Two-Dimensional Quantum Modelling of Heterojunction Field Effect Transistors

R. Drury, R.E. Miles, C.M. Snowden

Microwave and Terahertz Technology Group,
Dept. Electrical and Electronic Engineering,
University of Leeds,
Leeds, LS2 9JT, UK

Abstract

A new, fast, two-dimensional model is presented that couples the classical semiconductor transport equations with quantum mechanics. It is particularly suited to the simulation of single channel, pseudomorphic and multi-channel HFETs and delta doped structures, where the primary conduction path between source and drain is via carriers confined to a two-dimensional potential well. The model solves Poisson's and the current-continuity equation self consistently with the effective mass Schrödinger equation, the latter taken in slices perpendicular to the heterojunction. Current flow is modelled by restricting the discretised "quantum" electrons to two-dimensional motion, neglecting non-equilibrium dynamics. The model improves on previously reported versions by allowing a full two-dimensional treatment of the Fermi-level, allowing a non-equilibrium treatment of Schrödinger's equation.

Introduction

The increasing use of AlGaAs/InGaAs/GaAs heterostructure devices has lead to great interest in modelling the electrons confined within 2 Dimensional Electron Gas (2DEG) layers. Classical schemes are based upon the electron wavefunction being described as Bloch states, which in turn are derived from flat band conditions. When events occur that approach the size of the electron wavepacket, ie. the de-Broglie wavelength, this approximation is invalid and quantum effects have to be included. Unfortunately a rigorous solution of the quantum mechanical equations becomes very involved and computationally intensive, limiting their use within physical device modelling. For this reason a simplified scheme has been adopted whereby quantum effects are modelled by solving the effective mass Schrödinger equation (1) across the heterojunction but assuming the classical approximations to hold elsewhere.

$$-\frac{\hbar^2}{2q}\frac{\partial}{\partial y}\left(\frac{1}{m^*}\frac{\partial \xi_k}{\partial y}\right) + (V_{tot} - \lambda_k)\xi_k = 0 \qquad (1)$$

where

$$V_{tot} = -\psi + V_h + V_{xc} \qquad (2)$$

V_h is the heterojunction potential and V_{xc} the exchange-correlation energy [1]. This approach is justified as the smallest event in the x-direction is the gate which is at least an order of magnitude larger than the electron wavelength. The electron density is now described by equation (3), [2], instead of the classical Fermi-integral.

$$n = N_{c2D} \sum_k |\xi_k|^2 \log_e \left\{ 1 + \exp \frac{q}{kT}(\phi - \lambda_k) \right\} \quad (3)$$

The model therefore solves Poisson's equation self-consistently with the classical charge transport equation, with the modification that the electrons are divided into two classes. The first posessing "quantised motion" are only permitted to move parallel to the heterojunction, and are formed from the electrons whose intersub-band separation is greater than the thermal energy, k_BT. The second are normal three-dimensional electrons, which, in order to reduce the computational demands are approximated within the model by the Fermi-integral taken from a quasi-continuous conduction band edge shown in Figure 1.

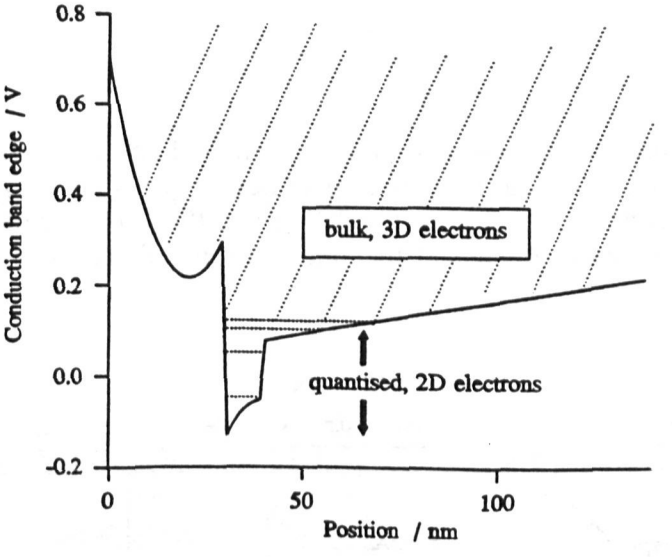

Figure 1. Conduction band edge of a pseudomorphic AlGaAs/InGaAs/GaAs HFET showing the separation of the two- and three-dimensional electrons.

