A SELF-CONSISTENT SOLUTION OF ONE-DIMENSIONAL SCHRODINGER-POISSON EQUATIONS BY NEWTON-RAPHSON ITERATION TECHNIQUE

S. Subramanian*

Department of Electrical and Computer Engineering, Oregon State University, Corvallis, OR 97331

* On leave of absence from the Tata Institute of Fundamental Research, Bombay, India.

ABSTRACT

A self-consistent, one-dimensional solution of Schrodinger-Poisson equations is obtained by Newton-Raphson iteration technique using a finite-difference method with a non-uniform mesh. The method is applied to the simulation of a Schottky barrier placed on the surface of a single quantum well structure. The capacitance of the structure is calculated directly from the solution of the a.c. Poisson equation. The simulated apparent carrier profile is shown to be in excellent agreement with the experimental carrier profile obtained by C-V measurements on a GaAs/InGaAs/GaAs strained layer single quantum well structure.

I INTRODUCTION

A number of papers in the literature deal with the self-consistent solution of one-dimensional Schrodinger-Poisson equations [1-4]. The most commonly used technique to obtain the required self-consistent solution is the so-called relaxation method. In this method, a trial potential distribution $V_{in}(x)$ is used to solve the Schrodinger equation and the resulting wavefunctions and the energy eigenvalues are used to calculate the charge density in the quantum well regions. Poisson equation is then solved using this charge density to get the new potential distribution $V_{out}(x)$. For the solution of Schrodinger equation in the next iteration, a linear combination of $V_{in}(x)$ and $V_{out}(x)$ given by

$$V'_{in}(x) = V_{in}(x) + f(V_{out}(x)-V_{in}(x)) \qquad ...(1.1)$$

is used as the input potential, where f is known as the relaxation factor. The whole procedure is repeated until convergence, viz. the input and the output potentials $V_{in}(x)$ and $V_{out}(x)$ are equal within the desired accuracy. A small value of f usually gives a safe but slow convergence. A number of methods have been described for the choice of f which give faster convergence [1]. Yet, the convergence of relaxation method is generally slow. In this paper, we describe an alternative method of obtaining the self-consistent solution by solving the Poisson equation by Newton-Raphson (NR) iteration technique. The application of NR method for the solution of non-linear Poisson equation when the charge density can be expressed explicitly as a function of the potential is well known. This paper basically extends this method to the case when the charge density calculation requires the solution of Schrodinger equation.

II NEWTON-RAPHSON METHOD

Newton-Raphson method in N dimension deals with the solution of N non-linear equations

$$F_i(x_1,x_2,.....x_N) = 0, \quad i=1,2,.....N. \qquad ...(2.1)$$

In the vector notation, eq.(2.1) is written as

$$\mathbf{F}(\mathbf{x}) = 0 \qquad ...(2.1a)$$

where $\mathbf{x}$ and $\mathbf{F}$ stand for the vectors $(x_1,x_2,....x_N)$ and $(F_1,F_2,....F_N)$, respectively. Eq. 2.1a is solved by starting with a trial vector $\mathbf{x}_0$, and adding to it a correction vector $\delta\mathbf{x}$ given by

$$\mathbf{F}(\mathbf{x}_0+\delta\mathbf{x}) = \mathbf{F}(\mathbf{x}_0) + \mathbf{J}.\delta\mathbf{x} = 0 \qquad ...(2.2)$$

or,

$$\mathbf{J}.\delta\mathbf{x} = -\mathbf{F}(\mathbf{x}_0) \qquad ...(2.2a)$$

where the elements of the Jacobian matrix **J** are given by

$$J_{ij} = \partial F_i / \partial x_j. \qquad ...(2.3)$$

The matrix equation 2.2a is solved by standard LU decomposition and the solution vector is found by

$$x_{new} = x_{old} + \delta x. \qquad ...(2.4)$$

III BASIC EQUATIONS AND THE ITERATIVE PROCEDURE

In this section, we summarize the basic equations and the iterative procedure that we used for the self-consistent solution. The one-dimensional Schrodinger equation is :

