Chapter 3
Numerical Modeling

3.1 Introduction

It is usually difficult to obtain closed-form expressions which satisfactorily describe the operation of modern semiconductor devices. There are also limitations of the degree of precision by the necessary approximations associated with analytic models. Numerical techniques may be used to solve the full set of semiconductor equations. but any approach for the solution of such a system consist essentially of three tasks. First; the domain (the geometry of the device has to be discretezed). The second; the differential equations are approximated by algebraic equations. The solutions of this algebraic equations consist on the third task. The finite difference method is adopted here for the reason which will be explained later.

We will consider the case of an n-p junction. The n side represents the active layer of the field effect transistor, the side p represents the substrate itself. The set of differential equations describing the transport mechanism are well known: The Poisson's equation relating electric fields with charge densities; continuity equations relating the rate of change of charge densities with current sources and sinks (generation-recombination). The equation defining the current as being caused by the locally existing fields and by diffusion if concentration gradients are present. The empirical function for the recombination mechanism for the carriers is usually needs to determinate the proportional deviation from equilibrium ($np-n_i^2$) and those describing the occupation of traps in band gap.

The finite difference method is largely used for numerical solution of the semiconductor equations because of the simplicity of implementing the numerical schemes. The majority of early devices simulations such as those of Gummel [8] Slotboom [9]and Scharfetter and Gummel [10] used one dimensional finite difference schemes; which are adequate in the case where the current flow and electric field are predominantly unidirectional. In some situations it may be preferable to use a nonuniform spacing when discretizing, if the electron and hole distribution is expected to change rapidly through a region. For this it may be necessary to use a small spacing between points in this area. However, for many device structures, even abrupt p-n junctions, uniform grid spacing is suitable.

This method offers the solutions for the physical variables p, n, ψ as descretized values at specific nodes contained within a mesh. The continues derivatives of the semiconductor equations are replaced by discretized finite approximations (see for example [4]). The discretized physical variables are represented by values obtained from solution of the discretized equations at each mesh point except where boundary conditions determine the values of the variables.

3.2 The phenomenological transport equations

The phenomenological transport equations in semiconductors is given by the Poisson formula which is;

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{q}{\varepsilon_s}(p - n + N_D - N_A + N_{TD}^{+} - N_{\bar{T}A}) \qquad 3.1$$

Where we consider two deep centers might be donors like centers and acceptors like centers; here we treat the steady state dc condition

Where ψ is the electron potential, $\varepsilon_s = 12.3015 \cdot 10^{-13}$ F/cm; n and p are the free electron and hole concentrations and $N_D - N_A = N_{TOT}$ which is the effective doping distribution.

The ionized defect density (for a donor) depend on the temperature and the position of defect level with respect to Fermi level. This relation is given by

$$N_{TD}^{+} = f \cdot N_{TD} \qquad 3.2$$

where f the occupation factor given by

$$f = \frac{1}{1 + \exp\left(\frac{E_F - E_{TD}}{K_B T}\right)} \qquad 3.3$$

E_{TD} is the energy level of the trap; and N_{TD} is its density. Since the hole density is given by

$$p = n_i \exp\left(\frac{E_i - E_F}{K_B T}\right) \qquad 3.4$$

E_i is the intrinsic level, then the Eq 3.2 will be written as

$$N_{TD}^{+} = N_{TD}\left(\frac{1}{1 + \frac{n_i}{p}\exp\left(-\frac{E_{TD} - E_i}{K_B T}\right)}\right) \qquad 3.5$$

In the same way, the ionized density of a deep acceptor is given as

$$N_{TA}^{+}=N_{TA}\left(\frac{1}{1+\frac{n_i}{n}\exp\left(\frac{E_{TA}-E_i}{K_BT}\right)}\right) \qquad 3.6$$

E_{TA} is the energy level of acceptor traps; N_{TA} is the total acceptor trap density.

The electron and hole conservation laws can be written :

$$\frac{1}{q}\cdot\frac{\partial J_n}{\partial x}-U=0 \qquad 3.7$$

$$\frac{1}{q}\frac{\partial J_p}{\partial x}+U=0 \qquad 3.8$$

While knowing that $C_n=\sigma_n\cdot v_{thn}$ and $C_p=\sigma_p\cdot v_{thp}$. The thermal generation rate of carriers for a single species of generation level take the following form,

$$U=\frac{n\cdot p-n_i^2}{\tau_p\left(n+n_1\right)+\tau_n\left(p+p_1\right)} \qquad 3.9$$

