ACCURATE AND EFFICIENT MODELING OF HETERO-FETS

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ABSTRACT

Efficient numerical methods which are usually used in e.m. field problems are applied to solve Schroedinger's equation in semiconductors. The energy band structure of microwave heterostructure FETs is obtained by solving Poisson's and Schroedinger's equations self-consistently. The obtained results are used together with a two dimensional Monte-Carlo code to simulate the physical operation of the device. The model offers an accurate and efficient way to determine the DC and RF characteristics.

INTRODUCTION

Submicrometer hetero-FETs are now widely applied in microwave and high speed digital circuits. Many authors investigated various physical models to characterize the operation and to optimize the performance of these devices. Although Monte-Carlo codes describe electron transport in bulk materials and in homo-FETs accurately, special treatments are required to take the physical phenomena in hetero-structures into account. These phenomena are determined accurately by solving Schroedinger-Poisson equations.

A number of authors investigated different methods to solve Poisson's and Schroedinger's equations self-consistently [1-3]. Finite-difference methods are usually used to solve Schroedinger's equation. The numerical efficiency of these methods is deteriorated by discretization and mesh size [3]. The obtained wave functions are just numerically given so that any further application of them in calculating the scattering rates and the carrier transport properties inside the semi-conductor material requires large CPU [1].

Considering Monte-Carlo models, two main methods are usually used to simulate the hetero-FET. The first method applies boundary conditions on the electron transport at the heterointerface and permits carrier transfer between the semiconductor layers under the conditions of conservation of energy and parallel momentums to the interface [4-6]. The size quantization effects are not included and hence these models are not able to simulate highly doped devices accurately.

The second method takes size quantization into account by introducing a two-dimensional electron gas region and studying the carrier transport in that region and in the three-dimensional one [7,8]. As the derivation of the two-dimensional scattering rates and of the coupling between 2D and 3D regions is not an easy task, the applicability of such models is limited. On the other hand, these models use an approximated triangular potential well to derive the scattering rates what may lead to some errors.

A more accurate determination of the scattering rates and of the carrier transport properties is obtained by a self-consistent solution of Poisson's and Schroedinger's equations. The conventional numerical methods leed, however, to too large CPU time thus preventing an efficient device simulation.

In the present work, an efficient method is introduced to simulate HFETs accurately. Numerical techniques which are usually used to solve the electro-magnetic wave equation [9] are implemented to obtain the solution of Schroedinger's equation. Then numerical difficulties which are overcome which result from mesh size and discretization [3].

The potential energy distribution inside the hetero-FET is determined from a self-consistent solution of Poisson's and Schroedinger's equations. The obtained results are used together with a two-dimensional Monte-Carlo code to determine the physical operation of the device. Validation and efficiency of our model are demonstrated by comparing the obtained results with those from classical models.

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ENERGY BAND MODELING

The energy band is modelled by solving Schroedinger's equation which is given by

$$-\frac{\hbar^2}{2\,m^*}\frac{\partial^2 \psi_l(y)}{\partial y^2} + V(y)\,\psi_l(y) = E_l\,\psi_l(y) \qquad (1)$$

$$V(y) = -e\,\phi(y) + V_h(y) + V_{ex}(y) \qquad (1.a)$$

where $\phi(y)$ means electrostatic potential , $V_h(y)$ potential step function at the hetero-interface, $V_{ex}(y)$ local exchange potential, E_l eigenenergy, $\psi_l(y)$ wave function corresponding to the eigenenergy E_l, e magnitude of electronic charge, m^* effective mass, and $\hbar$ Planck's constant. Finite difference methods are usually used to solve (1) numerically. Their accuracy is, however, limited by discretization and mesh size [2].

Instead of finite difference we apply the Rayleigh-Ritz method to obtain the solution in closed form. This method determines a finite set of eigenvalues and the corresponding eigenfunctions of (1) for given boundary conditions. For a semiconductor structure of width a, the eigenfunctions satisfy the boundary conditions $\psi(0)=0$, $\psi(a)=0$. They can then be expressed as

$$\psi_k = \sum_{n=1}^{N} a_{nk}\, f_n \qquad (2)$$

$$f_n = \left(\frac{2}{a}\right)^{1/2} \mathrm{Sin}\left(\frac{n\,\pi\,y}{a}\right) \qquad (2.a)$$

If N is chosen as infinite, the eigenfunctions will be identical with the set of true eigenfunctions. However, a finite N still leads to the required solution with good accuracy [9].

The problem is reduced now to determine the expansion coefficients a_{nk} which are used to obtain the eigenfunctions. They can be calculated from the set of homogeneous equations

$$\sum_{n=1}^{N} a_{nk}\left(T_{ln} - \frac{2\,m^*}{\hbar^2}\,E_k\,\delta_{ln}\right) = 0 \qquad l = 1,2,\ldots,N \qquad (3)$$

$$T_{ln} = T_{nl} = \int_0^a \left(\frac{df_n}{dy}\,\frac{df_l}{dy} + \frac{2\,m^*}{\hbar^2}\,V(y)\,f_l\,f_n\right) dy \qquad (3.a)$$

The wave functions are calculated if the potential energy function V(y) is known. This function is obtained from the solution of Poisson's equation. Different potential functions and their corresponding wave functions are shown in fig.1.

