Extended Abstracts of the 1994 International Conference on Solid State Devices and Materials, Yokohama, 1994, pp. 802-804 **PC-1-7**

# Electron Transport Modeling of Electron Waveguides in Nonlinear Transport Regime

H. Tsuchiya and T. Miyoshi

Department of Electrical and Electronics Engineering, Kobe University

Rokko-dai, Nada-ku, Kobe 657, Japan

The modeling of nonlinear quantum transport in electron waveguides is studied based on the Wigner function model. In particular, the phase-randomizing scatterings in contacts are carefully modeled in the quantum Liouville equation for the Wigner function by using the relaxation time approximation. Space-charge effects are also included by solving the Liouville equation and the Poisson's equation self-consistently. The current-voltage characteristics of electron waveguide is simulated at $T$ =0K. In the nonlinear transport regime, the space-charge significantly affects the current-voltage characteristics of the electron waveguide. Further, the possibility of the transistor operation of the electron waveguide is discussed at $T = 0$K.

## 1. INTRODUCTION

Recent advances in crystal growth and microfabrication technologies have allowed us to explore a new field of semiconductor device research. Instead of conventional devices described by the classical model, a variety of novel device concepts have been proposed based on the quantum mechanical features of carriers. As a preliminary modeling of quantum devices, the so-called transmission coefficient method has often been used because of its simplicity[1,2]. One major problem of this method is the fact that we have to assume the statistical distribution of carriers in advance. Thus, this model can be applied only to systems close to thermal equilibrium. On the other hand, the Wigner function model has been applied to the analysis of the transport problems including scattering effects and electron-electron interaction, and the dynamic properties[3-5]. The analogy between the two models is theoretically studied in the linear transport regime when the applied voltage is very small[6]. In this paper, the modeling of nonlinear quantum transport in quantum devices is studied based on the Wigner function model. In particular, the phase-randomizing scatterings in contacts are carefully modeled in the Liouville equation for the Wigner function by using the relaxation time approximation. Space-charge effects are also included by solving the Liouville equation for the Wigner function and the Poisson's equation self-consistently.

## 2.WIGNER FUNCTION MODEL FOR ONE-DIMENSIONAL ELECTRON WAVEGUIDE

### A. Quantum Liouville equation for Wigner function

As a simulation model, the one-dimensional electron waveguide with reservoirs as shown in Fig. 1 is considered, where the cross-sectional dimensions are $L_y$ and $L_z$. In the depth($z$) direction, only the fundamental mode is considered. For the infinite-confining

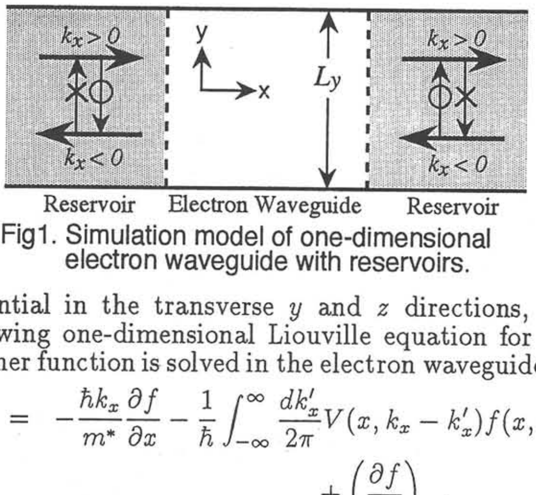


Fig1. Simulation model of one-dimensional electron waveguide with reservoirs.

potential in the transverse $y$ and $z$ directions, the following one-dimensional Liouville equation for the Wigner function is solved in the electron waveguide[3].

$$\frac{\partial f}{\partial t} = -\frac{\hbar k_x}{m^*}\frac{\partial f}{\partial x} - \frac{1}{\hbar}\int_{-\infty}^{\infty}\frac{dk_x'}{2\pi}V(x,k_x-k_x')f(x,k_x) + \left(\frac{\partial f}{\partial t}\right)_C, \quad (1)$$

where

$$V(x,k_x-k_x') = 2\int_0^{\infty} du_x\left[v\left(x+\frac{u_x}{2}\right) - v\left(x-\frac{u_x}{2}\right)\right] \times \sin[(k_x-k_x')u_x], \quad (2)$$

where $f(x,k_x)$ is the Wigner function integrated over the transverse momenta and coordinates. The scattering term $(\partial f/\partial t)_C$ is added phenomenologically to describe the phase-randomizing effects in reservoirs and the resistive effects in the waveguide.