where $n_1=\frac{e_n}{C_n}=N_c\exp-\left(\frac{E_c-E_T}{K_BT}\right)$ 3.10

$$p_1=\frac{e_p}{C_p}=N_v\exp-\left(\frac{E_T-E_v}{K_BT}\right) \qquad 3.11$$

At the thermal equilibrium $n_1\cdot p_1=n_i^2$

The minority excess carrier lifetimes are meaningful concepts for extrinsic semiconductors having a negligible density of deep centers and for small departure from thermal equilibrium:

$$\tau_n=\frac{1}{C_n\cdot N_T}\ ;\ \tau_p=\frac{1}{C_p\cdot N_T}$$

J_n is the electron current and J_p is the holes current given by

$$J_n=-qn\mu_n\frac{\partial\psi}{\partial x}+qD_n\frac{\partial n}{\partial x} \qquad 3.12$$

$$J_p=-qp\mu_p\frac{\partial\psi}{\partial x}-qD_p\frac{\partial p}{\partial x} \qquad 3.13$$

Since the velocity is proportional to the electric field as

$$v=\mu E$$

we have taken $\mu_n=\mu_{no}\cdot\frac{1}{1+\mu_{n0}\cdot\frac{E}{v_{nsat}}}$ and $\mu_p=\mu_{p0}\cdot\frac{1}{1+\mu_{p0}\cdot\frac{E}{v_{psat}}}$

where $v_{ns}=8\cdot10^6 cm/s$, $\mu_{n0}=7300F/cm$ and $v_{ps}=9.5\times10^6 cm/s$, $\mu_{p0}=425F/cm$

The relationship between D_n and μ_n in thermal equilibrium, for non degenerate semiconductors, and when n is much smaller than N_c is as know by Einstein relationship:

for the electron $D_n=\left(\frac{K_BT}{q}\right)\cdot\mu_n$ and for the hole $D_p=\left(\frac{K_BT}{q}\right)\cdot\mu_p$

where K_BT/q=0.0259 V at T=300°K

3.3 Discretization of the device

A partition of the structure n-p discretized in a uniform way. The meshpoint spacing is defined in the x-direction. We have take a fine spacing in order to detect any variation of parameters as a high field in a depletion layer. Such the active layer has a thickness of h_c=2μm and doping density of N_D=$10^{15}cm^{-3}$. The substrate has a thickness of $H_{sub}=20\,\mu m$. The structure is divided to NMAX points along its thickness L, the main points are denoted by N and the secondary points by M.

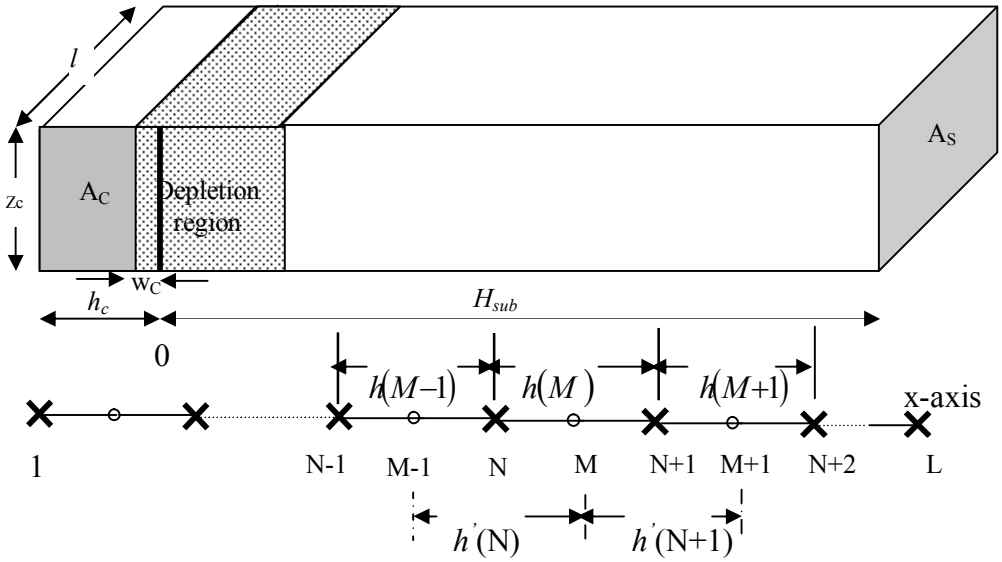

Fig 3.1: The special descretization of the structure

3.4 Numerical method of resolution

The basic equations (3.1); (3.7); (3.8) form the system for dc steady state analysis; given by

$$\begin{cases} \frac{1}{q}\cdot\frac{dJ_p}{dx}-(G-U)=0 \\ \frac{1}{q}\cdot\frac{dJ_n}{dx}+(G-U)=0 \\ \frac{\partial^2\psi}{\partial x^2}=-\frac{q}{\varepsilon_s}(p-n+N_D-N_A+N_{TD}^{+}-N_{TA}^{-}) \end{cases} \qquad 3.14$$

Assuming that no optical excitation or other generation sources as impact ionization, then $G=0$.

