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Wigner Function Model of Nonlinear Quantum Transport in a Split-Gate Electron Waveguide

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The nonlinear quantum transport in a split-gate electron waveguide is simulated by using the Wigner function model. First, the effects of the impurity scatterings on the quantized conductance of the electron waveguide are studied. The decrease of conductance and the deterioration of quantized steps due to the impurity scatterings are investigated. After that, the nonlinear conductance at the large bias voltage and the possibility of the transistor operation of the electron waveguide are discussed.

1.INTRODUCTION

An electron waveguide is a quantum wire that is so clean and so small that electron waves can propagate in guided modes. It is now possible to make it using molecular beam epitaxy in conjunction with high resolution electron beam lithography. The two terminal electrical conductance of an electron waveguide is quantized as a function of the width.[1)] Recently, we have succeeded in formulating the Wigner function model, which has been a promising tool for quantum transport modeling of quantum well electronic and optical devices,[2,3)] to simulate the quantum transport in the electron waveguide for the first time, and its static and dynamic behavior was examined in the linear ballistic transport regime.[4)] In this paper, the effects of the impurity scattering on the quantized conductance of an electron waveguide are studied first in the linear transport regime. Next, we will present the quantum mechanical simulation on the nonlinear quantum transport of the electron waveguide.

2.SPLIT-GATE ELECTRON WAVEGUIDE

In an electron waveguide with the split-gate HEMT structure, electron waves are confined by applying the negative bias voltage to the gate electrodes. As a result, the one-dimensional(1D) constriction of the electron waveguide gradually widens to embrace the two-dimensional(2D) contact as shown in Fig. 1 (a). In this paper, we assume that the gradual taper from the 2D contact to the 1D constriction is ideal, so that mode conversions and reflections at the interfaces are negligible. To model such an ideal 2D contact, the reservoirs are assumed to be attached to the 1D constriction as shown in Fig. 1 (b). For the infinite-confining potential in the transverse y and z directions, the following one-dimensional Liouville equation for the Wigner function is solved in the electron waveguide.[4)]

$$\frac{\partial F_n}{\partial t} = -\frac{\hbar k_x}{m^*}\frac{\partial F_n}{\partial x} - \frac{1}{\hbar}\int_{-\infty}^{\infty}\frac{dk'_x}{2\pi}V(x,k_x-k'_x)F_n - \frac{1}{<\tau_n(k_x)>}\left[F_n - F_n^0\int_{-\infty}^{\infty}dk'_xF_n\right] \quad (1)$$

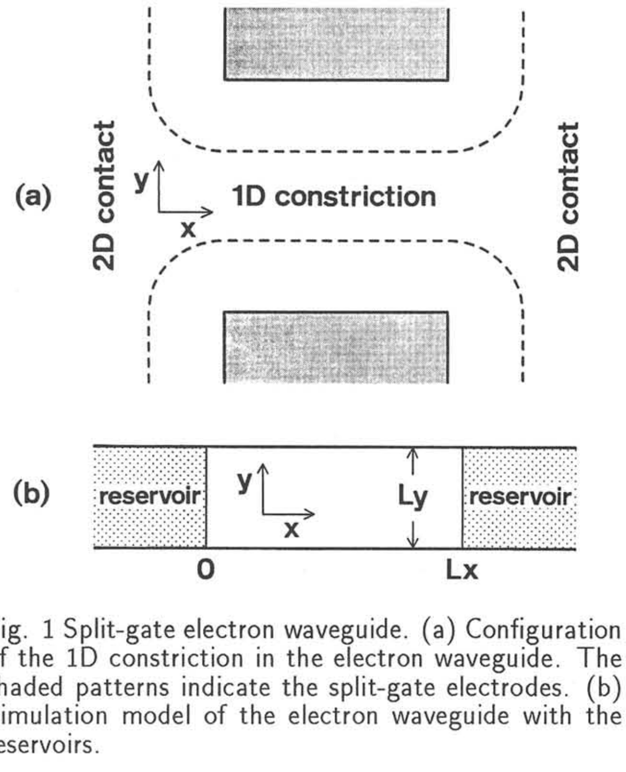

Fig. 1 Split-gate electron waveguide. (a) Configuration of the 1D constriction in the electron waveguide. The shaded patterns indicate the split-gate electrodes. (b) Simulation model of the electron waveguide with the reservoirs.