Simulation Details

The equations are discretised over a non-uniform rectangular mesh using central finite differences. Schrödinger's equation is solved, first by finding the eigenvalues via a bisection method based upon a "Sturm" sequence [3]. This method is both fast and robust, with the upper and lower bounds initially set using Gershgorin's theorem [4], and then updated using the last calculated eigenvalue. The eigenvalues are then substituted into Schrödinger's equation and eigenvectors found using a Newton iterative scheme. The current-continuity equation was formulated using current densities calculated at the half-nodes, assuming the independent variables ψ and ϕ vary linearly in between the nodes. This has the advantage that no "Scharfetter-Gummel" interpolation scheme is necessary, substantially simplifying the device equations.

The principle device equations are all highly non-linear in the independent variables ϕ, ψ. Consequently a modified Newton-Raphson iterative scheme was employed which requires the Jacobian, a matrix formed from the partial derivatives of the functions with respect to each of the variables. All of the terms in the two equations, with the exception of the partial derivative

of n_{2D} with respect to ψ are readily differentiable. This term depends explicitly upon the partial derivatives of ξ_k and λ_k, which are calculated using perturbation theory, equation (4)

$$\frac{\partial \lambda_k}{\partial \psi} = -1 \quad , \quad \frac{\partial \xi_k}{\partial \psi} = 0 \tag{4}$$

using this result it is evident by inspection of equation (3) that

$$\frac{\partial n_{2D}}{\partial \psi} = \frac{\partial n_{2D}}{\partial \phi} \tag{5}$$

Results

The model has been used to simulate several devices including single channel, pseudomorphic and multichannel FETs. A typical pseudomorphic device structure is shown in Figure 2. The ohmic contacts are assumed to extend to the 2DEG and thus the modelled region is truncated placing the source and drain contacts at the sides. A lumped access resistance is then added explicitly.

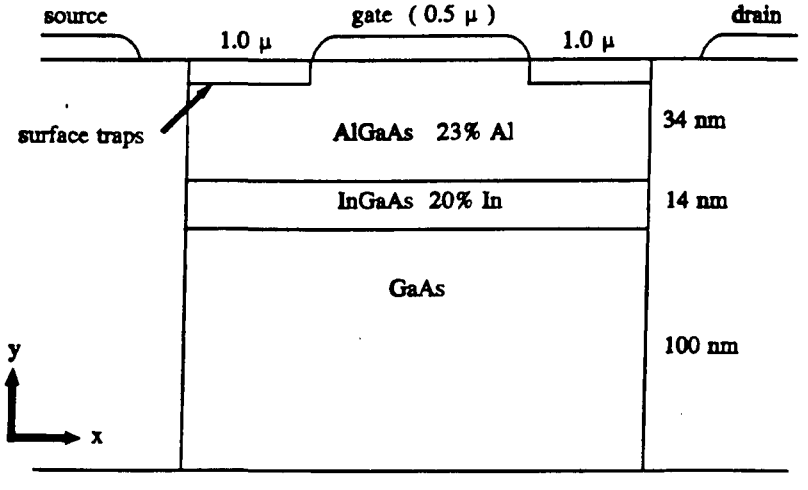

Figure 2. A typical pseudomorphic HFET structure used in the simulations.

Figures 3 and 4 show Fermi-level and conduction band edge profiles, taken at $V_{DS} = 1.7V$ and $V_{GS} = 0V$. The Fermi-level shows significant distortion around the gate, clearly perturbed from equilibrium, although in the InGaAs channel and GaAs substrate the gradient of the Fermi-level (driving force) is nearly parallel to the heterojunction. The conduction band edge shows the two-dimensional potential well formed in the InGaAs.

