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Preliminary Results of Quantum Directional Coupler Simulation Using a Beam Propagation Method

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Abstract

A simulation method for electron wave propagation in a quantum directional coupler is presented. As an example of the method, the switching behavior of quantum directional coupler is simulated.

1. Introduction

Recent advances in technology have enabled the fabrication of nano-scale devices, whose quantum effects can be put to use. The Quantum Directional Coupler (QDC) is an example of such a device which has been extensively investigated in the last three years [1-3]. A cross-section of a possible QDC structure is shown in Fig. 1. Space charge layers under the Schottky contacts create the required potential wells to confine the electrons in x-direction. The heterojunction between the undoped $Al_{0.3}Ga_{0.7}As$ and $GaAs$ layers confines the electrons in the y-direction. This creates two parallel quantum wires of two-dimensional electron gas (2DEG) with very high mobility at low temperature. If the separation between the wires is small enough, then the electrons propagating in these wires will interact with each other. For example, if initially the electron wave is in one wire, then after traveling some distance it will be transferred into the second wire. This can be viewed as the symmetric and antisymmetric modes beating with each other, causing the electrons to slosh between the two wires. The transfer length depends on the barrier height and upon the separation between the two wires. Therefore, by changing the voltages, one can switch the electron current from one wire to the other.

In previous papers [1-3], the two-dimensional Schrodinger's and Poisson's equations in the QDC structure were solved to calculate the electron eigenfunctions, and conclusions about the characteristics of the QDC were made. The purpose of this paper is to demonstrate the applicability of the beam propagation method (BPM), that has been used to simulate optical waveguides [4], to QDC simulation.

2. Physical model

To apply BPM one should assume that there is a preferred direction of wave propagation, along which the changes of electron wave-function are slow. In a QDC this is

the z-direction. We shall also assume that the QDC supports only two eigenfunctions: first symmetric and first antisymmetric modes [2], with nearly equal wave numbers k_z^s and k_z^a along the z-direction. Therefore the envelope of the electron wavefunction Ψ can be described as [2]

$$\Psi = \psi^s exp(-jk_z^s z) + \psi^a exp(-jk_z^a z) = \psi exp(-jk_z^s), \tag{1}$$

where ψ^s and ψ^a are z-independent wave functions, corresponding to the lowest symmetric and asymmetric modes, and $\psi = \psi^s + \psi^a exp[-j(k_z^a - k_z^s)z]$. If $k_z^a \approx k_z^s = k_z$ then ψ varies slow along the z-axis. Using this property of ψ we can use a *paraxial* approximation, $\mid k_z^2 \mid \gg \mid \partial^2\psi/\partial z^2 \mid$, to simplify Schrodinger's equation. In this study we shall assume that the electrons in the quantum wells are fully confined in the y-direction. Therefore it is sufficient to solve Schodinger's equation in 2D instead of in 3D. Substituting (1) into Schrodinger's equation, one can derive the following reduced equation for ψ [5]:

$$2jk_z\partial\psi/\partial z = [2m^*(E - E_c)/\hbar^2 - k_z^2]\psi + \partial^2\psi/\partial x^2. \tag{2}$$

Here m^* is the effective mass of electrons in $GaAs$, E is the electron energy, $E_c = -qV + E_g/2$ is the edge of the conduction band, V is the electrostatic potential, and E_g is the semiconductor bandgap.

3. Numerical method

The simulation method is as follows:

1. For given gate voltages and semiconductor layer parameters we solve Poisson's equation

$$\nabla \cdot (\epsilon_s\epsilon_0\nabla V) = -q(p - n + N_d^+ - N_a^-), \tag{3}$$

where the hole and electron concentrations p and n are calculated using a constant Fermi level approximation. This equation is solved for the "classical" case, where we neglect electrons in the localized states. After linearization and discretization on a non-uniform rectangular grid, we solve a system of linear algebraic equations with a five-diagonal symmetric matrix using the Incomplete Cholesky-Conjugate Gradient method.

2. For a given electron energy E and an initial electron wavefunction, we calculate k_z using the variational principle (as suggested in [6] for optical wave-guides):

$$k_z^2 = \frac{\int 2m^*(E - E_c)/\hbar^2 \mid \psi \mid^2 dx - \int \mid \partial\psi/\partial x \mid^2 dx}{\int \mid \psi \mid^2 dx}. \tag{4}$$

3. Next we solve (2) on the uniform x-grid, for one step in the z-direction starting from $z = 0$. We have compared several different first- and second-order integration methods, and have found that the Crank-Nicholson scheme gives the the best results.

4. If the contact geometry changes with z, we repeat steps 1-3 until we reach the end of the simulation region. For the particular QDC considered later, we need only repeat the third step.

All calculations were done on IBM PC AT/486 computer. The typical calculation time was 2 to 5 minutes for 40 × 70 spatial grid nodes in Poisson's equation, 200 nodes, and 100 to 200 z-steps in Schrodinger's equation.

4. Results and discussion

A QDC structure similar to the one investigated in [3] is considered in our simulation (see Fig. 1). The Schottky barrier height is 1.0 eV, and the lattice temperature T = 4.2 K. The length of the structure is 100 nm, which can be regarded as a reasonable value for ballistic electron motion length for such temperature [2]. A low voltage $V_{G1} = V_{G5} = 0.2$ V is applied to the gates G1 and G5, creating deep space charge regions which prevent electrons from moving out of the simulation region. A high voltage $V_{G2} = V_{G4} = 0.75$ V is applied to the gates G2 and G4, creating two quantum wires underneath them. The potential on gate G3 is varied to control the barrier height and the distance between these wires. To estimate the currents flowing in the wires we calculate the quantity $k_z \int \psi\psi^* dx$, where the integral is taken over the left or right sides with respect to the QDC centerline.

