUBROUTINE: BASEX DETERMINES THE EFFECTIVE IMPURITY ATOM CONCENTRATION OF THE SUBSTRATE-EPITAXY Redistribution, FOR THE TWO-STEP P-TYPE BASE DIFFUSION.

- BASEX SUBROUTINE: BASEX DETERMINES THE EFFECTIVE IMPURITY ATOM CONCENTRATION OF THE SUBSTRATE-EPITAXY Redistribution, FOR THE TWO-STEP P-TYPE BASE DIFFUSION.

- BASEX SUBROUTINE: BASEX DETERMINES THE EFFECTIVE IMPURITY ATOM CONCENTRATION OF THE SUBSTRATE-EPITAXY Redistribution, FOR THE TWO-STEP P-TYPE BASE DIFFUSION.

- BASEX SUBROUTINE: BASEX DETERMINES THE EFFECTIVE IMPURITY ATOM CONCENTRATION OF THE SUBSTRATE-EPITAXY Redistribution, FOR THE TWO-STEP P-TYPE BASE DIFFUSION.

- BASEX SUBROUTINE: BASEX DETERMINES THE EFFECTIVE IMPURITY ATOM CONCENTRATION OF THE SUBSTRATE-EPITAXY Redistribution, FOR THE TWO-STEP P-TYPE BASE DIFFUSION.

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- BASEX SUBROUTINE: BASEX DETERMINES THE EFFECTIVE IMPURITY ATOM CONCENTRATION OF THE SUBSTRATE-EPITAXY Redistribution, FOR THE TWO-STEP P-TYPE BASE DIFFUSION.

- BASEX SUBROUTINE: BASEX DETERMINES THE EFFECTIVE IMPURITY ATOM CONCENTRATION OF THE SUBSTRATE-EPITAXY Redistribution, FOR THE TWO-STEP P-TYPE BASE DIFFUSION.
```plaintext
223 CMI1) = 0.25*SSJ11 + (11,1) + (11,1111) + SYTJ11
BM1(1) = 0.25*SSY11 + (11,1) + (11,1111) + SYTJ11
DM1(1) = (C11,1) + (C11,11) + 0.25*SYT11 + (11,1) + (11,1111) + SYTJ11
 inconsistency = 0.5*SYT11 + (11,1111)
322 CONTINUE
DM1(1) = DM1(1) + CB1(1,4) + CA(1,4)
CONTINUE
CONTINUE
CONTINUE
CONTINUE
END
203 CONTINUE
C**********BOUNDARY CONDITIONS CHANGE TO DERIVATIVE EQUAL TO ZERO FOR************
C**********ENTIRE SURFACE******************************************************************************
C**********SET DIFFUSION CONSTANT*******************************************************************************
DO 101 I=1,100
DO 101 J=1,52
DO 223 K=1,10000
C**********HORIZONTAL EQUATIONS******************************************************************************
DO 223 L=1,43
L1 = F1(J,E0,110) + 300
AM1(L) = 0.25*SM11 + (11,1) + (11,1111) + SYT11
BM1(L) = 0.25*SSY11 + (11,1) + (11,1111) + SYTJ11
DM1(L) = (C11,1) + (C11,11) + 0.25*SYT11 + (11,1) + (11,1111) + SYTJ11
SC1(L) = 0.5*SSY11 + (11,1111)
GO TO 230
232 AM1(L) = 0.25*SM11 + (11,1) + (11,1111) + SYT11
BM1(L) = 0.25*SSY11 + (11,1) + (11,1111) + SYTJ11
DM1(L) = (C11,1) + (C11,11) + 0.25*SYT11 + (11,1) + (11,1111) + SYTJ11
SC1(L) = 0.5*SSY11 + (11,1111)
CONTINUE
C**********VERTICAL EQUATIONS******************************************************************************
DO 230 L=1,43
L1 = F1(E0,110) + 300
AM1(L) = 0.25*SM11 + (11,1) + (11,1111) + SYT11
BM1(L) = 0.25*SSY11 + (11,1) + (11,1111) + SYTJ11
DM1(L) = (C11,1) + (C11,11) + 0.25*SYT11 + (11,1) + (11,1111) + SYTJ11
SC1(L) = 0.5*SSY11 + (11,1111)
CONTINUE
C**********FIRST HORIZONTAL ROW EQUATIONS******************************************************************************
DO 236 L=1,43
L1 = F1(E0,110) + 300
AM1(L) = 0.25*SM11 + (11,1) + (11,1111) + SYT11
BM1(L) = 0.25*SSY11 + (11,1) + (11,1111) + SYTJ11
DM1(L) = (C11,1) + (C11,11) + 0.25*SYT11 + (11,1) + (11,1111) + SYTJ11
SC1(L) = 0.5*SSY11 + (11,1111)
CONTINUE
```
APPENDIX F