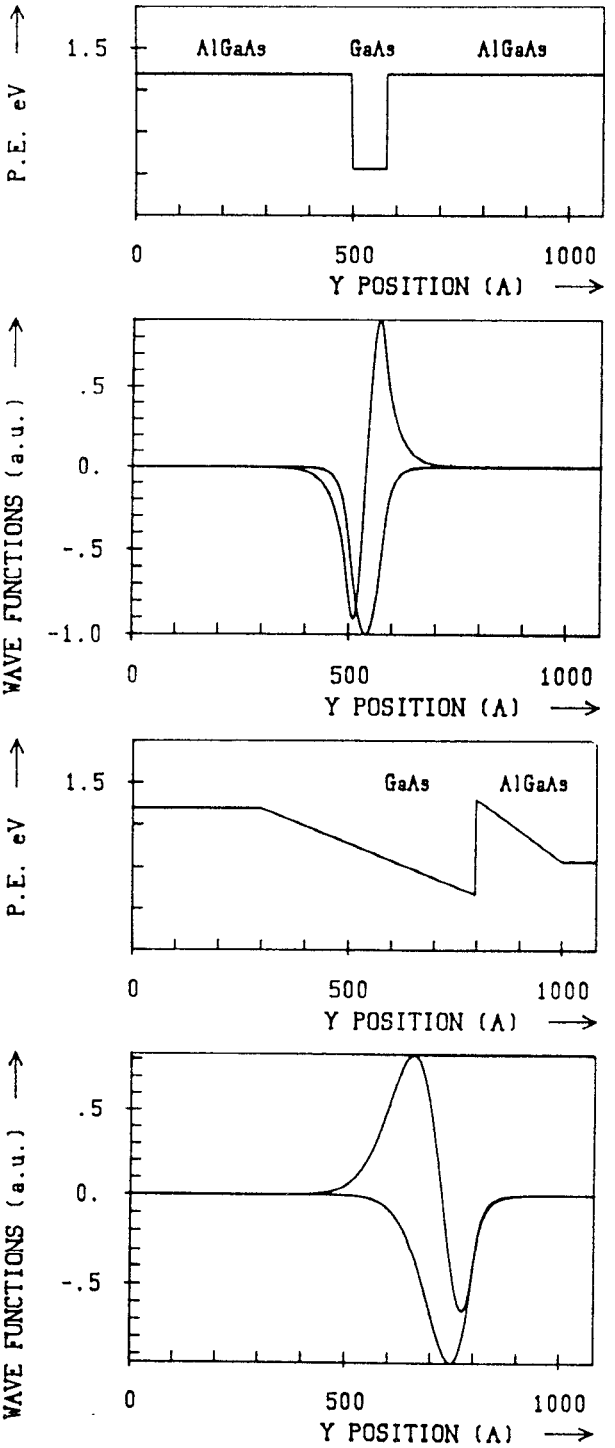

Fig.1 Potential energies and corresponding wave functions

SELF-CONSISTENT PROCEDURE

We believe that the solution of the Poisson-Schroedinger system of equations will become a common simulation tool for ultra-small and quantum devices. With our method the scattering rates inside complicated semiconductor structures and the carrier transport properties are easily obtained by using the closed forms of the wave functions (2).

Equation (1) and Poisson's equation are solved iteratively until a self-consistent solution is obtained. For the first iteration, the potential energy function V(y) and the corresponding wave functions are calculated by using the triangular wave approximation. The electrostatic potential $\phi(y)$ is then calculated by solving Poisson's equation. The boundary conditions imposed on the structure state that the differences between the Fermi level and the bottom of the conduction band are constant at both ends and equal to difference values in the bulk. These values are calculated by knowing the occupancy of the deep centers and the electron concentration [2].

The new potential energy function is then calculated using (1.a). For the next iteration, the effective potential energy function is expressed as a linear combination of new and old values of V(y) given by

$$V_{new}(y) = \omega\, V_{new}(y) + (1-\omega)\, V_{old}(y) \qquad (4)$$

where ω means relaxation constant which is introduced to obtain the solution safely [6]. From (3) and (3.a), the potential energy function V(y) is used to determine the wave functions which are used to recalculate the carrier distribution. The procedure is repeated until initial and final values of V(y), within the same iteration, differ by less than a specified error. The self-consistent algorithm is illustrated by the flow chart in fig.2

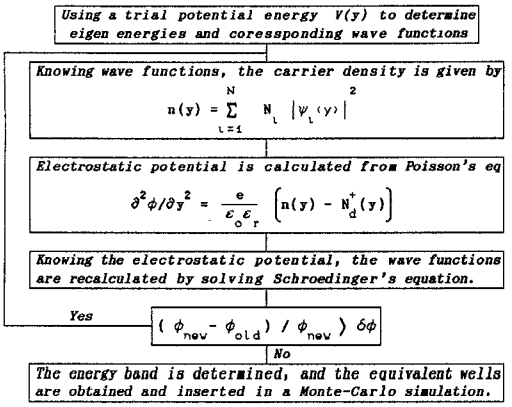

Fig.2 Self-consistent solution of Poisson-Schroedinger equations.

