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Guided Modes of Electron Wave in a Si-Quantum Wire

Yasushi OKAWA, Hideaki TSUCHIYA, and Tanroku MIYOSHI
Department of Electrical and Electronics Engineering, Kobe University
Rokko-dai, Nada-ku, Kobe 657, Japan

The eigenmodes of electron wave propagating through a Si-quantum wire are analyzed by self-consistent calculations of the two-dimensional Schrödinger equation and Poisson's equation. In the description of the Schrödinger equation, anisotropic effective mass in the six conduction band valleys is considered exactly. As a result, the eigenenergies of electron waves and the electron density distributions are found to be greatly affected by the electron-electron interaction. Further, it is demonstrated that the number of guided modes in the Si-quantum wire are controlled by the gate bias voltage.

1. INTRODUCTION

Recent progress of semiconductor crystal growth and microfabrication technologies make it possible to fabricate novel quantum devices with quantum wire structures. In particular, a Si-quantum wire is one of promising quantum devices, because it is possible to fabricate nanoscale wire structures through the use of its matured existing technologies and the quantized conductance has been observed at high temperature over 100K [1]. In this paper, the eigenmodes of electron wave propagating through a Si-quantum wire are studied by self-consistent calculations of the two-dimensional Schrödinger and Poisson's equations to include the electron-electron interaction within the limits of Hartree approximation. As a result, the eigenenergies of electron waves and the electron density distributions are found to be greatly affected by the electron-electron interaction. Further, it is demonstrated that the number of eigenmodes propagating in the wire can be controlled by applying the positive bias voltage to the gate electrode.

2. SIMULATION MODEL

A simulation model of Si-quantum wire used in this study is shown in Fig. 1, where a n-type silicon wire with a rectangular cross-sectional shape surrounded by SiO_2 is put on n-type (100) silicon substrate. A gate electrode is assumed above the wire to control guided modes of electron wave. For simplicity, $< 001 >$ axis is chosen as a propagation direction because only the diagonal components appear in the reciprocal effective mass tensor. Since there are three sets of energy levels doubly degenerated, corresponding to the three inequivalent alignments of conduction band valleys [2], the three Schrödinger equations are solved simultaneously to obtain the eigenmodes of electron waves propagating through the Si-quantum wire.

$$-\frac{\hbar^2}{2}\left[\frac{\partial}{\partial x}\left(\frac{1}{m_x^*}\frac{\partial \psi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{1}{m_y^*}\frac{\partial \psi}{\partial y}\right)\right] + V(x,y)\,\psi(x,y) = E\psi(x,y), \qquad (1)$$

where m_x^* and m_y^* are the spatially varying effective masses in x and y directions, respectively. The potential energy of the conduction band $V(x,y)$ is given by

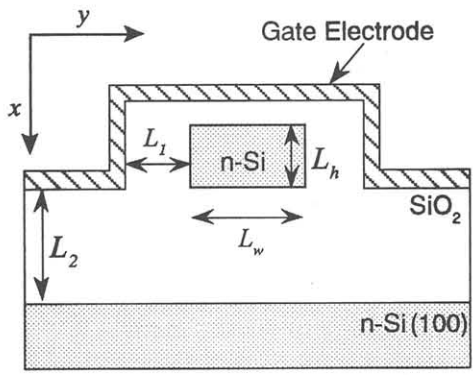

Fig. 1 Simulation model

$$V(x,y) = -e\phi(x,y) + \Delta E_c(x,y), \qquad (2)$$

where $\Delta E_c(x,y)$ denotes the conduction-band offset and $\phi(x,y)$ is the electrostatic potential which is determined by the Poisson's equation. The electron density distribution in the quantum wire is defined as

$$n(x,y) = \sum_i \psi_i(x,y)\,\psi_i^*(x,y)\,\frac{g\,(2m_z^* k_B T)^{\frac{1}{2}}}{\pi\hbar} F_{-\frac{1}{2}}(\eta), \qquad (3)$$