COMPUTER PROGRAMS FOR SEMICONDUCTOR DEVICE MODEL

Two computer programs have been generated to solve the hole and electron current continuity equations and Poisson's equation for the variables of electron concentration, hole concentration, and valence band edge potential. The integral formulation of the finite difference approximations is used in both programs to generate the three sets of algebraic equations from the linearized elliptic equations. The first computer program uses a nonlinear over-relaxation method (NLOR) to solve for the variables at each mesh node. This method which is a nonlinear version of the successive over-relaxation method (SOR) is about the most elementary but not the most efficient method of solving the three sets of algebraic equations. However, the elementary nature of the NLOR method greatly simplifies the analysis of numerical problem areas when they occur. The second computer program utilizes a quasi-linearization technique which is conceptually similar to Newton's method to linearize the equations and the Peaceman-Rachford alternating direction method (ADI) to solve the three sets of algebraic equations. The quasi-linearization-ADI method normally converges more rapidly than the NLOR method.

The two computer programs share the same subsidiary subroutines and differ mainly in the MAIN programs and the solution subroutines.
Both computer programs use the TRIAL subroutine to generate the initial trial solution for each variable at every mesh node. The values of the variables are basically the thermal-equilibrium values modified by first-order theory in the depletion areas and the contact areas. The MOAL subroutine calculates the hole and electron mobility as a function of the electric field and impurity concentration and determines the generalized Einstein relations for each outer iteration. The Fermi subroutine calculates the electron or hole concentrations for a given chemical potential or a chemical potential for a given concentration. The subroutine uses Boltzmann statistics for values of chemical potential below - 4.0, tabulated values of the Fermi-Dirac integral for chemical potentials between - 4.0 and 20.0, and a 2/3 power-law for chemical potentials above 20.0. The OUTPUT subroutine computes from the final values of the hole and electron concentrations and the valence band edge potentials the various current densities, the terminal currents, and the electric field.

The NLOR computer program uses the RELAX subroutine to calculate by iteration the values of hole and electron concentrations and valence band edge potentials. Both the outer and inner iteration loops are contained within this subroutine. The subroutine is blocked in that the new values of one variable are obtained at all mesh nodes before continuing to the next variable. The quasi-linearization-ADI method uses three separate subroutines to solve for the three sets of variables. The PSIV subroutine solves for the new values of the valence band edge potential, the ELECTC subroutine calculates the new
electron concentrations, and the HOLECO subroutine determines new hole concentrations. Each of these subroutines contains the inner iteration loop, and the outer iteration loop is in the MAIN program. The TRIDT subroutine is a modified Gaussian elimination program which solves the tridiagonal matrix equations. The MAIN program for both computer programs reads in and normalizes the input data, sets up the outer iteration loop, calls the subroutines, and determines the termination point of the iterative process.
141

CONTAINS:

MAIN PROGRAM 1 CALLING PROGRAM FOR ALL SUBROUTINES, AND CONTROLS THE ACCURACY OF THE SOLUTION BY THE NUMBER OF OUTER ITERATIONS.

RELAX SUBROUTINE COMPUTES NEW VALUES OF ELECTRON AND HOLE CONCENTRATIONS AND VALENCE BAND EDGE POTENTIALS BY A POINT NONLINEAR-RELAXATION METHOD.

TRIAL SUBROUTINE COMPUTES THE TRIAL SOLUTIONS OF THE ELECTRON CONCENTRATIONS, HOLE CONCENTRATIONS, AND PSI FROM FIRST-ORDER THEORY.

MOB SUBROUTINE COMPUTES MOBILITIES AND GENERALIZED EINSTEIN RELATIONS FOR EACH OUTER ITERATION.

DIHOC SUBROUTINE COMPUTES THE CHEMICAL POTENTIAL FOR A GIVEN PARTICLE CONCENTRATION ON COMPUTES THE PARTICLE CONCENTRATION FOR A GIVEN CHEMICAL POTENTIAL USING THE RELAX.

OUTPUT SUBROUTINE COMPUTES FINAL VALUES OF ELECTRIC FIELD, HOLE AND ELECTRON CURRENT DENSITIES, AND TOTAL CURRENT.

MAIN PROGRAM 1 CALLING PROGRAM FOR ALL SUBROUTINES, AND CONTROLS THE ACCURACY OF THE SOLUTION BY THE NUMBER OF OUTER ITERATIONS.