where F_n is the Wigner function integrated over the transverse momenta and coordinates for the n - th mode. F_n^0 is the normalized distribution function in thermal equilibrium and $< \tau_n(k_x) >$ is the relaxation time for the n-th mode electron. When the quantized conductance of the electron waveguide is discussed at low temperature, only the impurity scattering is taken into consideration in the formulation of $\tau_n(k_x)$.

For an electron waveguide with the dimensions of L_x, L_y, and L_z, the boundary conditions for the n-th mode Wigner function at the left and the right boundaries are given by

$$F_n(0, k_x) = 2f_{FD}(k_x, k_y^n, k_z^1) \quad , \quad k_x > 0 \tag{2}$$

$$F_n(L_x, k_x) = 2f_{FD}(k_x, k_y^n, k_z^1) \quad , \quad k_x < 0 \tag{3}$$

where f_{FD} is the Fermi-Dirac distribution function characterized by the Fermi level E_f, the temperature T. k_y^n and k_z^1 are the quantized wavenumbers in the y and z directions, respectively. The Liouville equation (1) is solved numerically based upon the finite-difference method as discussed in Ref. 4.

3.QUANTIZED CONDUCTANCE OF AN ELECTRON WAVEGUIDE

First, the two-terminal conductance of an electron waveguide with the impurities is calculated. The ionized impurities are assumed to be 15nm away outside from the center of the waveguide bottom and distributed straight in the transmission direction. The depth of the waveguide L_z is 30nm. The Fermi energy E_f is 10meV and the temperature T is assumed to be 0K. The applied bias voltage V is given as 50μV, so that the electron waveguide operates in the linear transport regime. Fig. 2 (a) shows the calculated two-terminal conductances of the electron waveguide as a function of the width. The impurity density N_D is given as $10^5\mathrm{cm}^{-1}$, $10^6\mathrm{cm}^{-1}$ and $4 \times 10^6\mathrm{cm}^{-1}$. The dotted line indicates the ideal quantized steps without any scatterings. The decrease of conductance and the deterioration of quantized steps due to the impurity scatterings are found to become more conspicuous as the impurity density increases. When N_D is more than $10^6\mathrm{cm}^{-1}$, the steps of quantization disappear due to the strong impurity scatterings. Next, we compare our quantum transport model with the classical transport model represented by using the electron mobility. In the classical model, the conductance is obtained by the following equation.

$$I = \sum_n \frac{N_n e \mu_n}{L_x} V, \tag{4}$$

where μ_n is the electron mobility estimated by the relaxation time due to the impurity scatterings and N_n is the one-dimensional electron density. The conductances calculated by the equation (4) are shown in Fig. 2(b). In the classical model, the conductance takes an extremely high value for the small impurity density because the electron mobility becomes very large. On the contrary, in the Wigner function model shown in Fig. 2 (a), the conductance is limited to its quantized value. As the impurity density increases,