The system of three equations of three unknowns (p,n,ψ) is obtained for each discretization point $x_i(0\le i\le 1001)$. Considering the following steps.

The first is that any function variable f_u (n, p, $\mu_{n,p}$, E, $D_{n,p}$) of x its derivation is

$$\frac{\partial f_u}{\partial x}=\frac{f_u(N)-f_u(N-1)}{x(N)-x(N-1)} \qquad 3.15$$

where $x(N)-x(N-1)=H1$ which represent the discretization of main grid

The second step is Scharfetter and Gummel [10] approximation which takes the potential difference between two adjacent nodes sufficiently smaller and cannot exceed $2KT/q$. This is achieved by increasing the total point number to produce a finite differences to avoid the negative values of electron density n. However; this lead to the reduction of computation efficiency and numerical instability in the solution. These can be avoided by allowing the electron density to follow an exponential variation between two mesh point. The current density equations J_n and J_p are integrated assuming: (1) the current densities equations J_n and J_p and mobilities are constant between two adjacent point N and $N+1$, (2) a linear variation of the electrostatic potential which is justified because the potential variation is smooth along a discretization interval. From eq (3.12); we have

$$\frac{1}{n}\frac{\partial n}{\partial x}=\frac{J_n}{K_BTn\mu_n}+\frac{q}{K_BT}\frac{\partial\psi}{\partial x} \qquad 3.16$$

According to the integration method of variation constant

$$n(x)=C_0(x)\exp\left(\frac{q}{K_BT}\psi\right) \quad 3.17$$

where $C_0(x)=\int\frac{J_n}{\mu_n K_BT}\exp\left(\frac{-q}{K_BT}\psi\right)$

Since J_n is constant along the interval $[x_i, x_{i+1}]$; we obtain

$$J_{n\frac{i+1}{2}}=\mu_n K_BT\frac{C_{i+1}-C_i}{\int_{x_i}^{x_{i+1}}\exp\left(-\frac{q\psi}{K_BT}\right)dx} \quad 3.18$$

where $C_{i+1}=n_{i+1}\exp\left(-\frac{q\psi_{i+1}}{K_BT}\right)$

$$C_i=n_i\exp\left(-\frac{q\psi_1}{K_BT}\right)$$

with same way for holes current density

$$J_{p\frac{i+1}{2}}=-\mu_p K_BT\frac{C'_{i+1}-C'_i}{\int_{x_i}^{x_{i+1}}\exp\left(\frac{q\psi}{K_BT}\right)dx} \quad 3.19$$

where $C'_{i+1}=p_{i+1}\exp\left(\frac{q\psi_{i+1}}{K_BT}\right)$

$$C'_i=p_i\exp\left(\frac{q\psi_1}{K_BT}\right)$$

Then from eqs (3.18); (3.19); the current density equations are treated implicitly as differential equations in n and p. An approximation given to ψ as

$$\psi=ax+b$$

where $a=\frac{\psi_{i+1}-\psi_i}{x_{i+1}-x_i}$; $b=\psi_i-ax_i$

Gummel and Shraffeter inferred the expressions for J_n and J_p as:

$$J_{n\frac{i+1}{2}}=q\mu_n\frac{n_{i+1}\exp-\frac{q}{K_BT}(\psi_{i+1}-\psi_i)-n_i}{\exp-\frac{q}{K_BT}(\psi_{i+1}-\psi_i)-1}\cdot\frac{\psi_{i+1}-\psi_i}{x_{i+1}-x_i} \quad 3.20$$

$$J_{p\frac{i+1}{2}}=q\mu_p\frac{p_i\exp-\frac{q}{K_BT}\left(\psi_{i+1}-\psi_i\right)-p_{i+1}}{\exp-\frac{q}{K_BT}\left(\psi_{i+1}-\psi_i\right)-1}\cdot\frac{\psi_{i+1}-\psi_i}{x_{i+1}-x_i} \quad 3.21$$

hence, the novel expressions are given by

$$J_p=-\frac{q\mu_pE}{1-e^{\theta Ex}}\left(p(0)e^{\theta Ex}-p(x)\right) \quad 3.22$$

$$J_n=-\frac{q\mu_nE}{1-e^{\theta Ex}}\left(n(0)e^{-\theta Ex}-n(x)\right) \quad 3.23$$

where $\theta=\frac{q}{K_BT}$ is the thermal voltage and E is the electric field derived from ψ as $E=-\frac{d\psi}{dx}$.