RELAX SUBROUTINE COMPUTES NEW VALUES OF ELECTRON AND HOLE CONCENTRATIONS AND VALENCE BAND EDGE POTENTIALS BY A POINT NONLINEAR-RELAXATION METHOD.

TRIAL SUBROUTINE COMPUTES THE TRIAL SOLUTIONS OF THE ELECTRON CONCENTRATIONS, HOLE CONCENTRATIONS, AND PSI FROM FIRST-ORDER THEORY.

MOB SUBROUTINE COMPUTES MOBILITIES AND GENERALIZED EINSTEIN RELATIONS FOR EACH OUTER ITERATION.

DIHOC SUBROUTINE COMPUTES THE CHEMICAL POTENTIAL FOR A GIVEN PARTICLE CONCENTRATION ON COMPUTES THE PARTICLE CONCENTRATION FOR A GIVEN CHEMICAL POTENTIAL USING THE RELAX.

OUTPUT SUBROUTINE COMPUTES FINAL VALUES OF ELECTRIC FIELD, HOLE AND ELECTRON CURRENT DENSITIES, AND TOTAL CURRENT.

CONTAINS:

PROCEDURE FOR COMPUTING THE STEADY-STATE PARAMETERS OF SEMICONDUCTOR DEVICES.
CALL TRIE(90)
DO 407 J=2,99
427 PS1(1+J)=NP(1)-J
GOTO 606

C**CREATION OF HORIZONTAL ADU EQUATIONS*******************************

DO 606 J=1,44,21
LI=J
AMP(J)=S(Y(11)+X(I1)+X(05*J1))
CHP(J)=S(Y(11)+X(05*J1))
DH(J)=AMP(J)+CHP(J)+CPI(J)

606 CONTINUE
DO 609 J=1,44,21
LI=J
AMP(J)=S(Y(11)+X(I1)+X(05*J1))
CHP(J)=S(Y(11)+X(05*J1))
DH(J)=AMP(J)+CHP(J)+CPI(J)

CALL TRS(J)

609 CONTINUE
GOTO 606

C**Determination of Fermi potential
DO 615 J=1,44,49
LI=J
AMP(J)=S(Y(11)+X(I1)+X(05*J1))
CHP(J)=S(Y(11)+X(05*J1))
DH(J)=AMP(J)+CHP(J)+CPI(J)

615 CONTINUE
DO 630 J=1,44,21
LI=J
AMP(J)=S(Y(11)+X(I1)+X(05*J1))
CHP(J)=S(Y(11)+X(05*J1))
DH(J)=AMP(J)+CHP(J)+CPI(J)

CALL TRS(J)

630 CONTINUE
GOTO 606

ENDIF.
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C**VERTICAL EQUATIONS FOR COLUMNS 0-21;33-49;61-85;AND 93-97**********

DO 429 J=1,2,3,92100 TO 629
IF(J,EQ.1)GOTO 629
IJP(J)=1
JNP(J)=1

CALL TRS(J)

429 CONTINUE
GOTO 606

C**VERTICAL EQUATIONS FOR COLUMNS 4-21;33-49;61-85;AND 93-97**********

DO 630 J=2,3,51
IF(J,EQ.1)GOTO 630
IJP(J)=1
JNP(J)=1

CALL TRS(J)

630 CONTINUE
GOTO 606

ENDIF.
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C**Fermi Subroutine Calculates the Hole or Electron Concentration
DO 120 J=1,99
IJP(J)=1
JNP(J)=1

CALL TRS(J)

120 CONTINUE
GOTO 629

C**Verticle Equations For Concentration
IF(J,EQ.1)GOTO 629

CALL TRS(J)

629 CONTINUE
GOTO 606

C**Computations for Concentration
IF(J,EQ.1)GOTO 629

CALL TRS(J)

606 CONTINUE

C**Fermi Subroutine Calculates the Hole or Electron Concentration
DO 120 J=1,99
IJP(J)=1
JNP(J)=1

CALL TRS(J)

120 CONTINUE
GOTO 629

C**Verticle Equations For Concentration
IF(J,EQ.1)GOTO 629

CALL TRS(J)

629 CONTINUE
GOTO 606

C**Computations for Concentration
IF(J,EQ.1)GOTO 629

CALL TRS(J)

606 CONTINUE
computing hole current in y-direction

calling total current in x-direction

computing terminal currents

continue

calling output of electric field

calling output of currents

continue

calling total current in x-direction

calling terminal currents

continue

calling collector currents

do 107 i=1,492

continue

calling collector currents

do 907 j=1,492

continue

calling total current in x-direction

calling collector currents

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