An Accurate and Efficient Method to Characterize Heterostructure Devices

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Abstract
Electronic states inside heterostructure devices are obtained by solving Poisson's and Schroedinger's equation self-consistently. Schroedinger's equation is efficiently solved by using variational techniques to obtain the wave functions in terms of a number of expansion functions. The present method is used to characterize the operation of single-well and pseudomorphic heterostructures, to characterize quantum wire devices, to calculate the two-dimensional scattering rates, and in Monte-Carlo codes.

I Introduction

The physical phenomena which are taking place in ultra-small and highly doped heterostructure devices require accurate physical models to characterize device operation and to optimize the structures. The main difficulty is that the behavior in the two dimensional electron gas (2DEG) region depends in a complicated manner on the device geometry and on bias conditions. The self-consistent solution of Poisson's and Schroedinger's equations is one of the most accurate models which is used to characterize heterostructure semiconductors to overcome these difficulties [1,2].

Previous self-consistent calculations generally used the finite difference technique to solve Schroedinger's equation [3-5]. The mesh size and the discretization method deteriorated the accuracy of the obtained results. We have recently introduced an efficient method to solve Schroedinger's equation by using variational techniques [6]. In the present work, we apply this method to characterize different heterostructure devices.

II Modeling

The effective mass, one-dimensional Schroedinger equation is given by

$$-(\hbar^2/2m^*)(\partial^2\psi_i(x)/\partial x^2) + V(x)\psi_i(x) = E_i\psi_i(x) \qquad (1)$$

where V(x) means potential energy, E_i eigenenergy, $\psi_i(x)$ wave function corresponding to the eigenenergy E_i, m^* effective mass, and $\hbar$ Planck's constant. For a semiconductor structure of width a, the wave functions can be expanded as

$$\psi_k = \sum_{n=1}^{N} a_{nk} \sin\left(\frac{n \pi x}{a}\right) . \qquad (2)$$

If N is infinite, the obtained wave functions are identical with the true ones. However, a finite N still leads to very good accuracy. The coefficients a_{nk}, the eigenenergies, and the corresponding wave functions are determined by solving the matrix equation resulting from the variational integral for E_i [6].

III Application

The previous method is applied to characterize a modulation doped structures by solving Poisson's and Schroedinger's equations self-consistently. The 2DEG density, the energy levels, the wave functions, and the transconductance are displayed versus the total gate voltage in figs. 1,2,3, and 4 respectively. The total gate voltage represents the sum of the applied external voltage and the Schottky barrier equivalent voltage. Good qualitative agreement between the calculated results and those from both experiments and Monte-Carlo calculations [7] is obtained.

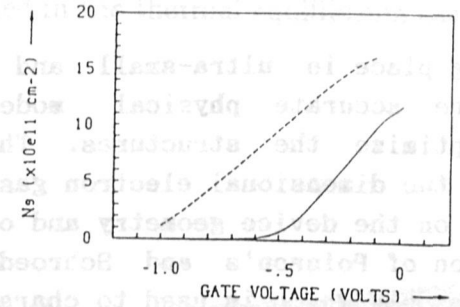


Fig.1 2DEG density versus gate voltage in single-well (solid line) and pseudomorphic (dashed line) structures.

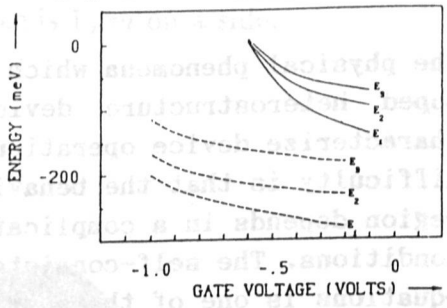
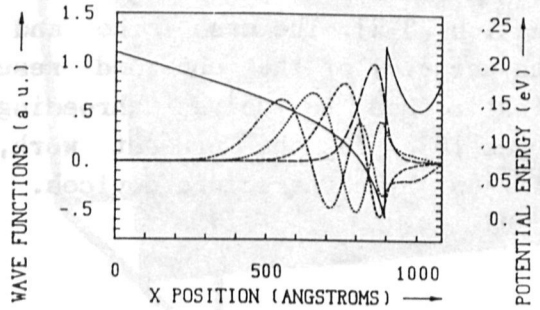
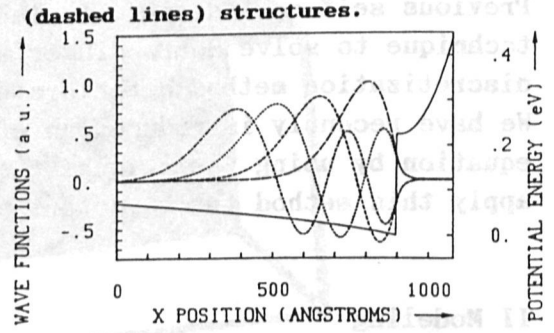