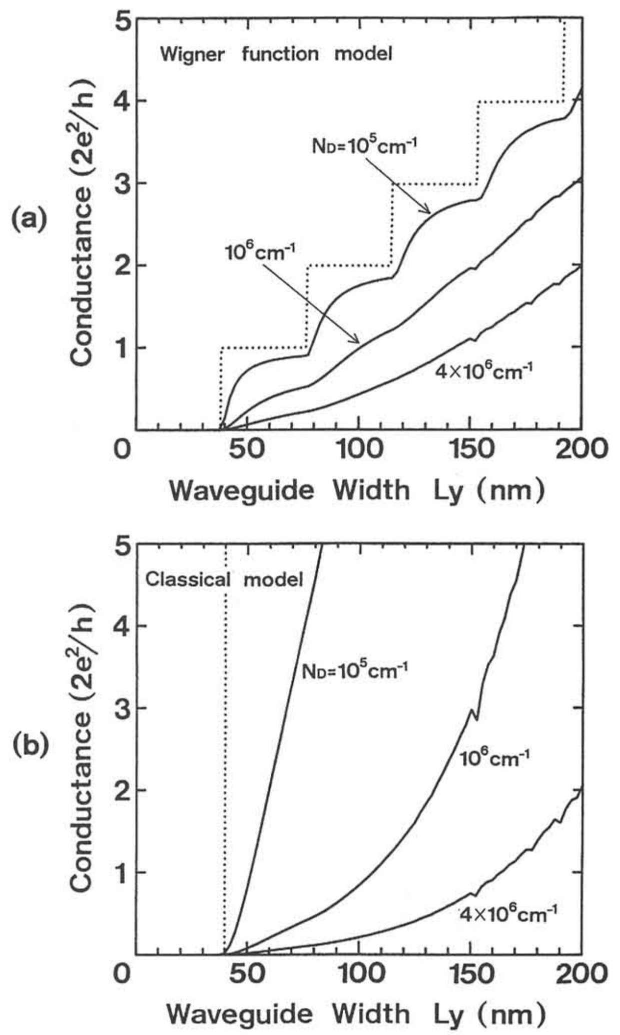

Fig. 2 Comparison between the Wigner function model and the classical model. Conductances are calculated by (a)the Wigner function model and (b)the classical model for the impurity densities of $10^5\mathrm{cm}^{-1}$, $10^6\mathrm{cm}^{-1}$ and $4 \times 10^6\mathrm{cm}^{-1}$.

the conductance decreases in both models. It should be noted that in case of $N_D = 4 \times 10^6\mathrm{cm}^{-1}$, the two models give almost the same conductance. The dips in conductance are seen for the waveguide wider than 150nm, that will occur when electrons in the lower modes are coupled strongly to the higher mode traveling backward.

4.NONLINEAR QUANTUM TRANSPORT OF AN ELECTRON WAVEGUIDE

We further examine the nonlinear quantum transport of the electron waveguides at the large bias voltage. First, the current-voltage characteristics of the waveguide in Fig. 3(a) are simulated at 0K. In Fig. 3(a), the ionized impurities are assumed to be distributed two-dimensionally in the plane parallel to the waveguide layer. The impurity density is given as $2.8 \times 10^{11}\mathrm{cm}^{-2}$ and the distance between the waveguide and the impurity layer z_0 is 100nm. Fig. 3(b) shows the I-V curves for various waveguide widths, where L_y is varied around the first step in Fig. 3(a). 44nm corresponds to the rising of the first step, 60nm

