Edited by H. Ryssel, P. Pichler - September 1995

Coupled 2D-microscopic/macroscopic simulation of nanoelectronic heterojunction devices

Carsten Pigorsch[1], Roland Stenzel[1] and Wilfried Klix[2]

[1] Dresden University of Technology and Economics
Friedrich-List-Platz 1, D-01069 Dresden, Germany
[2] Dresden University of Technology
Mommsenstr. 13, D-01062 Dresden, Germany

Abstract

A two dimensional self consistent solution of the Schrödinger and the Poisson equation is obtained. This is coupled with a three dimensional drift-diffusion model to simulate nanometer heterojunction devices with respect to the microscopic properties of the electrons. Some examples of calculated III-V semiconductor structures are represented.

1. Introduction

The development of the semiconductor technology has made possible the production of structures and devices with small dimensions. For the simulation of these nanometer devices it is necessary to consider the wave properties of the carriers. Generally the Schrödinger equation is used to describe the microscopic energy quantisation which appears at heterojunctions [1]-[4]. The starting point of our work is the three dimensional (3D) device simulator SIMBA [5] based on a macroscopic drift-diffusion model, which is adapted to the simulation of heterostructures. The aim is the improvement of the simulation model by inserting the two dimensional (2D) Schrödinger equation. We make a point of an efficient numerical algorithm. The solution of the Schrödinger equation takes place by choice 1D or 2D depending on the structure design.

2. Simulation Model

The coupled 2D-microscopic/macroscopic model consists essentially of the microscopic Schrödinger equation and a macroscopic drift-diffusion model.

The behaviour of the electrons is described by the wave function ψ as the solution of the 2D Schrödinger equation [1], [2]

$$-\frac{\hbar^2}{2m^*}\Delta\psi(x,y) + V(x,y)\psi(x,y) = E\psi(x,y). \quad (1)$$

Here m^* is the effective mass and E are the discrete energy levels. The potential energy V is

$$V(x,y) = -q\phi(x,y) + \Delta E_C + V_{xc}(x,y) + V_{im}(x,y), \quad (2)$$

where ϕ is the electrostatic potential, ΔE_C is the conduction band discontinuity and V_{xc} is the local exchange correlation potential energy, V_{im} is the image potential [3], [6], [7]. V_{xc} and V_{im} has been neglected at first [1].
With the wave functions ψ and the corresponding energies E we obtain the microscopic electron density [2], [3], [6]

$$n(x,y) = \sum_i |\psi_i(x,y)|^2 n_i + n_{bulk} \qquad n_i = \frac{1}{\pi}\left(\frac{2m^* kT}{\hbar^2}\right)^{1/2} F_{1/2}\left(\frac{E_{Fn} - E_i}{kT}\right). \qquad (3), (4)$$

The 3D bulk electron density n_{bulk} contains the carriers in an assumed energy band above the considered discrete energies.
For the calculation of the electrostatic potential the Poisson equation is solved. The macroscopic part of the simulation model consists of the 3D continuity and transport equations for hole and electron current densities as described in [5].

3. Numerical Method

The 2D coupled algorithm is shaped as an inner iteration of the Schrödinger and the Poisson equation and an outer iteration where the transport model is solved [6].
Usually the inner iteration delivers a self consistent solution of Poisson and Schrödinger equation but for a good convergence of the whole algorithm often it is favourable to consider the transport equations after some or only one loop of the inner iteration. For a sure and successful iteration the change of the electrostatic potential is damped. The principle of the numerical algorithm is shown in Fig. 1.
The coupling of the microscopic and the macroscopic parts of the model takes place in a way described in [6]. It is based on the assumption that the sheet electron density at the heterojunction delivered by the microscopic Schrödinger equation and the density calculated by the transport equations have to be equal. For the solution of the microscopic density n by equations (3), (4) a Fermi level W_{Fn} is searched so that the integral of the electron densities in the quantum well realizes the condition above. The Fermi energy is assumed as constant in the whole area of the quantum well.
The Schrödinger equation is transformed into an eigenvalue problem by the Rayleigh-Ritz method. The wave function ψ is expressed as a sum of expansion functions in the form