and by knowing that

$$J_p(M)=-\frac{q\mu_p(M)}{\theta\cdot h(M)}\left[p(N+1)-p(N)\right]-\frac{q\mu_p(M)}{\theta\cdot h(M)}\left[\psi(N+1)-\psi(N)\right]\frac{p(N)+p(N+1)}{2} \quad 3.24$$

$$J_n(M)=-\frac{q\mu_n(M)}{\theta\cdot h(M)}\left[n(N+1)-n(N)\right]+\frac{q\mu_n(M)}{\theta\cdot h(M)}\left[\psi(N+1)-\psi(N)\right]\frac{n(N)+n(N+1)}{2} \quad 3.25$$

Eqs (3.24); (3.25) can be put in simple way:

$$J_p(M)=\frac{q}{h(M)}\left[\alpha_{p1}(M)p(N)+\alpha_{p2}(M)p(N+1)\right] \quad 3.26$$

$$J_n(M)=\frac{q}{h(M)}\left[\alpha_{n1}(M)n(N)+\alpha_{n2}(M)n(N+1)\right] \quad 3.27$$

where

$$\alpha_{p1}=\mu_p(M)\frac{\psi(N)-\psi(N+1)}{1-\exp\left(-\beta(M)\right)} \quad \text{and} \quad \alpha_{p2}=\mu_p(M)\frac{\psi(N)-\psi(N+1)}{1-\exp\left(\beta(M)\right)}$$

$$\alpha_{n1}=\mu_n(M)\frac{\psi(N)-\psi(N+1)}{1-\exp\left(\beta(M)\right)} \quad \text{and} \quad \alpha_{n2}=\mu_n(M)\frac{\psi(N)-\psi(N+1)}{1-\exp\left(-\beta(M)\right)}$$

with $\beta(M)=\theta\cdot\left[\psi(N)-\psi(N+1)\right]$

The system (3.14) become after descritezation:

$$\begin{cases} \frac{1}{q}\cdot\frac{J_p(M)-J_p(M-1)}{h\cdot(N)}+U(N)=0 \\ \\ \frac{1}{q}\cdot\frac{J_n(M)-J_n(M-1)}{h\cdot(N)}-U(N)=0 \\ \\ \gamma_1(N)\psi(N-1)+\gamma_2(N)\psi(N)+\gamma_3(N)\psi(N+1)=-\frac{q}{\varepsilon}\left[p(N)-n(N)+N_D(N)-N_A(N)+N_{TD}^{+}(N)-N_{\bar{T}A}(N)\right] \end{cases} \quad 3.28$$

where the coefficient $\gamma_i(i=1,2,3)$ are given by :

$$\gamma_1(N)=\frac{1}{h(M-1)h\cdot(N)}$$

$$\gamma_2(N)=\frac{1}{h\cdot(N)}\left[\frac{1}{h(M-1)}+\frac{1}{h(M)}\right]$$

$$\gamma_3(N)=\frac{1}{h(M)h\cdot(N)}$$

Like the currents densities, the recombination rate and the ionized traps density involve nonlinear functions. Assuming that the function is continues, single valued function of x of continues derivatives. So these are linearized by the first order approximation obtained from Taylor expansion:

$$J_p(M)\approx J_p^0(M)+\frac{\partial J_p^0(M)}{\partial p(N)}\delta p(N)+\frac{\partial J_p^0(M)}{\partial p(N+1)}\delta P(N+1)+\frac{\partial J_p^0(M)}{\partial \psi(N)}\delta\psi(N)+\frac{\partial J_p^0(M)}{\partial \psi(N+1)}\delta\psi(N+1) \quad 3.29$$

$$J_n(M)\approx J_n^0(M)+\frac{\partial J_n^0(M)}{\partial n(N)}\delta n(N)+\frac{\partial J_n^0(M)}{\partial n(N+1)}\delta n(N+1)+\frac{\partial J_n^0(M)}{\partial \psi(N)}\delta\psi(N)+\frac{\partial J_n^0(M)}{\partial \psi(N+1)}\delta\psi(N+1) \quad 3.30$$

$$U=U^0(N)+\frac{\partial U^0(N)}{\partial p(N)}\delta p(N)+\frac{\partial U^0(N)}{\partial n(N)}\delta n(N) \quad 3.31$$

$$N_{TD}^{+}(N)=N_{TD}^{+\,0}(N)+\frac{\partial N_{TD}^{+\,0}}{\partial p(N)}\delta p(N) \quad 3.32$$

$$N_{\bar{T}A}(N)=N_{\bar{T}A}^{\,0}(N)+\frac{\partial N_{\bar{T}A}^{\,0}}{\partial n(N)}\delta n(N) \quad 3.33$$

Where the quantities defined at the origin of expansion are denoted by superscript 0 are determined from the initial conditions p_0, n_0 and ψ_0. After the linearization of the continuity equations aforementioned and the substitution of Taylor expansion in.

