Two-Dimensional Simulation of Negative Resistance Effects Using Quantum Moment Equations

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The need for adequate simulations of quantum transport in semiconductor heterostructures has become more and more important as new advances in processing techniques have permitted the fabrication of devices that are expected to be controlled by quantum phenomena. Here we use a model based on the quantum moment equations derived from the Wigner distribution function to simulate a double barrier structure in two dimensions. The expected negative resistance effect is clearly seen in the current vs voltage characteristics of the device at 300 K. Other information, such as the electron concentration, can also be obtained with this method.

1. Introduction

In recent years, the great improvement in material quality and processing techniques (particularly heteroepitaxial technology) has permitted the fabrication of semiconductor structures and devices so small that their size is indeed comparable to the coherence length of the electrons. Since the operation of these devices is expected to be dominated by quantum interference effects, a precise simulation of quantum transport is very important. Several methods have been used to improve the classical Boltzmann transport equation, which is no longer valid for ultra-submicron sizes. For example, negative resistance effects in resonant tunneling devices have been successfully simulated in one dimension using the Wigner distribution function [1], but this method is not expected to be suitable for multidimentional device simulation since it is very demanding in terms of memory storage and computation time. As an alternative, quantum moment equations derived from the Wigner function [2] have been employed to simulate ultra-small GaAs MESFET's [3]. In this communication we present a multidimensional simulation of negative resistance effects using quantum moment equations. To our knowledge, this is the first time such a result has been reported.

2. Calculation Method and Results

The Wigner distribution function can be defined by

$$P_W(x,p,t)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dy\,\psi^*(x+y/2)\psi(x-y/2)e^{ipy/\hbar}, \quad (1)$$

where x is the space coordinate, p is the momentum coordinate, and $\psi(x)$ represents the state of the system. Assuming that $\psi(x)$ satisfies the Schrödinger equation for a system with Hamiltonian $H=p^2/2m+V(x)$, the Wigner distribution function satisfies the time evolution equation

$$\frac{\partial P_W}{\partial t}+\frac{p}{m}\frac{\partial P_W}{\partial x}+\theta\cdot P_W=0, \quad (2)$$

where

$$\theta\cdot P_W=-\frac{2}{\hbar}\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)!}\left(\frac{\hbar}{2}\right)^{2n+1}\frac{\partial^{2n+1}V(x)}{\partial x^{2n+1}}\cdot\frac{\partial^{2n+1}P_W}{\partial p^{2n+1}}. \quad (3)$$

A Wigner-Boltzmann transport equation can be obtained [2] by adding to Eq. (2) a collision term expressing phenomena not included in the classical Boltzmann equation.

$$\frac{\partial P_W}{\partial t}+\frac{p}{m}\frac{\partial P_W}{\partial x}+\theta\cdot P_W=\left(\frac{\partial P_W}{\partial t}\right)_{coll.} \quad (4)$$

Multiplication of Eq. (4) by an appropriate function of momentum (p^0, p, $p^2/2m$, ...) and integration over all momenta result in the moment equations. The first three moments are of particular importance because they represent the density, momentum and energy, respectively, of a physical system. For a wavefunction of the form $\psi(x,t)=A(x,t)\exp(iS(x,t)/\hbar)$, we have:

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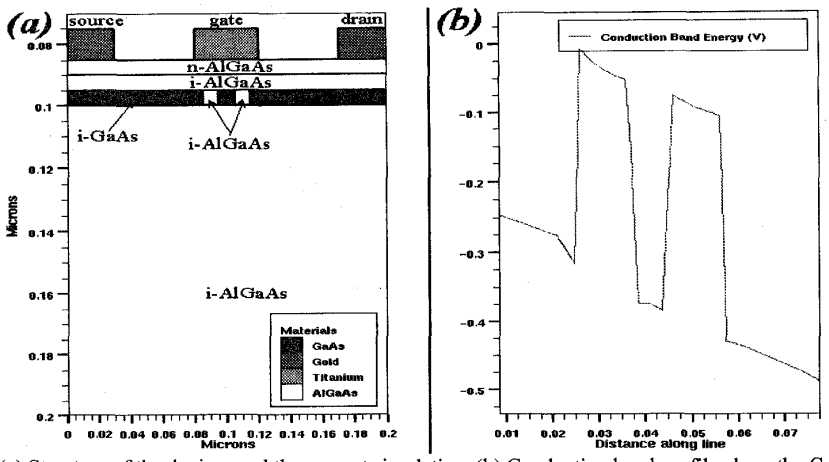

Fig. 1.- (a) Structure of the device used the present simulation. (b) Conduction band profile along the GaAs channel.

$$\langle p^0 \rangle = \rho(x,t), \tag{5}$$

$$\langle p^1 \rangle = mv\rho, \tag{6}$$

$$\langle p^2 \rangle = (mv)^2 \rho - \frac{\hbar^2}{4} \rho \frac{\partial^2}{\partial x^2} \ln \rho, \tag{7}$$

where $\rho(x,t)$ is the probability density. The quantum corrections appear in the terms containing an explicit dependence on $\hbar$. When $\hbar$=0, Eqs. (5)-(7) become the classical moment equations.

Using these moments, the quantum corrections can be explicitly incorporated in an energy representation as

$$E = \frac{1}{2} m^* v^2 + \frac{3}{2} k_B T + U_q, \tag{8}$$

where m^* is the electron effective mass, v is the electron velocity, T is the electron effective temperature, and the quantum potential U_q is given by

$$U_q = -\frac{\hbar^2}{8m^*} \nabla^2 \ln(n). \tag{9}$$

Since the quantum potential is proportional to the second-order gradient of the carrier concentration log, the effect of the quantum correction will be to smooth the carrier concentration, especially when sharp changes take place.