$$-\hbar^2/2m^*(x)\, d^2y(x)/dx^2 + V(x)y(x) = E\, y(x) \qquad ...(3.1)$$

where y(x) is the wavefunction, E is the energy eigen value, m^* is the effective mass and V(x) is the potential energy. With a given potential energy distribution V(x), eq. 3.1 is solved numerically to get the energy eigenvalues E_k and the corresponding wavefunctions $y^k(x)$. The electron density distribution in the quantum well region is given by

$$n(x) = m^*/\pi\hbar^2\, \Sigma_k\, kT \ln(1+\exp((E_F-E_k)/kT))\, |\, y^k(x)\, |^2 \qquad ...(3.2)$$

where the summation (Σ_k) is carried out over all the allowed bound states in the well and E_F is the Fermi energy. The electron density distribution in the regions outside the quantum well is given by the conventional 3-D Fermi-Dirac statistics, viz.

$$n(x) = 2/\sqrt{\pi}\, N_c\, F_{1/2}\, [(E_F-V(x))/kT] \qquad ...(3.3)$$

where N_c is the effective density of states in the conduction band, and $F_{1/2}$ is the Fermi-Dirac integral. The Poisson equation in one-dimension is

$$d^2\Phi(x)/dx^2 = -\, \rho(x)/\varepsilon(x) \qquad ...(3.4)$$

where Φ is the electrostatic potential, $\varepsilon(x)$ is the dielectric constant, and the charge density $\rho(x)$ is given by

$$\rho(x) = q(N_d^+(x) - n(x)). \qquad ...(3.5)$$

In eq. 3.5, $N_d^+(x)$ and n(x) are the ionized donor density and the electron density distribution, respectively. The Poisson equation 3.4 is solved numerically by Newton-Raphson method as described in section **IV**. The potential energy V(x) for the solution of Schrodinger equation in the next iteration is calculated from the electrostatic potential $\Phi(x)$ through the relation

$$V(x) = -q\Phi(x) + E_g(x) \qquad ...(3.6)$$

where E_g is the bandgap of the semiconductor. In eq. 3.6, the exchange-correlation term is neglected and the zero of energy is taken to be the valence band maximum. The whole procedure is repeated until the potential energy distribution V(x) is equal for successive iterations, within a desired accuracy.

IV NUMERICAL SOLUTION OF POISSON EQUATION

In order to apply Newton-Raphson (NR) method for the solution of Posisson equation, we first rewrite eq. 3.4 in the form of eq.2.1 using a three point finite difference scheme and a non-uniform mesh:

$$F_i = R_i\Phi_{i-1} - (1+R_i)\Phi_i + \rho_i/\varepsilon_i h_i^2 R_i(1+R_i)/2 + \Phi_{i+1} = 0, \quad i=1...N, \qquad ...(4.1)$$

where h_i is the width of the i'th grid and $R_i=h_{i+1}/h_i$. As described in section **II**, eq. 4.1 can be solved by starting with a trial vector Φ^0, and adding a correction vector given by the solution of the matrix equation

$$\mathbf{J}.\delta\Phi = -\mathbf{F}. \qquad ...(4.2)$$

The Jacobian matrix **J** is seen to be of the familiar tridiagonal form with elements given by

$$J_{ij} = \partial F_i / \partial \Phi_j \qquad ...(4.3)$$

$$= R_i, \qquad j = i-1, \qquad ...(4.3a)$$

$$= 1, \qquad j = i+1, \qquad ...(4.3b)$$

$$= -(1+R_i)+h_i^2 Ri(1+R_i)/2\varepsilon_i\, d\rho_i/d\Phi_i, \qquad j=i, \qquad ...(4.3c)$$

$$= 0, \qquad \text{otherwise}. \qquad ...(4.3d)$$

The $d\rho_i/d\Phi_i$ term required in eq.4.3c is obtained by differentiating eq.3.5:

$$d\rho_i/d\Phi_i = q\{dN_d^+(\Phi_i)/d\Phi_i + dn(\Phi_i)/d\Phi_i\}. \quad ...(4.4)$$