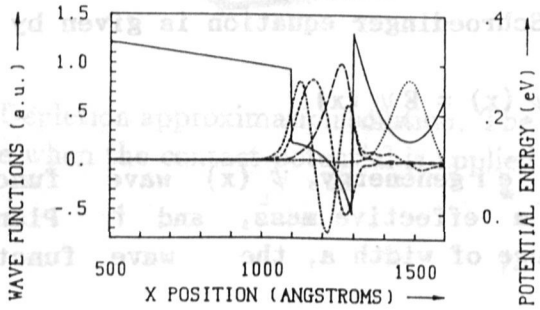
Fig.2 Subband energies versus gate voltage in single-well (solid lines) and pseudomorphic (dashed lines) structures.



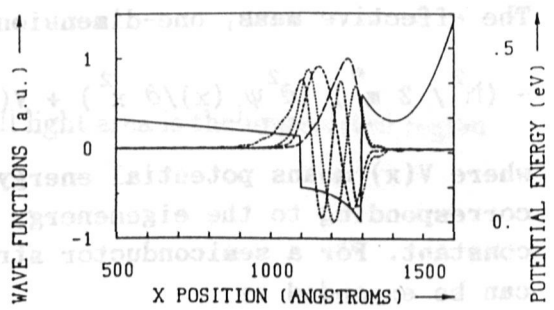
(a) Single-well (Vg = -0.1 Volt).



(b) Single-well (Vg = -0.5 Volt).



(c) Pseudomorphic (Vg = -0.1 Volt).



(d) Pseudomorphic (Vg = -0.5 Volt).

Fig.3 Energy-band (dashed line) and wave functions (solid lines) for

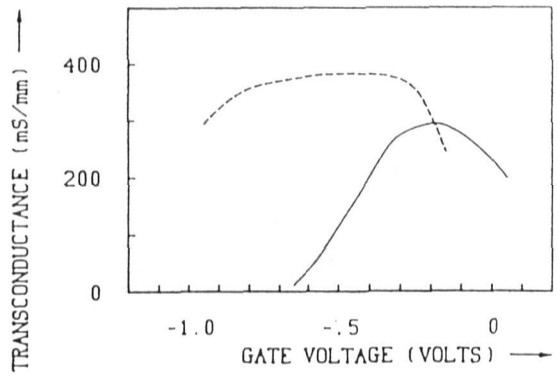


Fig.4 Transconductance versus gate voltage in single-well (solid line) and pseudomorphic (dashed line) structures.

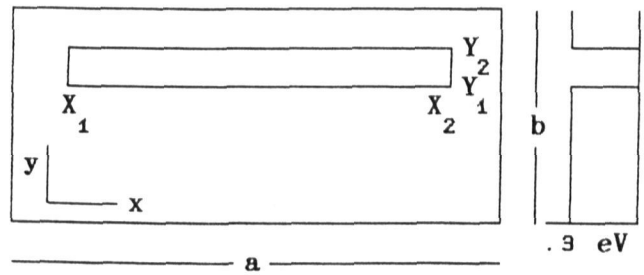


Fig.5 Schematics of the simulated structure. a=b=100nm, X1=20nm, X2=80nm, Y1=60nm, Y2=70nm

Quantum wire structures, shown in fig.5, can also be characterized by solving Schroedinger's equation in two dimensions using Rayleigh-Ritz method to obtain the two-dimensional wave functions (fig.6). The present method has the advantageous that it requires resonable CPU time, it is straight forward, and it overcomes the limitations of previous models arising from mesh size and discretization.