$$\psi(x,y) = \sum_i \sum_j v_i(x)\, w_j(y).$$

In our simulations we have used Sinus functions [4] as well as B-Splines [8] for the expansion functions v_i, w_j. The advantage of Sinus functions is the independence of the number of expansion functions from the spatial discretization of the structure. The number of the expansion functions $(i \cdot j)$ is equal to the dimension of the eigenvalue problem. The resulting matrices of the eigenvalue problem are symmetric, which simplifies the solution method. We solve the problem by tridiagonalizing the symmetric matrix and than using the Sturm sequence and a bisection method to find the required eigenvalues. So the solution is less expensive than a finite difference or element method.
The Poisson equation and the transport equations are solved by the finite difference method with a non equidistant discretization.

4. Results and Discussion

The coupled microscopic/macroscopic method is applied to several heterojunction

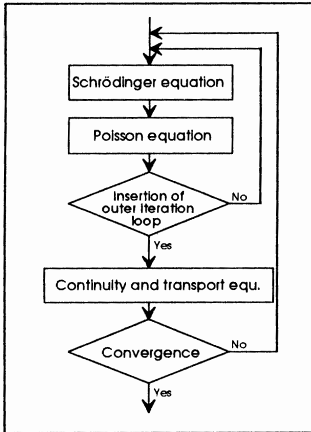

Fig. 1. Flowchart of the microscopic/macroscopic simulation (Inclusion of more model equations is possible)

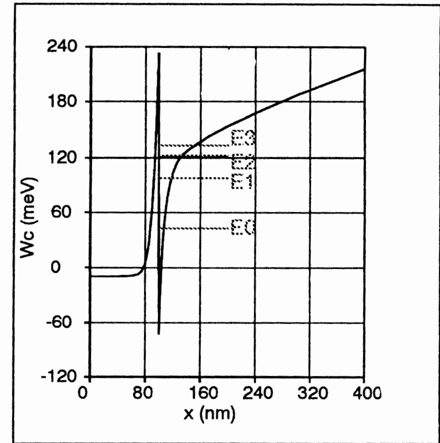

Fig. 2. Conduction band edge and discrete energy levels at a AlGaAs/GaAs heterojunction

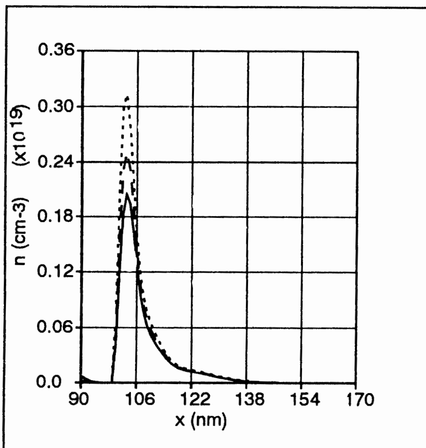

Fig. 3. Electron density at a AlGaAs/GaAs heterojunction (bias V = 0 solid line, 0.1V dashed line,0.2V dotted line)

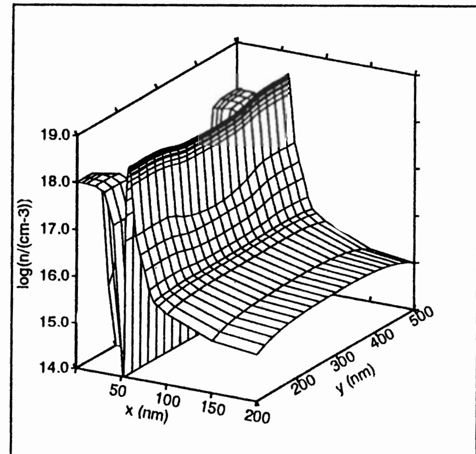

Fig. 4. Electron density distribution of a AlGaAs/GaAs-HEMT structure (L_G = 200 nm, V_{GS} = -0.5V, V_{DS} = 0)

structures. First we regard a simple abrupt GaAs/$Al_{0.3}Ga_{0.7}As$ heterojunction. The GaAs is undoped, the $Al_{0.3}Ga_{0.7}As$ is 10^{18} cm^{-3} n-doped. Fig. 2 is the calculated conduction band edge with the discrete energy levels at the heterojunction. With increasing bias the resulting electron density in the two dimensional electron gas increases (see Fig. 3).