Thereby allowing to find a new system which involve only fundamental variable increments as unknowns. Written in matrix-vector as follow:

$$A(N)\delta y(N-1)+B(N)\delta y(N)+C(N)\delta y(N+1)=F(N)\ ,\ 2\le N\le L-1 \qquad 3.34$$

For the differentials boundary conditions for $\delta p,\delta n,\delta\psi$ respectively are zero at $N=1$ and $N=L$. A,B,C are the square matrixes of nine elements and F is a vector of three elements.

Where the elements of matrix A are defined as;

$$A_{11}=-\frac{1}{qh'(N)}\frac{\partial J_p^0(M-1)}{\partial p(N-1)};\quad A_{13}=-\frac{1}{qh'(N)}\frac{\partial J_p^0(M-1)}{\partial \psi(N-1)}$$

$$A_{22}=-\frac{1}{qh'(N)}\frac{\partial J_n^0(M-1)}{\partial n(N-1)};\quad A_{23}=-\frac{1}{qh'(N)}\frac{\partial Jn(M-1)}{\partial \psi(N-1)}$$

$$A_{33}=\frac{1}{h(M-1)h'(N)}$$

$$A_{21}=0\ ;\ A_{12}=0\ ;\ A_{31}=0\ ;\ A_{32}=0$$

For the matrix B

$$B_{11}=\frac{1}{qh'(N)}\left[\frac{\partial J_p^0(M)}{\partial p(N)}-\frac{\partial J_p^0(M-1)}{\partial p(N)}\right]+\frac{\partial U^0(N)}{\partial p(N)};\quad B_{12}=\frac{\partial U^0(N)}{\partial n(N)}$$

$$B_{13}=\frac{1}{qh'(N)}\left[\frac{\partial J_p^0(M)}{\partial \psi(N)}-\frac{\partial J_p^0(M-1)}{\partial \psi(N)}\right]$$

$$B_{21}=-\frac{\partial U^0(N)}{\partial p(N)}$$

$$B_{22}=\frac{1}{qh'(N)}\left[\frac{\partial J_n^0(M)}{\partial n(N)}-\frac{\partial J_n^0(M-1)}{\partial n(N)}\right]-\frac{\partial U^0(N)}{\partial n(N)};\quad B_{23}=\frac{1}{qh'(N)}\left[\frac{\partial J_n^0(M)}{\partial \psi(N)}-\frac{\partial J_n^0(M-1)}{\partial \psi(N)}\right]$$

$$B_{31}=\frac{q}{\varepsilon_s}\left[1+\frac{\partial N_{TD}^{+\,0}}{\partial p(N)}\right];\quad B_{32}=\frac{-q}{\varepsilon_s}\left[1+\frac{\partial N_{TA}^{+\,0}}{\partial n(N)}\right];\quad B_{33}=-\frac{1}{h'(N)}\left[\frac{1}{h(M-1)}+\frac{1}{h(M)}\right]$$

The matrix C;

$$C_{11}=\frac{1}{qh'(N)}\cdot\frac{\partial J_p^0(M)}{\partial p(N+1)};\quad C_{13}=\frac{1}{qh'(N)}\cdot\frac{\partial J_p^0(M)}{\partial \psi(N+1)}$$

$$C_{22}=\frac{1}{qh'(N)}\cdot\frac{\partial J_n^0(M)}{\partial n(N+1)};\quad C_{23}=\frac{1}{qh'(N)}\cdot\frac{\partial J_n^0(M)}{\partial \psi(N+1)}$$

$$C_{33}=\frac{1}{h(M)h'(N)}\ ;C_{12}=0\ ;C_{21}=0\ ;C_{31}=0\ ;C_{32}=0\ .$$

For the matrix F

$$F_1 = -\frac{1}{qh'(N)}\cdot\left[J_p^0(M) - J_p^0(M-1)\right] - U^0(N)$$

$$F_2 = -\frac{1}{qh'(N)}\cdot\left[J_n^0(M) - J_n^0(M-1)\right] + U^0(N)$$

$$F_3 = -\frac{q}{\varepsilon_s}\cdot\left[N_D - N_A + p^0(N) - n^0(N) + N_{TD}^{+\,0}(N) - N_{\bar{T}A}^{\;0}(N)\right] - \gamma_1(N)\psi^0(N-1) - \gamma_2(N)\psi^0(N) - \gamma_3(N)\psi^0(N+1)$$

