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Elastic Scattering and Depletion Effects on Current-Voltage Characteristics of Gated Resonant Tunneling Diodes

Chomsik Lee

Hyundai Semiconductor R&D LAB 2
Ichon-kun, Kyoungki-do, Korea 467-860

Numerical solutions to the two-dimensional Poisson's equation and the continuity equation have been used to calculate the lateral depletion region and carrier concentrations by the finite difference method. Simulation of the GRTD using a self-consistent quantum model shows depletion effects on current-voltage characteristics. In the bias conditions whereby the GRTD reaches zero-dimension in the well region, we consider elastic scattering mechanisms and the presence of evanescent modes to calculate resonant tunneling transmission coefficients. We present the effects of subband mixing and elastic scattering in a two-dimensional simulation of the current-voltage characteristics of the GRTD. The effect of this scattering results in shifting and broadening the tunneling probability, and reducing its peak value.

1. INTRODUCTION

There are a number of papers in the literature dealing with the calculation of the transmission probabilities and current-voltage charact ristics in heterostructure systems. Mukherji and Nag[1] attempted to include nonparabolicity of the band structure in the calculation of the transmission probability. A self-consistent numerical solution of the Poisson and Schrödinger equations was made by Vassell *et al.*[2] in a one-dimensional model of the RTD. Frensley[3] studied that the potential and density of the resonant tunneling diode by the self-consistent Wigner function. Lent[4] has considered edge state currents in a circular dot in a magnetic field. One of the central questions concerning carrier transport in quantum tunneling devices is to determine what affects the tunneling transmission coefficient and the eigenenergy levels in a confined geometry. In addition, one of the active research questions is why the theoretical results of the peak-to-valley current ratio of the negative-differential-resistance (NDR) features are larger than experimental results. Although double-barrier resonant tunneling has received considerable attention in recent years, there has been very little research into two or three-dimensional heterostructures. Reed *et al.*[5] experimentally investigated electronic transport through a three-dimensional confined quantum dot. Bryant has studied the effects of subband mixing in harmonic-oscillator states at 0 K temperature in a two-terminal device structure[6]. Bagwell introduced evanescent modes in quasi-one-dimensional wires[7].

The purpose of this work is to study the resonant tunneling and current-voltage characteristics in two-dimensional models of the gated resonant tunneling diode(GRTD)[8]. Such a device involves the integration of a double-barrier tunnel structure with a field-effect transistor in which the electrical size of the channel within the vertical resonant tunneling diode (RTD) is directly controlled by a simple, self-aligned rectifying electrode in the low-doped GaAs material. The GRTD consists of the following: the molecular-beam epitaxially grown layers 200Å of GaAs (Si doped and graded from $2 \times 10^{18} cm^{-3}$ to $10^{16} cm^{-3}$) on n^+ - GaAs substrate, 50Å undoped GaAs spacer layer, 50Å undoped $Al_{.3}Ga_{.7}As$ barrier, 50Å undoped GaAs well layer, 50Å undoped $Al_{.3}Ga_{.7}As$ barrier, 50Å undoped GaAs spacer layer, 200Å of GaAs (Si doped and graded from $2 \times 10^{18} cm^{-3}$ to $10^{16} cm^{-3}$), followed by a 0.5 μm - GaAs surface layer (n^+). The ohmic contact of the emitter was used as a shadow mask for nonconformal deposition of chromium on the etched MBE surface. Details of the fabrication of such a device have been previously reported[9]. The gate was placed the low-doping concentration region (lower than $10^{17} cm^{-3}$) to ensure a large depletion region. The most important new feature of the method proposed here is its use of the exact solution of the Schrödinger equation with four open channels. It also uses a very compact, and so numerically efficient, version of the scattering transfer matrix.

2. THEORY AND METHOD

The application of a potential difference across the gate and the common-emitter will cause lateral depletion, and this leads to a reduced cross-section for electron transport. It is demonstrated that three-dimensional confinement of carriers with a gate potential is feasible. A two-dimensional method for the solution of the classical transport equation has been obtained with a nonuniformly doped three-terminal diode(GRTD). Finite difference methods(FDM) were used to calculate electrostatic potential (Ψ), quasi-Fermi level for electrons (ϕ), doping concentration(N_d), and electron concentration (n). In the numerical analysis, the emitter and collector are described as a ohmic contacts. An assumption is made that the average electron velocity is dependent on the local electric field.