We have used ATLAS, a commercial device simulator software from Silvaco International that incorporates this quantum moment approach. Since initial solutions with this model can be difficult, a damping factor is included to allow for gradually increasing the level of quantum moments applied to the solution until the full amount is included. This also includes a projection and trapping method for aid in reaching convergence. Our research group and Silvaco have been in contact for some time to try to develop a comprehensive tool for the study of quantum transport in semiconductor heterostructures.

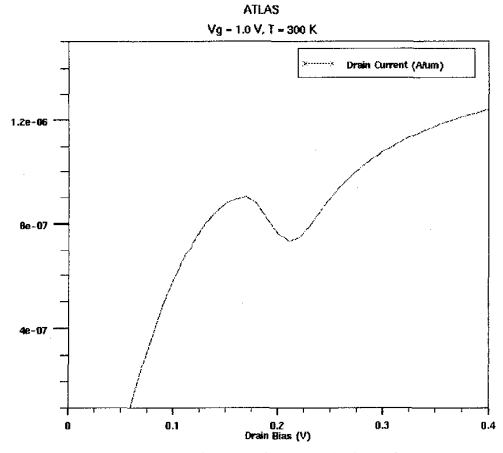

Fig. 2.- Current vs voltage characteristics for the device at a temperature of 300 K.

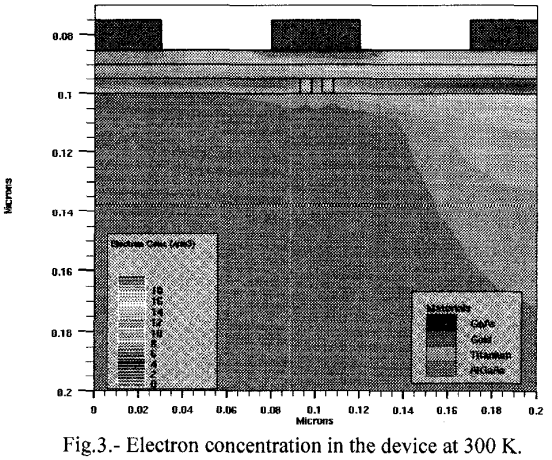

Fig.3.- Electron concentration in the device at 300 K.

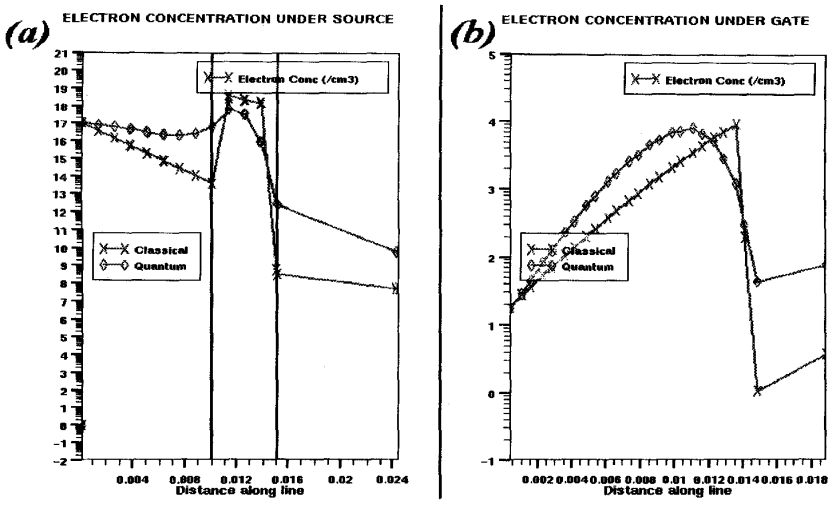

Fig.4.- Electron concentration under source (a) and gate (b) of the device, showing the smoothing effect caused by quantum corrections.

In this simulation we have used the HEMT-like structure shown in Fig. 1. The top n-$Al_{0.3}Ga_{0.7}As$ layer has a doping concentration n = 1×10^{17} cm^{-3}, while the background doping concentration is p = 1×10^{14} cm^{-3}. The double barrier region consists of a 5-nm-wide quantum well of GaAs bounded by identical 5-nm-wide barrier layers of $Al_{0.3}Ga_{0.7}As$. The number of points in the mesh employed to discretize the problem was around 700. A temperature of 300 K was assumed in the simulation.

The I-V characteristics of the device are calculated by applying an incremental bias voltage to the gate and then sweeping for a given range of drain voltages. Figure 2 shows an example of the simulated I-V characteristics at 300 K. The region of negative resistance is clearly seen for a drain voltage around 0.2 V. Similar results were obtained for other temperatures.

Besides the I-V curves, other information can be obtained with this simulation technique using quantum moment equations. This includes carrier concentration, electric field and current density in the device, among others. As an example, Fig. 3 shows a two-dimensional map of the electron concentration in the structure. One-dimensional cuts under source and gate are shown in Fig. 4, where the smoothing of the carrier concentration caused by the quantum corrections is clearly seen.

3. Conclusion

We have performed a two-dimensional simulation of a double barrier structure in the size range of a few nanometers, where quantum effects are expected to be dominant. The simulation model is based on the quantum moment equations derived from the Wigner distribution function. The results show that the quantum corrections introduced in the model do give the expected effects. In particular, a region with negative resistance was clearly observed in the current vs voltage characteristics of the device used in this simulation.

Acknowledgements

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