Solving this matrix vector equations mean solving the tridiagonal square matrix of order N. The global system has the form:

$$[U][\delta] = [F] \qquad 3.35$$

where $[U]$ is the Jachobian matrix of the system of (L-2).(L-2) elements; and each matrix element itself corresponding to a single node x_i has nine scalar elements;

$$U_{ij} = \begin{bmatrix} \frac{\partial F_p^i}{\partial p_j} & \frac{\partial F_n^i}{\partial p_j} & \frac{\partial F_\psi^i}{\partial p_j} \\ \frac{\partial F_p^i}{\partial n_j} & \frac{\partial F_n^i}{\partial n_j} & \frac{\partial F_\psi^i}{\partial n_j} \\ \frac{\partial F_p^i}{\partial \psi_j} & \frac{\partial F_n^i}{\partial \psi_j} & \frac{\partial F_\psi^i}{\partial \psi_j} \end{bmatrix};$$

$$\delta = \begin{bmatrix} \delta p_j \\ \partial n_j \\ \partial \psi_j \end{bmatrix}$$

For the problem that the total number of scalar elements is so large; a direct application of the Gaussian elimination method without modification is not recommended. A commonly accepted way to expedite computation is to exclude all zero elements. If this is done, only nine elements per line are stored in memory. If the elementary matrixes U_{ij} are viewed as blocks; the previous solution method can be extended in such a way that each element is block matrix instead of scalar. This is solved using a recursive method.

In addition to the semiconductor equations and the domain, boundary and initial conditions have to be specified. Suitable for this, Dirichlet boundary conditions are usually used where the potential and carrier concentrations are pre-defined at the contacts.

The absence of current and applied bias set the device at thermal equilibrium. Under the space charge neutrality condition, the initial carrier densities values are:

$$n^0 = N_D - N_A, \quad p^0 = n_i^2/N_D - N_A \qquad \text{at active layer (n side)} \qquad 3.36.a$$

$p^0=N_A-N_D$, $n^0=n_i^2/N_A-N_D$ at substrate (p side) 3.36.b

In equilibrium; the current is zero. So that from eqs (3.11); (3.12) we can get

$$q\mu_n \cdot n \cdot d\psi = q \cdot D_n \cdot dn \quad \text{and} \quad q\mu_p\, pd\,\psi = q \cdot D_p \cdot dp$$

Integrating these equations and the substituting n^0 and p^0 the initial values of the potential is given by;

$$\psi^0 = \begin{cases} \frac{1}{q}\ln\left[\frac{N_D-N_A}{n_i}\right] & \text{at the contact of the n-side} \\ \frac{1}{q}\ln\left[\frac{-n_i}{N_D-N_A}\right] & \text{at the contact of the p-side} \end{cases} \qquad 3.37$$

For any external polarization the initial values of n and p are unchanged while those of the potential are changed in a proportional way . so that the new trial values are given

$$\psi_T(N)=\left[1-\frac{V_{ap}}{\psi_1(1)-\psi_1(L)}\right]\cdot\psi_1(N)+\frac{V_{ap}}{\psi_1(1)-\psi_1(L)}\cdot\psi_1(L) \qquad 3.38$$

where the voltage V_{ap} referred the voltage applied and $\psi_1(1)$and $\psi_1(L)$ are the are the potential of starting condition. The next step is to solve the system with a recursive technique .

First; equation(3.34) which has unknowns vectors at three point is transformed to an equation involving unknowns vectors at two points as;

$$B'(N)\delta y(N)+C'(N)\delta y(N+1)=F'(N) \qquad 3.39$$

Or $\delta y(N)=B'(N)^{-}F'(N)-B'(N)^{-}C'(N)\delta y(N+1)$ 3.40

Second; substituting $\delta y(N)$ in the equation (3.34) knowing that division point N is decreased by one; we can found

$$\begin{cases} B'(2)=B(2) \\ C'(2)=C(2) \\ F'(2)=F(2) \end{cases} \qquad 3.41$$

For N=2 , the direct comparison of eq(3.39) with eq(3.34) yields to $\delta y(1)=0$

$$\begin{cases} B'(N)=B(N)-A(N)B'(N-1)^{-1}C'(N-1) \\ C'(N)=C(N) \\ F'(N)=F(N)-A(N)B'(N-1)^{-1}F'(N-1), \quad 3\le N\le L-1 \end{cases} \tag{3.42}$$

Thus, starting with equations (3.41) in equation (3.42) are determined for N=3, 4, ..., L-1, where the inverse matrix B' is obtained from the Sylvester's formula.

The last step is to calculate $\delta y(N)$ starting with N=L-1, L-2, ……, 2 using equation (3.39). where $\delta y(L)$=0 is used at the starting condition.

As in all iterative methods the problem is in deciding when is the time to stop and what criteria are set. The Newton method is significantly sensitive to correction terms set after each iteration. An overestimation given to the initial solution results in divergence.