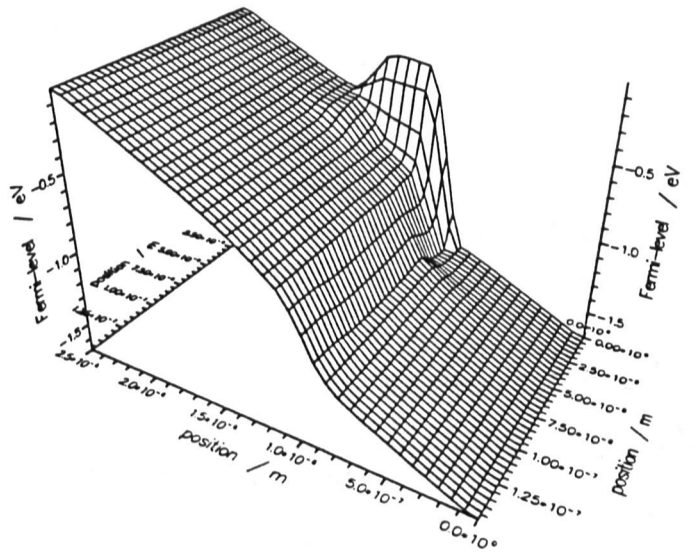

Figure 3. Fermi-level for a pseudomorphic HFET.

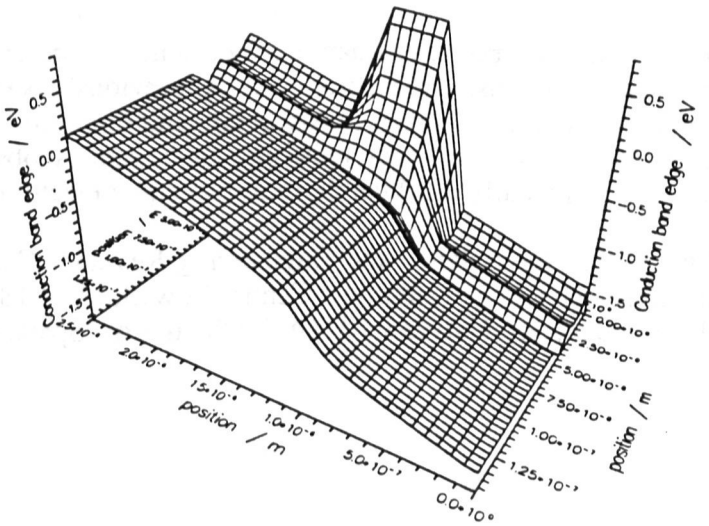

Figure 4. Conduction band edge for a pseudomorphic HFET.

Figure 5 shows the I_{DS}-V_{DS} characteristics for this device, comparing quantum (solid lines) with classical Fermi-integral solutions, from which it is evident that the quantum simulation has a lower output current. This is mainly attributable to the reduced carrier density produced by this scheme, as current flow in the y-direction is mainly limited by the high access resistances to the 2DEG regions which are populated by three-dimensional electrons in both cases.

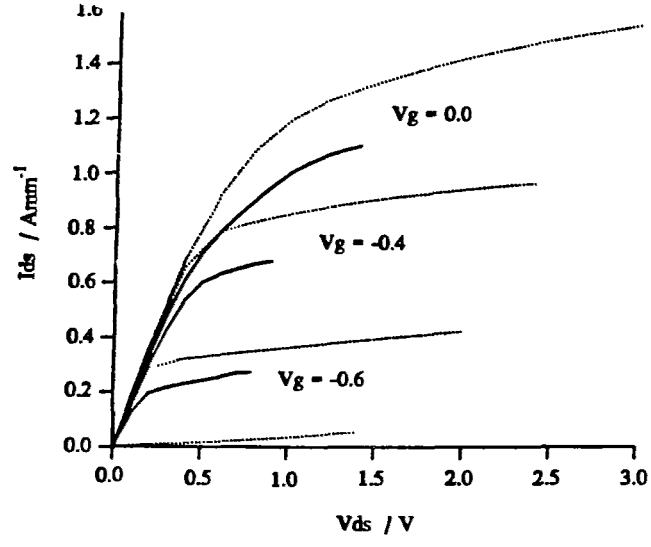

Figure 5. I_{DS}-V_{DS} curves for the quantum and classical simulations.

Conclusions

A two-dimensional HFET model incorporating quantum mechanics is presented that solves Schrödinger's equation in a more self-consistent fashion than has previously been reported. The quantisation in electron motion is explicitly taken into account, and found to have little effect in the final current-voltage curves. A significant reduction in current is observed between quantum and classical models, principally attributable to a lower free electron density.

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