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. 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, 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. 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.

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

![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.](image-url)
where $F_n$ is the Wigner function integrated over the transverse momenta and coordinates for the $n$-th mode. $F_{0n}^\theta$ is the normalized distribution function in thermal equilibrium and $\langle \tau_n(k_x) \rangle$ 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

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

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

where $f_{FD}$ is the Fermi-Dirac distribution function characterized by the Fermi level $E_F$, the temperature $T$. $k_y^0$ and $k_z^1$ are the quantized wavenumbers in the $y$ and $z$, 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 $10^5$cm$^{-1}$, $10^6$cm$^{-1}$ and $4 \times 10^6$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 $10^6$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.

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

where $\mu_n$ 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, the conductance decreases in both models. It should be noted that in case of $N_D = 4 \times 10^6$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 $2.8 \times 10^{10}$cm$^{-3}$ 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...
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 $E_y = (n\hbar \pi)^2/(2m^* L_y^2)$. 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.

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.

REFERENCES

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