We have solved the two-dimensional Poisson equation[10]

$$\nabla^2 \Psi(x,z) = e(N_d - n)/\epsilon(x,z),$$

and continuity equation which includes a generation - recombination term

$$\nabla \cdot J(x,z) = R_g.$$

More detailed boundary condition of each interface for FDM have been published in Ref.[9]. The full explanations have been published in Ref.[11]. In our model, the transmission probability can be calculate by a transfer-matrix formalism. First, we solve the two-dimensional Poisson equation and the continuity equation to find the depletion region and initial condition of the conduction band structure. This provides a reasonably good description of the electronic band structure. Following this, we solve the Schrödinger and Poisson equations over a smaller region of interest. There will be finite number of evanescent modes existing if any quasi-bound states are present above the Fermi energy.

The Schrödinger equation for a structure having effective mass differences in the z direction is where the confinement potential V_t is dependes only on the transverse direction (x) and V_{sc} is the potential of any defects or impurities, V_l is the applied bias, m^* effective mass, E total energy, and ψ is electron wave function. For each position z along the device, we can write the dependence of the wave function along x as a sum over a set of coefficients $\phi_n(z)$. The complete set of eigenfunctions is given by

$$\psi(x,z) = \sum_{n=1}^{M} \phi_n(x)\phi_n(z).$$

Now consider the wave function of $\phi(z)$, the wave equation with the potential discontinuity (V_{sc}) is given by where M is the total number of modes and wave vector k_n is

$$k_n^2 = \frac{2m^*}{\hbar^2}[E - \Xi_x - V_l(z)]$$

and

$$\Omega_{nm} = \frac{2m^*}{\hbar^2}\int \phi_n^*(x)V_{sc}\phi_m(x)dx, \qquad (1)$$

where the scattering potential is given by $V_{sc} = \beta\delta(z)\delta(x - x_j)$, Ω_{nm} are mode coupling constants, and β is the coupling strength. The matching conditions of longitudinal direction (z) in the equal lateral confinement region are

$$\phi_j(z) = \phi_{j+1}(z), \qquad (2)$$

and

$$\frac{1}{m_j}\frac{d\phi_j^n(z)}{dz} = \frac{1}{m_{j+1}}\frac{d\phi_{j+1}^n(z)}{dz} + \sum_{n=1}^{M}\Omega_{nm}\phi_m(z). \qquad (3)$$

After we normalized the coefficient of the incident electron wave function to 1, the equation can be reduced where T transmission coefficient in region n, R reflection coefficient in region 1, and M_{tot} is given by the matrix product. $M_{tot} = C_x' M_z$, C_x' can be calculated by lateral boundary condition. For one propagating wave function, the matrix M_z is

$$M_z = \frac{1}{2}\begin{pmatrix} 1 & 1/ik_{n1} \\ 1 & -1/ik_{n1} \end{pmatrix} T_m(L,0) \begin{pmatrix} 1 & 1 \\ ik_{01} & -ik_{01} \end{pmatrix}, \qquad (4)$$

where

$T_m(L,0) = [M(L)\cdot M^{-1}(L-1)\cdot M_{sc}^{-1}(j)M(j)\cdots M^{-1}(0)]$, T_m is the resultant of the product of the transfer matrices coupling the first region to the end of the region. M_{sc} is the transfer matrix by V_{sc}. $k_{0l}^2 = 2m^*(E - E_{xl})/\hbar^2, k_{jl}^2 = 2m^*((E - E_{xl}) + eV(z_j))/\hbar^2$, l is integer.

The wave function has a plane-wave form in the well region, and is an exponentially-decaying wave in the barriers. It is now possible to find the scattering transfer matrix using the matching conditions of $\phi(z)$. If there is one V_{sc} at the region j, then

$$\begin{aligned} M_{sc}^{-1}(j)M(j) &= M^{-1}(j)M(j)M_{sc}^{-1}(j)M(j) \\ &= M^{-1}(j)S_jM(j). \end{aligned}$$

A detailed derivation has been published Ref [11]. After using the scattering matrix S_j, we can reduce the number of the transfer matrices and cancel complex number i in matrix calculation.