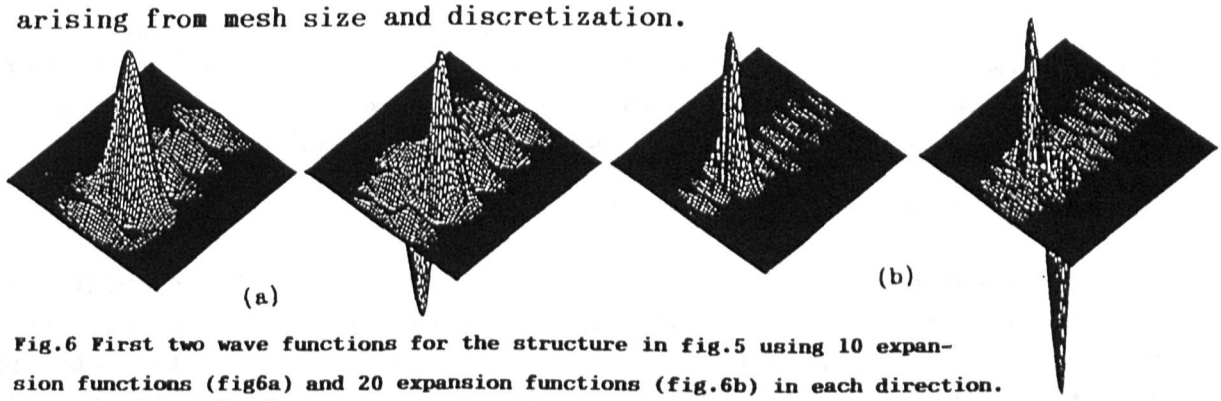


Fig.6 First two wave functions for the structure in fig.5 using 10 expansion functions (fig6a) and 20 expansion functions (fig.6b) in each direction.

IV Calculation of the two-dimensional scattering rates

The two-dimensional scattering rates are calculated by defining the matrix element for scattering between the *i*th and the *j*th subbands according to

$$| M_{ij} |^2 = \int | M(Q,q) |^2 | I_{ij}(q) |^2 dq \qquad (3)$$

where Q, q are the phonon wave-vector components parallel and normal to the hetero-interface, and $I_{ij}(q)$ means overlap integral

$$I_{ij}(q) = \int \psi_i(x) \psi_j(x) \exp(iqx) dx . \qquad (4)$$

$\psi(x)$ is the normalized envelope wavefunction. Both Rayleigh-Ritz and finite difference methods are applied to calculate the subband energies and the corresponding wavefunctions of an AlGaAs/GaAs heterostructure. Using Rayleigh-Ritz method, the required CPU time (fig.7b) to calculate the 2D scattering rates (fig.8) versus the number of subbands is nearly constant while it greatly changes using the finite difference method (fig.7a). This makes the application of the present method more practical in particular for device simulation.

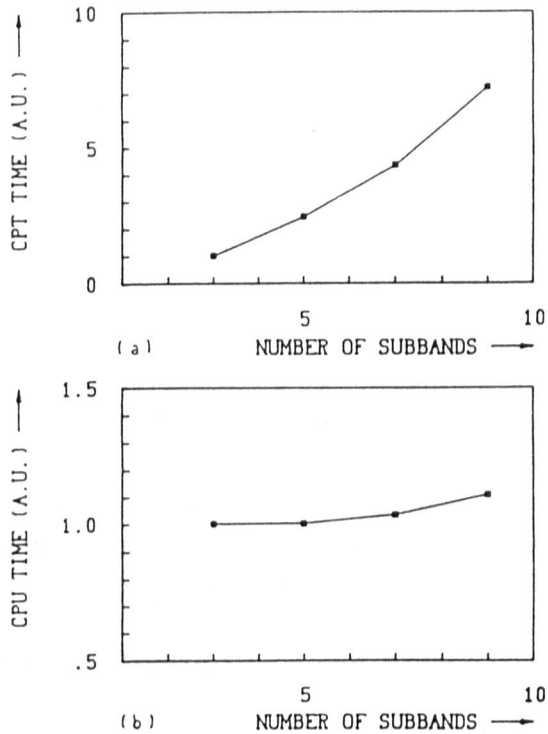


Fig.7 Required CPU time to calculate the 2D scattering rates versus number of subbands. a) finite difference, b) Rayleigh-Ritz method.