At iteration k+1 the solution $p^{(K)},n^{(K)},\psi^{(K)}$ are corrected follows:

$$\text{for } \delta\psi^{(*)} \qquad \begin{cases} \delta\psi^{(*)}=\delta\psi^{(K)} & \text{if } \delta\psi^{K}\le\dfrac{K_BT}{q} \\ \delta\psi^{(*)}=\dfrac{\left|\delta\psi^{(K)}\right|}{\delta\psi^{(K)}}\cdot\dfrac{K_BT}{q} & \text{if } \delta\psi^{K}\rangle\dfrac{K_BT}{q} \end{cases} \tag{3.43}$$

for $\delta n^{(K)},\delta p^{(K)}$ the corrective factor at iteration k+1is as follow:

Since n and p are Boltzman-Maxwell functions then $\delta n^{(K)},\delta p^{(K)}$ are calculated as exponential functions of $\delta\psi^{(K)}$ where;

$$n^{(K+1)}=n^{(K)}\exp\left(\frac{q\,\delta\psi}{K_BT}\right) \tag{3.44}$$

therefore by developing at the first order allowing to

$$\left|\frac{\delta n}{n^{(K+1)}}\right|\le\frac{q}{K_BT}\delta\psi \tag{3.45}$$

and in similar way

$$p^{(K+1)}=p^{(K)}\exp\left(\frac{q\,\delta\psi}{K_BT}\right) \tag{3.46}$$

$$\left|\frac{\delta p}{p^{(K+1)}}\right| \leq \frac{q}{K_B T}\delta\psi \qquad 3.47$$

which lead to $\begin{cases} \left|\frac{\delta n}{n^{(K+1)}}\right| \leq 1 \\ \left|\frac{\delta p}{p^{(K+1)}}\right| \leq 1 \end{cases}$ 3.48

It is necessary to set an other criterion to control the carrier densities solutions to avoid negative and weaker values which can affect the convergence. With a simple precaution that each negative or zero value is be replaced by a weaker and positive number of the order of 10^{-30}.

To stop the process, we just set the condition : $\left|\frac{\partial y}{y}\right| \leq e_{re}$. If this condition is satisfied at certain number of iterations, the simulation is achieved unless it may continues to a maximum permitted where therefore no convergence.

To realize this; a program developed at Brunel University (UK) is used and the flow chart of this program is shown in figure 3.2