APPLICATIONS AND RESULTS

A two-dimensional Monte-Carlo code is investigated to simulate the hetero-FET structure shown in fig.3. The energy band is obtained by applying the previous self-consistent solution of Poisson's and Schroedinger's equations. It is then approximated by various shape functions for the potential well which are subsequently used in a Monte-Carlo code. The height of the well is equal to the eigenenergy E_l, while the well width is given by the distance over which the square of ψ_l is maximum. The wave functions and equivalent energy wells at different sections along the channel are displayed in fig.4.

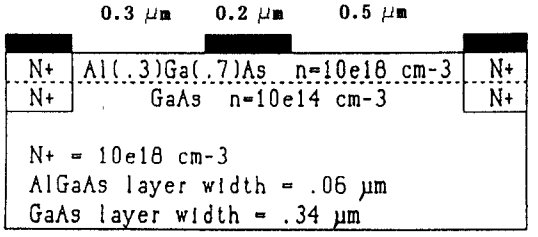

Fig.3 Simulated AlGaAs/GaAs Hetero-FET

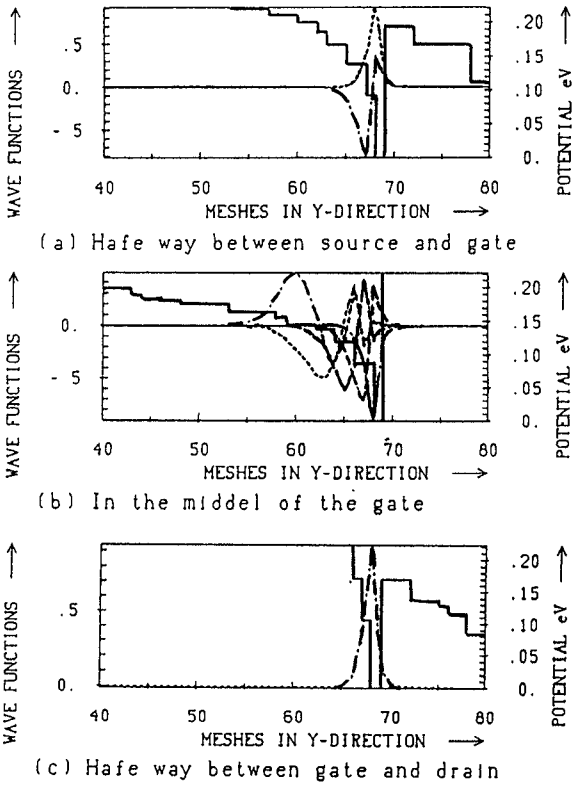

Fig.4 Energy wells (solid lines) and wave functions (dashed lines) at different positions (mesh size 50 Å)

The present model takes the size quantization into account because the electrons which have energies less than the barrier height can only move in two dimensions. Moreover the transfer between the different regions is simpler than in other models because no extra scattering rates are required to be derived. The carrier distributions inside the device with and without including the energy band into the simulation are shown in fig.5.

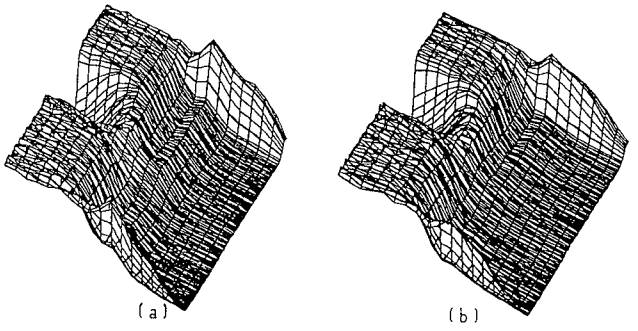

Fig.5 Carrier distribution in the channel
(a) The present model (b) Classical model

V CONCLUSIONS

An accurate and efficient method is presented to simulate heterostructure devices. By using the Rayleigh-Ritz method to solve Schroedinger's equation, the wave functions are obtained in closed form which offers an advantage in calculating the scattering rates and the carrier transport properties in heterostructures. For simple hetero-structures, the present method is shown to be efficient and accurate and the extension for determining the scattering rates and the carrier transport properties in complicated structures is expected to be straightforward.

The obtained wave functions are used to approximate the energy band inside the semiconductor device by a number of potential wells. This method offers an accurate way to model heterostructure devices in a reasonable CPU time. The capture of the carriers in the two-dimensional electron gas region is well simulated (fig. 5) and the transfer between hetero-structure layers is modelled in a simpler and more efficient way than with other simulators.

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