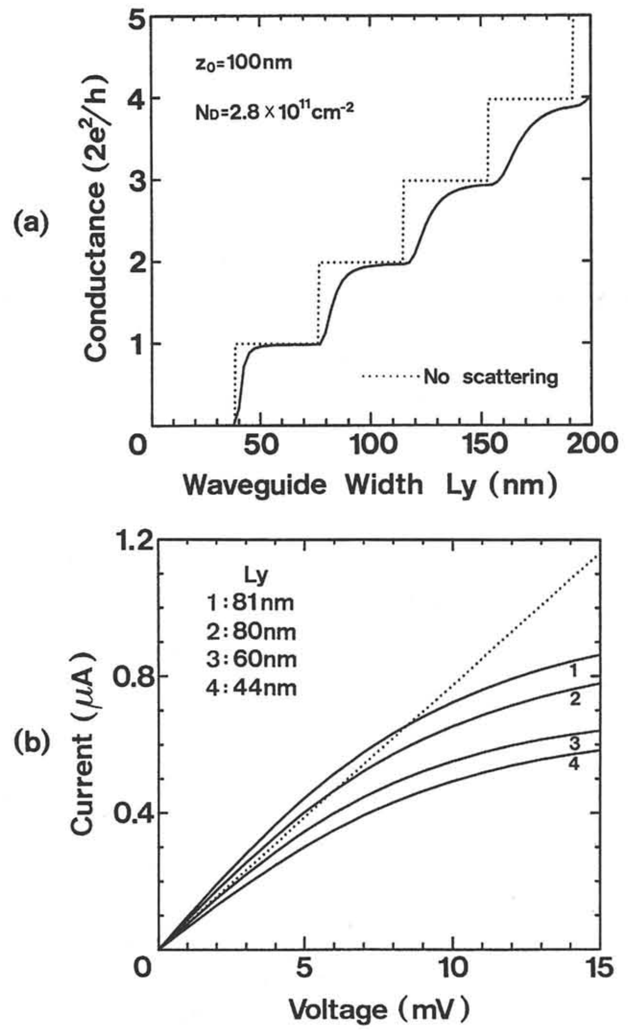

Fig. 3 (a)Calculated conductance of the electron waveguide with the two-dimensional impurity layer. (b) Calculated current-voltage characteristics of the electron waveguide at 0K for various waveguide widths. The dotted line indicates the relation of $I = (2e^2/h)V$.

the center of the first plateau, and 80 and 81nm the onset of the second step. The dotted straight line indicates the relation of the perfect quantization of conductance given by $I = (2e^2/h)V$. Even for 60nm as well as other width, the I-V curves are found to deviate from the dotted line as the applied voltage increases. This is due to the fact that the electron waves are reflected more by the potential variation in the constriction as the bias voltage becomes large. Such a nonlinear behavior has been reported experimentally in the quantum point contact structure.[5)]

Next, we will discuss the possibility of the transistor operation of the electron waveguide at room temperature. To include the various scattering processes in addition to the impurity scatterings at room temperature, 0.1ps of the relaxation time is assumed simply for all waveguide widths. Fig. 4 shows the calculated current-voltage characteristics of the electron waveguide at room temperature for various waveguide widths. At a small applied voltage, the current flows in proportion to the bias voltage. However, due to the balance of acceleration and reflection of electron wave caused by the electric field, the current saturates at the high voltage. In addition, the saturation current is found to increase with the waveguide width L_y. This is because the amount of electrons propagating in the transmission direction increases with L_y due to the decrease of the quantized energy in the y direction according to $E_y^n = (n\hbar\pi)^2/(2m^* L_y^2)$. Such a FET-like transistor operation will be expected in the split-gate structure, since the waveguide width can be varied by the external gate voltage.

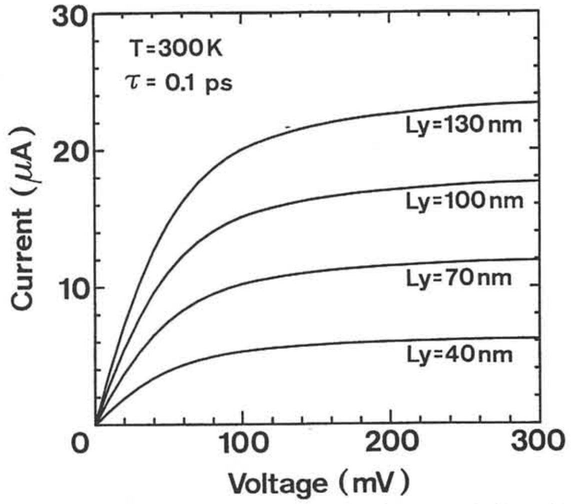

Fig. 4 Calculated current-voltage characteristics of the electron waveguide at room temperature for various waveguide widths.

5.CONCLUSION

The linear and nonlinear quantum transport in electron waveguides was studied by using the Wigner function model. In the linear transport regime, the decrease of conductance and the deterioration of quantized steps due to the impurity scatterings were discussed at low temperature. In the nonlinear transport regime, the nonlinear behavior of an electron waveguide was first simulated at low temperature. Further, the possibility of the transistor operation of an electron waveguide was demonstrated at room temperature.

In the Wigner function model described above, the lateral discontinuities at the contact electrodes in the split-gate structure, and the space charge effects in the waveguide are not included. Further study on these two problems will be necessary to analyze the practical waveguide devices.

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