We have calculate the electron density of a high electron mobility transistor (HEMT) by the 2D algorithm (Fig. 4). The HEMT consists on a 50 nm-$Al_{0.3}Ga_{0.7}As$-layer (10^{18} cm^{-3} n-doped) on a GaAs-substrate (undoped) with a gate length of 200 nm. Furthermore results of two quantum wire structures are shown. Fig. 5 shows a GaAs-corner in an $Al_{0.3}Ga_{0.7}As$-area, Fig. 6 is a square GaAs-area surrounded by $Al_{0.3}Ga_{0.7}As$.

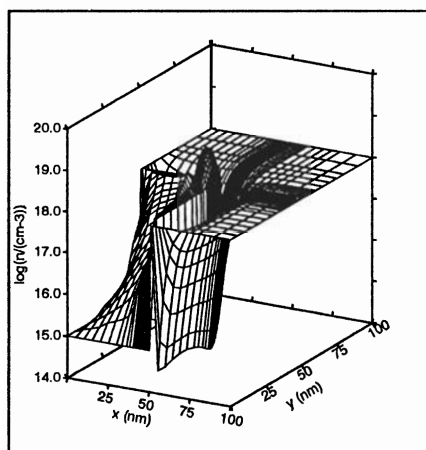

Fig. 5. Electron density distribution of a quantum wire at a AlGaAs/GaAs corner

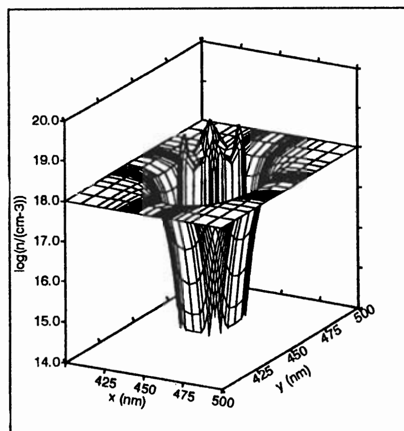

Fig. 6. Electron density distribution of a quantum wire of a (25 x 25) nm^2 GaAs area, surrounded by AlGaAs

5. Conclusion

In this paper we present a coupled microscopic/macroscopic simulation model with a complete 2D solution of the Schrödinger equation. An efficient solver for the differential equation and the resulting eigenvalue problem has been realized. The differences to the solution of a pure macroscopic model were shown by examples of several structures with III-V heterojunctions.

6. Acknowledgements

This work was supported by the German Ministry of Research and Technology under contract 01 BT 306/8.

References

[1] S. E. Laux, Numerical Methods for Calculating Self-Consistent Solutions of Electron States in Narrow Channels, Proc.of NASECODE V, pp. 270-275, 1987
[2] S. E. Laux, A. C. Warren, Self-Consistent Calculation of Electron States in Narrow Channels, IEEE IEDM 1986, pp. 567-570
[3] T. Kerkhoven et al., Efficient numerical solution of electron states in quantum wires, J. Appl. Phys., Vol. 68, No. 7, pp.3461-3469, 1990
[4] A. Abou-Elnour, K. Schuenemann, An Efficient and Accurate Self-Consistent Calculation of Electronic States in Modulation Doped Heterostructures, Solid States El., Vol. 37, No. 1, pp. 27-30, 1994
[5] R. Stenzel et al., Device Simulation of Novel In-Plane-Gated Field-Effect Transistors, Jpn. J. Appl. Phys., Vol. 33, No. 3A, pp. 1243-1247, 1994
[6] T. Wang, C. H. Hsieh, Numerical analysis of nonequilibrium electron transport in AlGaAs/InGaAs/GaAs pseudomorphic MODFET's, IEEE Trans. ED, Vol. 37, No. 9, pp. 1930-1938, 1990
[7] F. Stern, S. Das Sarma, Electron energy levels in GaAs-Ga(1-x)Al(x)As heterojunctions, Physical Review B, Vol. 30, No. 2, pp. 840-848, 1984
[8] J. Sánchez-Dehesa et al., Electronic energy of quantum-well wires, J. Appl. Phys., Vol. 73, No. 10, pp. 5027-5031, 1993