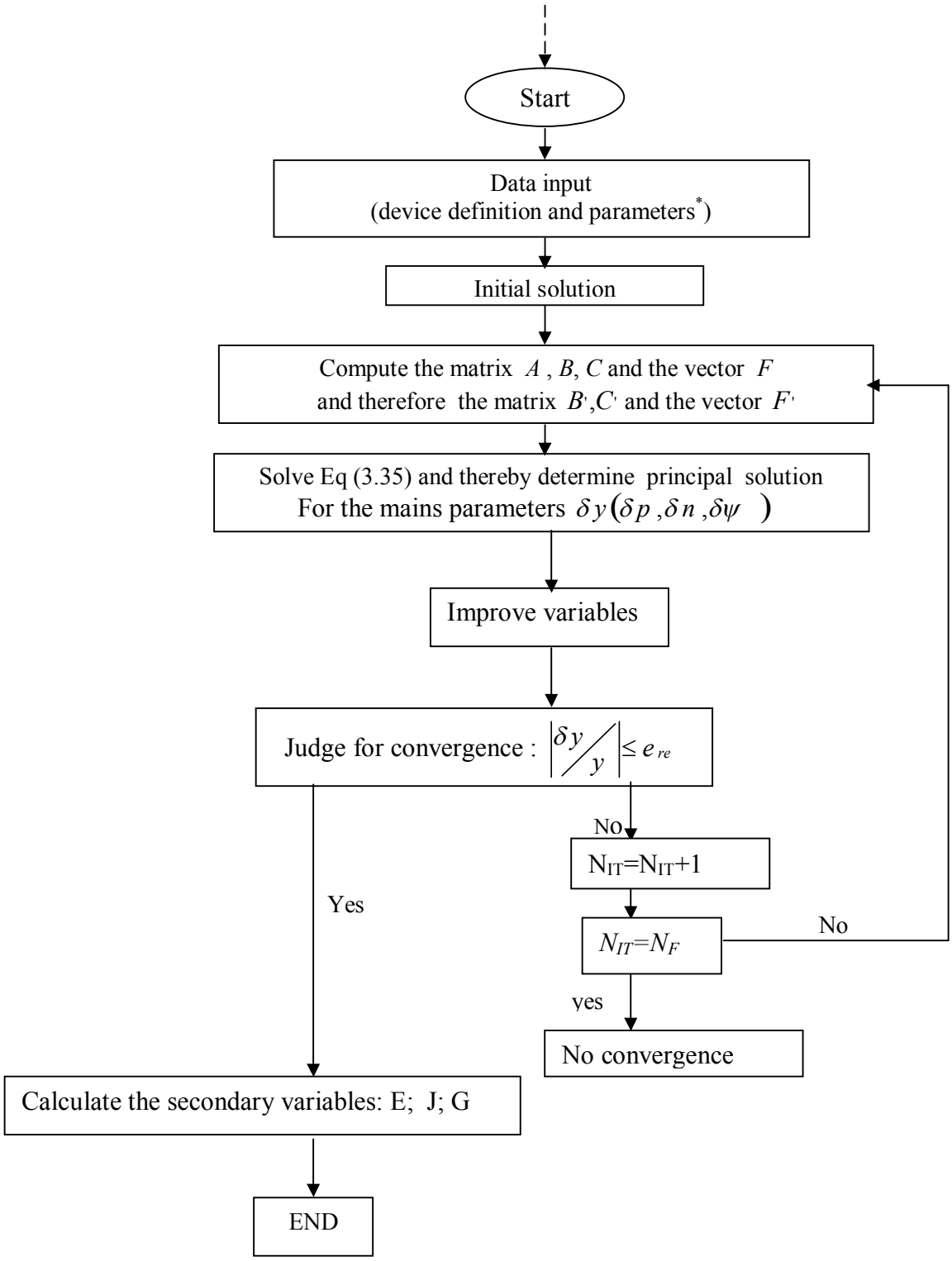

Fig3.2 Flow Chart for Numerical-Solution Procedure

*: Applied Bias (V), the maximum number of iterations, E_C-E_T in eV for the deep acceptors level, density of the deep acceptors level (in cm^{-3}), E_T-E_V in eV for the deep donors level, density of the deep donors level (in cm^{-3}), minority carrier lifetime (S), Device area (cm^2), a uniform generation rate (Normally 0), Temperature (K)

The program uses two input files and produce two output files.

Device definition

The device is divided into a number of points determined by the program taken at *NMAX*=1001, the spacings between the grid is constant given by $x_{step} = d / (NMAX - 1)$, after defining the one dimensional grid we give the shallow acceptor and donor at each point.

Run definition

This field provide the uses parameters it gives the reverse bias and minority lifetime. A clue to the items that must be included in this field may be summarized in the subroutine setrun.

Code output

The program produce two output files. The largest of the output files give the various distributions through the device (distance, the net shallow doping density, electron and hole concentrations, various current for the electron and holes, thermal generation-recombination rate and density of filled acceptors and donors).

The second files produced provides other information as applied bias; current; conductance.

3.5 The channel conductance and substrate current modeling

The backgating (the channel conductance reduction) is studied by calculating the space charge induced by depletion of the channel by the applied substrate voltage to reduce its effective thickness. By charge neutrality an equal and opposite charge is induced in the substrate. The relation between the conductance G and the width of the channel ($h_c - w_C$) is given by

$$G=\frac{\sigma A_C}{l}=\frac{qn\mu_n Z_c\left(h_c-w_C\right)}{l} \qquad 3.48$$

where $\sigma=qn\mu_n\approx qN_D\mu_n$ is the channel conductivity, n is the free electron density in the channel (we suppose that the channel doping is uniform so that $n=N_D$); $Ac=Z_c(h_c-w_C)$ is the channel cross section area. Z is the channel height, l is its length.

The incremental change dG in the conductance is given by

$$dG=\frac{\sigma dA_c}{l}=\frac{qn\mu_n Z_c\, d\left(h_c-w_c\right)}{l} \qquad 3.49$$

where dA_c is the incremental change in the channel cross section area, given by

$$dA_c=d\left(h_c-w_c\right)=-dw_c \qquad 2.50$$

since h_c is constant quantity and w_c is the depletion width in channel side which changes (reduction) with an applied voltage to the substrate. This reduction (w_C) will reduce the area of the channel through which the current passes and the conductance for the channel is then calculated using the reduced area and given by integrating equation (3.49).

$$G=\frac{q\mu_n Z_c}{l}\int_{-h_c}^{0} ndx=\frac{q\mu_n Z_c}{l}\int_{-h_c}^{-w_c} ndx$$

the upper integral limit is ($-w_c$) instead of (0) since in the depletion region ($-w_C<x<0$) the electron density is negligible.

The normalized conductance is then $G_{Vb}\big/G_{Vb=0}$

Where V_b is the backgating voltage applied to substrate.

The current through the substrate is calculated by solving the equations (3.9) and (3.10) after numerical solving for (p,n,ψ).