In the case of one propagating mode and one evanescent mode ($E_{x1} < E < E_{x2}$), since one subband is occupied in the emitter region, then the scattering matrix S_j (2x2) is where $\kappa_{jl}(z_j) = -ik_{jl}(z_j)$. If $V_{sc} = 0$, then S_j is unit matrix.

In the case of two propagating modes when two subbands are occupied in the emitter region and one evanescent mode ($E_{x2} < E < E_{x3}$), the transfer matrix is in Ref [11].

The scattering matrix S_j for two propagating modes is

$$S_j = \begin{pmatrix} 1 & 0 & 0 & 0 \\ \Omega_{11} + \alpha\Omega_{31} & 1 & \Omega_{12} + \alpha\Omega_{32} & 0 \\ 0 & 0 & 1 & 0 \\ \Omega_{21} + \alpha_1\Omega_{31} & 0 & \Omega_{22} + \alpha_1\Omega_{32} & 1 \end{pmatrix}$$

where $\alpha = -\Omega_{13}/(2\kappa_{j3} + \Omega_{33}), \alpha_1 = -\Omega_{23}/(2\kappa_{j3} + \Omega_{33})$. The S_j is also unit matrix if $V_{sc} = 0$.

The current through the device is then calculated by integrating the charge density times the tunneling probability and the carrier group velocity $v_g(E)$. If an external bias V_l is applied to the barrier, the net current flowing through it is the difference between the current from left to right and that from right to left. Generally, the current density J may be computed as the average of the product of the transmission coefficient and the group velocity:

$$J = \frac{e}{\pi\hbar}\sum_i \int_{Ec}^{\infty} T(E)[f(E) - f(E + eV_l)]dE,$$

where 0D is in the well region, $f(E)$ is the Fermi-Dirac distribution, the summation being done over occupied emitter subbands. The calculation is repeated the full applied voltage range and the current density as a function of applied bias.

3. DISCUSSION OF COMPUTATIONAL RESULTS

Tunneling current of the GRTD with a double-barrier structure is studied at low temperatures. If the gate area is on 2 x $10^{18}cm^{-3}$ area, the depletion width is about 220 Å (abrupt junction). The position of the depletion edge will be pinned by the heavily doped layer. If the gate is on $10^{16}cm^{-3}$ doping channel area, the depletion width is about 3800 Å with low gate bias. The depletion is greatest where the doping density is lowest, which is in the layers adjacent to the resonant tunneling barriers and well. Therefore, the width of the conducting channel between source and drain is expected to be a minimum at the undoped well. Evanescent modes are existed in the GRTD when the channel is strongly quantized. The number of evanescent modes, as well as band levels, are changed in each region as the lateral confinement is varied with the application of gate bias. In a confined geometry, such as the GRTD, the presence of evanescent modes affect the scattering boundary conditions.

We assume there are three different lateral confinement region, such as collector, emitter, and well area. In our calculations, the heights of the barriers are V=0.65(1.247x), their width 50Å, and their separation is 50Å, the gate-to-gate space is L=3600Å, and the mole fraction of Al x=0.3. The mass of

the electron is taken to be (0.067 +0.083x)m_0 in the barrier and 0.067m_0 outside of it. We have found that the transmission coefficient is changed by the location of scattering potential and the number of defect points. At the strong coupling strength with two attractive scattering potentials in the well, the peak positions are split into two ones in Fig. 1. The double barrier structure is no longer symmetry at the bias V_l=0.06 V, so the resonant tunneling probabilities are not one. If defects only exist outside of the well region, elastic scattering effects are very low on I-V curve. Because of multipeak, the valley current is increased, compared to no evanescent mode effect. When the incident electron energy aligns with the subbands of lateral confinement (E≈ E_x), the probability of occupying the evanescent mode increases. We find that scattering is enhanced if the scattering strength increased, but over all current is reduced.