The Liouville equation (1) is solved numerically based on the boundary conditions and the finite-difference method as discussed in Ref. 3.

### B. Modeling of reservoirs

Electron waves entering into a reservoir from a waveguide are phase-randomized in short time to reach the thermal equilibrium states. To describe such phase-randomizing scatterings in a reservoir phenomenologically, the following relaxation time approximation is introduced in our Wigner function model. Scattering process in reservoirs is schematically represented in Fig. 1. For simplicity, only the scattering process in the left reservoir is explained here.

When we assume that all left-going electron waves injected into the left reservoir from the device are absorbed without any reflection, the transitions from the left-going wave($k_x < 0$) to the right-going wave($k_x > 0$) can be neglected, and thus only the reverse coupling from the right-going wave to the left-going wave is considered in the left reservoir. The scattering term representing the above processes is written as

$$\left(\frac{\partial f}{\partial t}\right)_C = -\frac{1}{\tau_r}\left[f(x,k_x) - \frac{f_{eq}(x,k)}{\int_0^\infty dk'_x f_{eq}(x,k'_x)} \times \int_0^\infty dk'_x f(x,k'_x)\right] \quad ,k_x > 0 \quad (3)$$

$$= -\frac{1}{2\tau_r}\left[f(x,k_x) - \frac{f_{eq}(x,k)}{\int_{-\infty}^\infty dk'_x f_{eq}(x,k'_x)} \times \int_{-\infty}^\infty dk'_x f(x,k'_x)\right] \quad ,k_x < 0 \quad (4)$$

where $\tau_r$ and $f_{eq}$ are the relaxation time and the distribution function in thermal equilibrium, respectively. Here, note that the lower limits of integration are different for $k_x > 0$ and $k_x < 0$ in the above representations. In the right reservoir, the similar representations of the scattering term are obtained. In this paper, we will study the low temperature properties of the electron waveguide, and thus any scatterings in the waveguide region are ignored.

C. Space-charge effects

In the linear regime, the space-charge effects are not important because a small bias voltage induces a small charge imbalance in the device. On the other hand, in the nonlinear regime, a large amount of charge accumulation and depletion are expected to deform the potential profile significantly. Thus, to include the space-charge effects in the analysis of the exact nonlinear quantum transport of electron waveguide, the following Poisson's equation should be solved simultaneously with the Liouville equation for the Wigner function.

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = -\frac{e}{\varepsilon}[\Gamma(x,y,z) - n(x,y,z)] \quad (5)$$

where $\Gamma$ is the doping density. In this paper, we simplify the equation(5) to a quasi-one-dimensional problem by using the solutions when the bias voltage is removed, $\psi_0(x,y,z)$ and $n_0(x,y,z)$. When the both changes of $\psi$ and $n$ in the $y$ and $z$ directions are assumed to be negligibly small even after the bias voltage is applied, the quasi-one-dimensional Poisson's equation with respect to $x$-direction is derived as

$$\frac{d^2\psi}{dx^2} = -\frac{e}{\varepsilon}\left[\bar{n}_0(x) - \bar{n}(x)\right] \quad (6)$$

where $\bar{n}_0$ and $\bar{n}$ are the average electron densities per unit volume represented by

$$\bar{n}(x) = \frac{1}{L_yL_z}\int_{-\frac{L_z}{2}}^{\frac{L_z}{2}}\int_{-\frac{L_y}{2}}^{\frac{L_y}{2}} dzdyn(x,y,z) = \frac{n(x)}{L_yL_z} \quad (7)$$

$$\bar{n}_0(x) = \frac{1}{L_yL_z}\int_{-\frac{L_z}{2}}^{\frac{L_z}{2}}\int_{-\frac{L_y}{2}}^{\frac{L_y}{2}} dzdyn_0(x,y,z) = \frac{n_0(x)}{L_yL_z} \quad (8)$$

The Liouville equation(1) and the Poisson's equation(6) are mutually related through the one-dimensional electron density

$$n(x) = \int_{-\infty}^{\infty}\frac{dk_x}{2\pi}f(x,k_x) \quad (9)$$

and the potential energy $v(x) = -e\psi(x)$.