The first term in eq.4.4 is easily evaluated all points. The second term in eq.4.4 is also easily evaulated at points outside the quantum well region. In order to evaluate the second term of eq.4.4 in the quantum well region, we make the approximation that the wavefunctions and the energies of the bound states with respect to the bottom of the well do not change for a small change in potential $d\Phi$. Our numerical experience shows that this approximation is generally quite valid. Thus, assuming

$$d|y_i^k|^2/d\Phi_i = 0, \text{ and } d(E_k-E_F) = -qd\Phi_i, \quad ...(4.5)$$

eq.3.2 can be differentiated to give

$$dn(x)/d\Phi_i = (m^*/\pi\hbar^2)\,\Sigma_k\, 1/(1+\exp((E_k-E_F)/kT))\,|y_i^k|^2 \quad ...(4.6)$$

in the quantum well region. Thus, $d\rho_i/d\Phi_i$ is evaluated at all points including the quantum well region, and hence all the elements of the Jacobian matrix can be calculated using eqs. 4.3, and the correction vector $\delta\Phi$ can be found by solving eq. 4.2. The new potential for the solution of Schrodinger equation in the next iteration is given by

$$\Phi_{new} = \Phi^0 + \delta\Phi, \quad ...(4.7)$$

and the whole procedure can be iterated.

V NUMERICAL SOLUTION OF SCHRODINGER EQUATION

Schrodinger equation 3.1 is discretized using a three point difference scheme and using a non-uniform mesh:

$$-\hbar^2/2m^*\,\{R_i y_{i-1} - (1+R_i)y_i + y_{i+1}\}/(h_i^2 R_i(1+R_i)/2) + V_i\, y_i = E\, y_i, \qquad i=1,2,.....N \quad ...(5.1)$$

where, once again, h_i is the width of the i' th grid and $R_i = h_{i+1}/h_i$. Eq. 5.1 can be written in the matrix form

$$\mathbf{H}.\mathbf{y} = E\,\mathbf{y} \quad ...(5.2)$$

where the Hamiltonian matrix **H** has the tridiagonal form given by

$$\begin{aligned} H_{ij} &= -(\hbar^2/2m^*)/\{h_i^2 R_i(1+R_i)/2\}R_i, && j=i-1, && ...(5.3a)\\ &= -(\hbar^2/2m^*)/\{h_i^2 R_i(1+R_i)/2\}, && j=i+1, && ...(5.3b)\\ &= V_i + (1+R_i)\,(\hbar^2/2m^*)/\{h_i^2 R_i(1+R_i)/2\}, && j=i, && ...(5.3c)\\ &= 0, && \text{otherwise}, && ...(5.3d) \end{aligned}$$

and $\mathbf{y} = (y_1, y_2, ...y_N)$ is a column vector. We used an inverse iteration procedure to solve eq. 5.2. Starting with a trial eigenvalue α_k and a corresponding normalized trial eigenvector $\mathbf{y}^k$, the solution of the following equation

$$(\mathbf{H} - \alpha_k\mathbf{I}).\mathbf{b}^k = \mathbf{y}^k \quad ...(5.4)$$

where **I** is the unit matrix, gives an improved eigenvector $\mathbf{b}^k$, and

$$E_k = \alpha_k + 1/(\mathbf{b}^k.\mathbf{y}^k) \quad ...(5.5)$$

gives an improved estimate of the energy eigenvalue. The procedure is iterated by normalizing $\mathbf{b}^k$ and using in place of $\mathbf{y}^k$ until E_k and $\mathbf{y}^k$ are determined to the desired accuracy. The whole procedure is repeated until the eigenvalues and the eigenvectors of all the possible bound states in the quantum well are obtained.