The Fig. 2 shows evidence of subband mixing in the case in which one or more subbands are occupied in the emitter. At low bias(V_l), the subband is higher than the electron energy, there is no current flow. As the applied bias voltage is increased, the current starts to flow at V_{ce}=0.2 V and the number of bound states are added to one , two, or three. When the reverse gate bias(V_g) is increased from -1.2 to -1.26 V in Fig. 2, the current density is reduced at fixed V_{ce} =0.33 V. However, the peak current (I_{ce}) at V_g=-1.23 V is higher than at $V_g = -1.2$ V in fixed bias V_{ce} =0.37 V, which indicates negative transconductance. There is always a continuum of states which can mixed by other interactions. Figure 2 clearly illustrates the resonance peak shift in energy as a function of the gate bias. It is important to notice that the resonance peak shift monotonically in energy from 0.001 to 0.02 eV in going from no V_{sc} to increasing scattering potential. The current-voltage characteristic obtained for the above does not necessarily match the experimental da a precisely since we consider some limited cases.

4. CONCLUSION

We have analyzed depletion effects on current-voltage curve with scattering potential and without it. The presence evanescent modes leads to changes the scattering matrices and thus, the transmission coefficient is changed dramatically in the presence of a strong scattering potential. The scattering destroys the coherence of the wave function, so that the peak current from resonances are reduced. The valley current results from an anti-resonance, so the current off-resonance is increased. As the gate bias increases, the emitter region shows strong quantization. This quantization causes the resonant transmission peak to shift to higher bias in the current-voltage characteristics. Fine structure is observed because the density of states is discrete and thus the band mixing is significant in the I-V characteristics.

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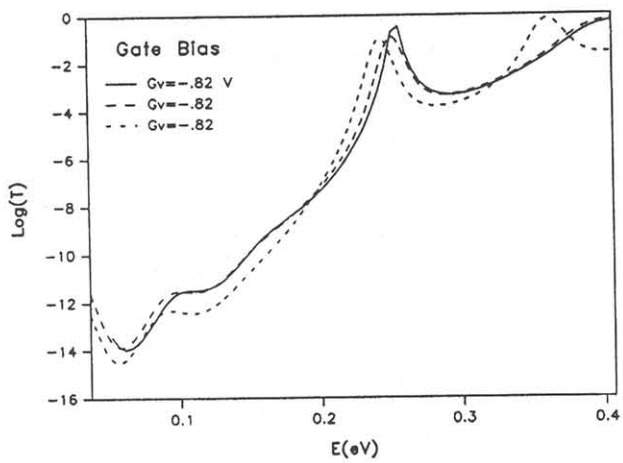

Fig. 1 Logarithmic plots of transmission probabilities as a function of electron energy at 77 K, $\beta_1 = 50$(solid line), $\beta_2 = -50$(dashed line), $\beta_3 = 0.5$(dot line) $feV \cdot cm^2$, one subband is occupied in the emitter region at V_l=0.06 V, localized 4 scattering potentials in the well.

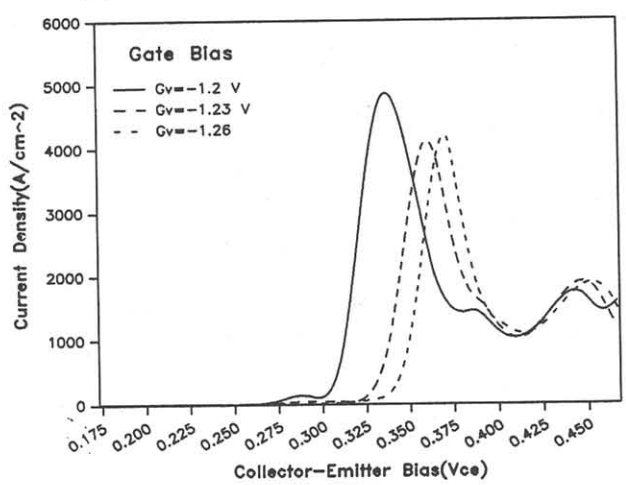

Fig. 2 Current-Voltage characterics at 77 K, $\beta = 1.5$ $feV \cdot cm^2$, gate bias=-1.2 V(solid line), -1.23(dashed line), -1.26(dot line). As increasing applied bias, occupied subbands in the emitter region are added. There is negative transconductance.