## 3. NONLINEAR $I-V$ CHARACTERISTICS OF ELECTRON WAVEGUIDES

First, the current-voltage characteristics of an one-dimensional electron waveguide are calculated at $T = 0$K. Since the waveguide region is assumed to be perfectly ballistic, voltage drops are expected to exist only near the both ends of the waveguide due to the so-called spreading resistance. Thus, as an initial potential distribution in the iterative calculation, a step potential drop as shown in Fig. 2 is employed. The waveguide structure is chosen so that only one width mode can propagate in the wire. Fig. 3 shows the calculated $I-V$ curves at $T = 0$K, where the phase-breaking time in the reservoirs is given as 10fs. The dashed line is the result neglecting the space-charge effects, and the dotted line indicates the relation of the perfect quantization of conductance. First, the $I-V$ curves are found to deviate from the dotted line as the bias voltage increases. Such a nonlinear behavior has been reported experimentally[7]. In addition, when the bias voltage is larger than 5mV, the solid curve diverges from the dashed one. This result means that the space-charge effects play an important role, particularly, in the nonlinear transport regime. Next, Fig. 4 and 5 show the electron density and the potential distributions for various bias voltages, respectively. It is found from Fig. 4 that the electrons are accumulated in the left reservoir and depleted in the right reservoir. This is due to the phase-breaking scatterings and the acceleration of electron waves by the electric field induced in the reservoirs as found in Fig. 5. Further, it is first found from Fig. 5 that as the bias voltage increases, the abrupt voltage drops at the both ends of the waveguide disappear due to such a space-charge effect. As a result, the electron density oscillation inside the waveguide, which has been obtained in the linear transport regime[6], disappears in the nonlinear transport regime. Further,

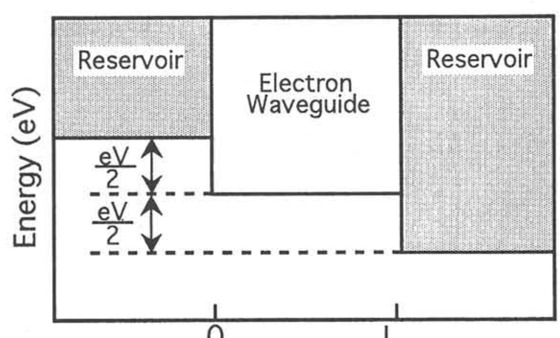

Fig. 2 Initial potential distribution in the iterative calculation at T=0K.

there is no saturation in current in the self-consistent solution. This is due to the fact that the electrons are accelerated in the cathode by the electric field induced by the space-charge effect. In addition, it is found from further investigation of the nonlinear behaviors by varying relaxation times that the $I-V$ curves similar to Fig. 3 are obtained although more electrons are accumulated in the left reservoir and depleted in the right reservoir for the shorter relaxation time.

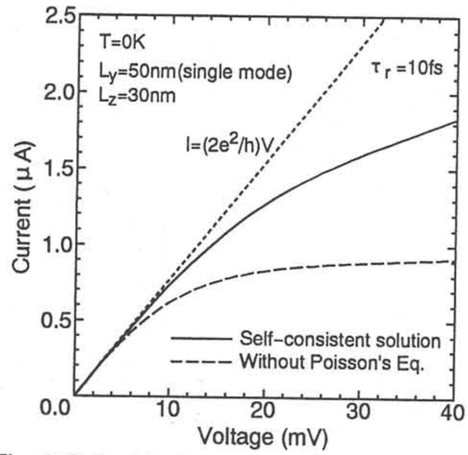


Fig. 3 Calculated current–voltage characteristics of electron waveguide at T=0K.