The initial $\psi(x)$ distribution simulates the injection of electrons into the left wire. From Fig. 2 we see that changing V_{G3} from 0 to 0.3 V can easily change the potential barrier between the wires from quite a large value to almost zero. This results in a different transmission probability, and in turn changes the length required for electrons to penetrate from the left wire to the right one (see Fig. 3). Calculating the currents for the given QDC dimension in z-direction for different V_{G3} values, we obtain *current-voltage* characteristics (see Fig. 4). A few remarks about the method in general and these results are appropriate.

1. The *paraxial* approximation is not important for our method. In fact, one can derive an equation slightly more complicated than (2) using a *wide angle* approximation. However we have found that all these approximations give only small differences in the final results (at least for our particular device).

2. Calculations made in [1] show that the occupancy levels of highest eigenstates decrease drastically with decreasing temperature. Therefore we suppose that for very low temperatures, which are required to obtain the reasonable values of collision-free electron length, our method will be accurate.

3. The results of Fig. 3 and 4 depend on the chosen value of electron energy and initial $\psi(x)$ distribution, which have been chosen arbitrarily in the present study. Therefore one should be cautious about drawing specific conclusions from those figures, but rather consider them only as an illustration of the possibilities of the proposed simulation method.

4. Future QDC structures will be non-uniform in z-direction [2,3] as our investigated QDC is. Moreover, to account for impurity de-ionization, electron concentration on the localized states, and other Fermi level related effects, one should solve a three-dimensional Schrodinger's equation instead of the two-dimensional one (2). However with suitable modifications, our method can handle these changes, and we hope that it still will be faster than a standard approach [1-3].

References

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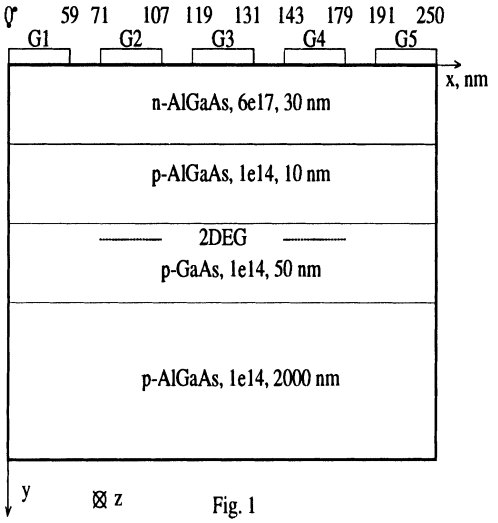

Fig. 1

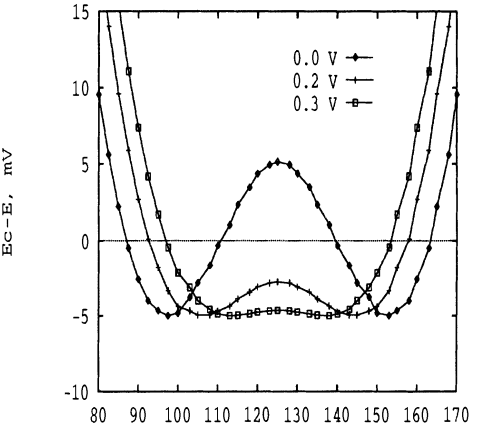

Fig. 2

Fig. 1. A cross-section of a quantum directional coupler. Lateral dimensions are in nanometers.

Fig. 2. $E_c - E$ distribution for y = 41 nm for various V_{G3} values.

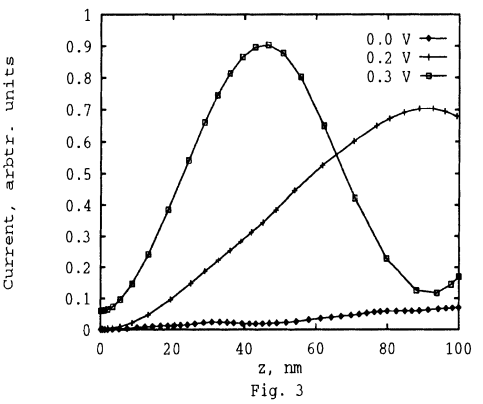

Fig. 3

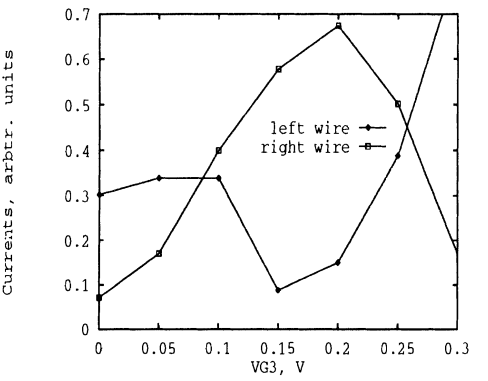

Fig. 4

Fig. 3. Right wire current dependence on z-distance for various V_{G3} values.

Fig. 4. Dependence of the output currents in the right and left wires on V_{G3}.