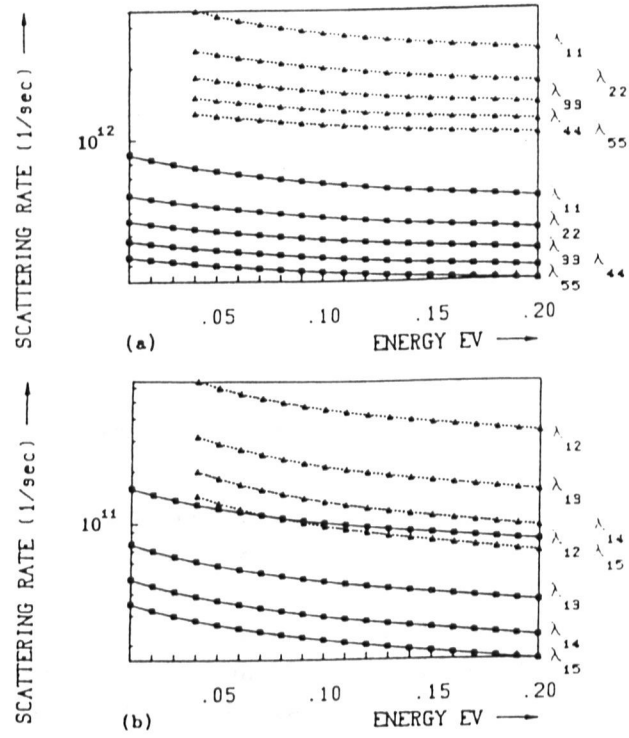


Fig.8 2D polar optical phonon scattering rate absorption (solid lines), emission (dashed line) a) intrasubband, b) intersubband scattering.

V Monte-Carlo simulation of Hetero-FETs

A two-dimensional Monte-Carlo code is investigated to simulate the hetero-FET structure shown in fig.9. Poisson's and Schroedinger's equations are sovled self consistently along the device and the obtained results are used to express the conduction band by a number of step functions. The wave functions and equivalent energy wells at different sections along the channel are displayed in fig. 10.

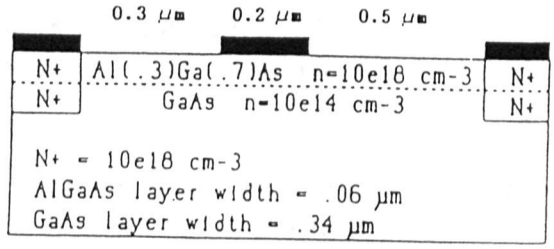


Fig.9 Simulated AlGaAs/GaAs Hetero-FET.

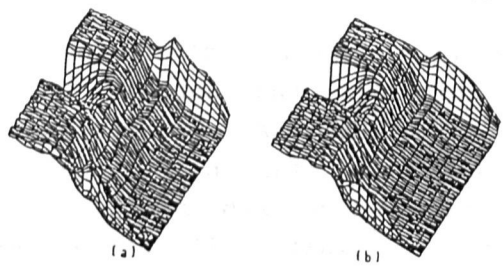


Fig.11 Carrier distribution in the channel (a) the present model (b) classical model.

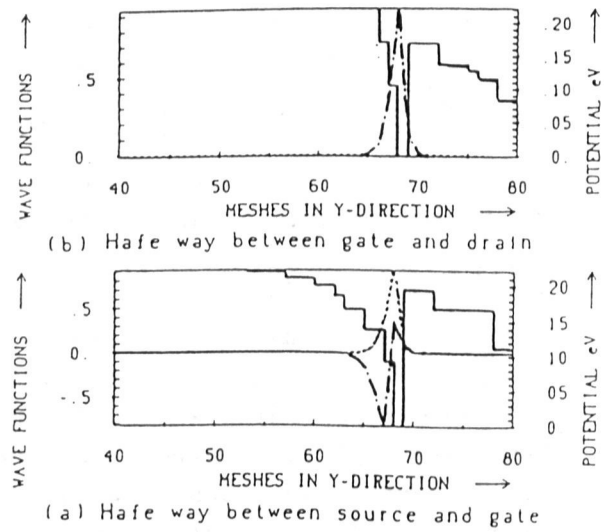


Fig.10 Energy wells (solid lines) and wave functions (dashed lines) at different positions [mesh size 50A].

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. Our model leads to a higher carrier concentration in the channel region than the classical models, fig. 11, because the carrier capture in the 2DEG region is better simulated.

VI Conclusions

An efficient computational tool is used to determine the electronic states inside heterostructure. The present model overcomes the limitations of the previous models which arise from mesh size and discretization. The closed forms of the wave functions makes the calculations of the two-dimensional scattering rates easier. This method can also be efficiently used together with Monte-Carlo codes to characterize semiconductor devices.

Acknowledgement

The authors are thankful to Prof. Dr. A. S. Omar for fruitful discussions and to the Deutsche Forschungsgemeinschaft for financial support.

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