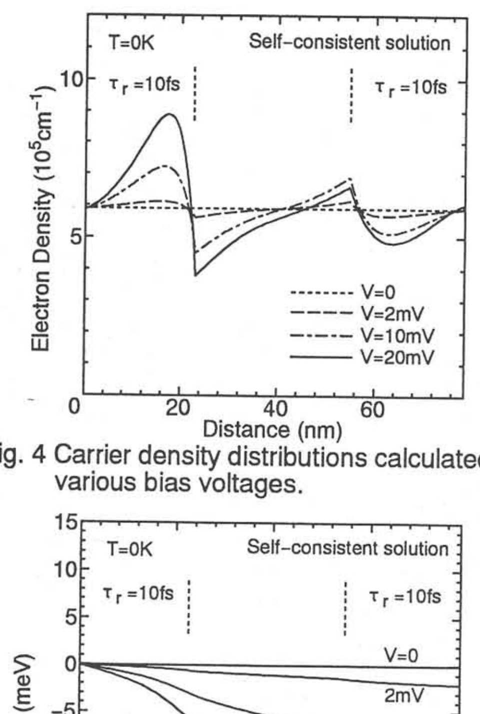


Fig. 4 Carrier density distributions calculated for various bias voltages.

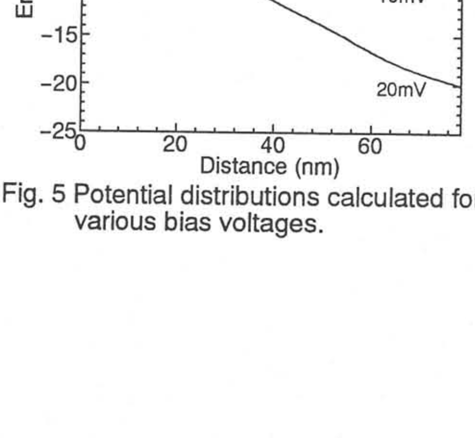


Fig. 5 Potential distributions calculated for various bias voltages.

Finally, we will present the transistor operation of the electron waveguide. Fig. 6 shows the $I-V$ curves at $T$ = 0K for various waveguide widths. The current is found to increase with $L_y$ since the width mode in the waveguide increases with the waveguide width. Such a FET-like transistor operation will be expected in the split-gate structure, because the waveguide width can be varied by the external gate voltage.

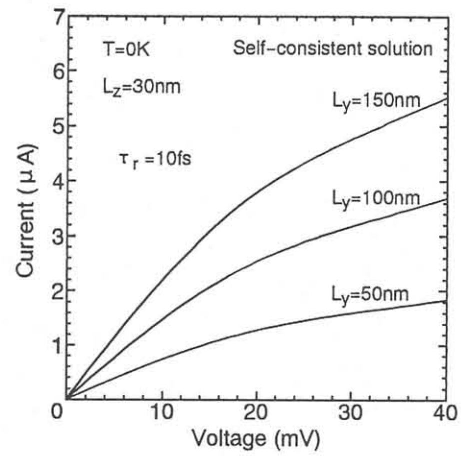


Fig. 6 Calculated current–voltage characteristics at T=0K for various waveguide widths.

## 4. CONCLUSION

The modeling of nonlinear quantum transport in quantum devices is studied based on the Wigner function model. In particular, the phase-randomizing scatterings in contacts are carefully modeled in the Liouville equation for the Wigner function by using the relaxation time approximation. In addition, space-charge effects are also included by solving the Liouville equation for the Wigner function and the Poisson's equation self-consistently. As a simulation model, one-dimensional electron waveguide is considered. The current-voltage characteristics of electron waveguide is simulated at $T$ = 0K. As a result, it is found that in the nonlinear transport regime, the space-charge significantly affects the current-voltage characteristics of the electron waveguide. Further, the possibility of the transistor operation of the electron waveguide is demonstrated at $T$ = 0K. In our Wigner function model, the high temperature performance of the electron waveguide can be obtained if the LO phonon scattering processes are included properly through the relaxation time approximation.

REFERENCES

[1]R. Tsu and L. Esaki, Appl. Phys. Lett., **22** (1973)562.

[2]M. Büttiker, Phys. Rev. **B38**(1988) 9375.

[3]H. Tsuchiya et al., Jpn. J. Appl. Phys., **30**(1991) 3853.

[4]H. Tsuchiya et al., IEEE Trans. on Electron Devices, **39**(1992) 2465.

[5]H. Tsuchiya et al., Jpn. J. Appl. Phys., **31**(1992) 745.

[6]M. J. McLennan et al., Phys. Rev. **B43**(1991) 13846.

[7]L. P. Kouwenhoven et al., Phys. Rev. **B39**(1989) 8040.