VI CALCULATION OF CAPACITANCE

We calculate the capacitance of the structure by directly solving the a.c. Poisson equation [5]. The change in the electrostatic potential distribution for a small change δV in the bias across the device is given by the solution of the a.c. Poisson equation (obtained by differentiating eq. 3.4)

$$d^2u(x)/dx^2 = -(d\rho(x)/d\Phi)u(x)/\varepsilon(x) \quad ...(6.1)$$

where $u(x) \equiv d\Phi(x)/dV$. From Gauss's law, the total charge per unit area can be obtained from the surface

electric field:

$$Q = -\varepsilon \, d\Phi/dx \, |_{x=0} \qquad ...(6.2)$$

The small signal capacitance is given by

$$C = dQ/dV = -\varepsilon \, du(x)/dx \, |_{x=0} \qquad ...(6.3)$$

Thus, by solving eq. 6.1 using the values of $d\rho(x)/d\Phi$ obtained in section **IV**, and using eq. 6.3 the capacitance of the structure is easily determined.

VII RESULTS AND DISCUSSION

The method was applied to the simulation of a strained GaAs/InGaAs/GaAs single quantum well structure grown by metal-organic chemical vapor deposition (MOCVD). A Schottky barrier was assumed to be placed on the surface of the sample and the simulations were carried out to calculate the capcitance of the structure for different voltages applied to the Schottky contact with respect to the bottom GaAs layer. From the calculated capacitance-voltage (C-V) data, the apparent carrier concentration profile was calculated using the standard relations,

$$\hat{n}(x) = 2/(q\varepsilon A^2 dC^{-2}/dV), \text{ and } x = \varepsilon A/C, \qquad ...(7.1)$$

where x is the depth below the Schottky barrier plane, and A is the area of the device. The only fitting parameter used for the simulation was the band offset ΔE_c. All the other parameters required for the simulation, such as the quantum well width, the nominal Indium composition in the well, etc. were estimated from the growth conditions. Figure 1 shows a comparison between the simulated and the experimental carrier profiles. To demonstrate the sensitivity of the simulated profile to the value of the fitting parameter ΔE_c, the simulations are shown for two different values of ΔE_c. Excellent agreement between the simulated and the measured profiles is obtained for $\Delta E_c = 0.165$ eV. We have also developed a modified Kroemer's analysis for the determination of ΔE_c directly from the experimental carrier profile [6]. From this analysis we get $\Delta E_c = 0.162$ eV in excellent agreement with the value obtained from simulation.

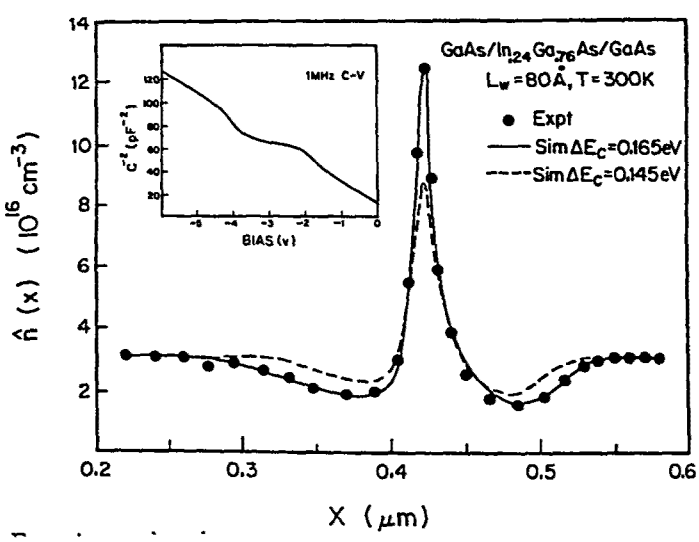

Fig1. Experimental and simulated carrier profiles of GaAs/InGaAs/GaAs strained SQW structure.

REFERENCES

1. F. Stern, J. Computational Physics **6**, 56 (1970).
2. M.B. Patil and H. Morkoc, Solid St. Electron. **33**, 99 (1990).
3. M.B. Patil and U. Ravaioli, Solid State Electron. **33**, 953 (1990).
4. A.M. Cruz Serra and H.A. Santos, J. Appl. Phys. **70**, 2734 (1991).
5. S. Subramanian, J. Appl. Phys. **64**, 1211 (1988).
6. S. Subramanian, et. al., J. Appl. Phys. **74**, 7618 (1993).