where $F_{-1/2}(\eta)$ is the Fermi-Dirac integral of order $-1/2$ and given by

$$F_{-\frac{1}{2}}(\eta) = \int_0^\infty \frac{1}{x^{\frac{1}{2}}\left[1+\exp(x-\eta)\right]}dx, \qquad (4)$$

where $\eta = (E_F - E_i)/k_B T$. m_z^* is the effective mass in the z direction, which is assumed to be different for Si and SiO_2 regions. g denotes the valley degeneracy equal to 2 for $< 001 >$ direction. E_F the Fermi energy and E_i the eigenenergy of i-th mode. In the self-consistent calculation of the Schrödinger equation (1) and the Poisson's equation, the potential change $\delta\phi$ is evaluated by the following equation.

$$\frac{\partial}{\partial x}\left(\varepsilon\frac{\partial \delta\phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\varepsilon\frac{\partial \delta\phi}{\partial y}\right)-\frac{e}{\varepsilon_0}\delta\phi\delta n = -\left[\frac{\partial}{\partial x}\left(\varepsilon\frac{\partial \phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\varepsilon\frac{\partial \phi}{\partial y}\right)\right]-\frac{e}{\varepsilon_0}(N_d - n), \qquad (5)$$

where N_d denotes the ionized donor density distribution and n is the electron density distribution defined in the equation (3), and δn, the electron density change due to $\delta\phi$, is represented by

$$\delta n = e\sum_i \psi_i\psi_i^* \frac{g}{\pi\hbar}\left(\frac{2m_z^*}{k_BT}\right)^{\frac{1}{2}} \frac{dF_{-\frac{1}{2}}(\eta)}{d\eta}. \qquad (6)$$

The simulation region is shown in Fig. 2. The Poisson's equation and the Schrödinger equation are discretized by the finite difference method in the regions enclosed by the solid and the dashed lines, respectively. Only for the discretization of the Poisson's equation, a nonuniform mesh is used. The boundary conditions for the Poisson's equation are $\partial\phi/\partial y = 0$, $\phi = 0$ and $\phi = V_g$ at the boundaries C_1, C_2 and C_3 ,respectively. As for the Schrödinger equation, the boundary condition of $\psi = 0$ is given. For simplicity, it is assumed that all donors are ionized and no surface charge exists at the Si-SiO_2 interface.

In the simulation, the Schrödinger equation and the Poisson's equation are solved iteratively for each gate bias condition until the self-consistent solution is obtained. In this paper, the iteration is continued until the change of potential energy becomes less than 0.01meV at any position.

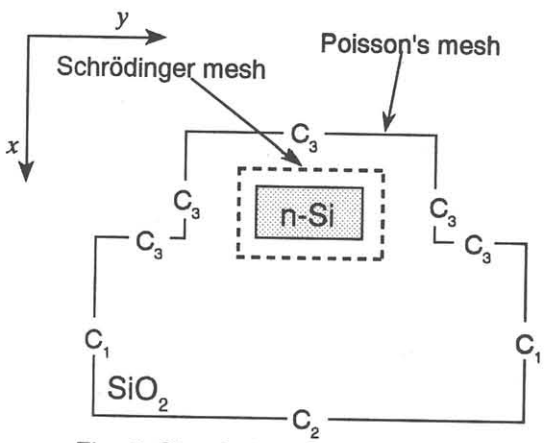

Fig. 2 Simulation regions of two-dimensional Schrödinger equation(dashed line) and Poisson's equation(solid line).

3. SIMULATION RESULTS

In the numerical calculation, the anisotropic effective mass in Si is taken as $m_t^* = 0.19m_0$ and $m_l^* = 0.98m_0$, and the isotropic effective mass of $0.5m_0$ is assumed in SiO_2 [3]. The static dielectric constant ε is given as 11.9 and 3.8 for Si and SiO_2 regions, respectively. The conduction band discontinuity at the Si-SiO_2 interface is assumed to be 3.25eV [4]. The height L_h and the width L_w of the wire are given as L_h =6nm and L_w=20nm, respectively, and N_d is assumed to be 10^{14}cm^{-3}. The thicknesses of SiO_2 surrounding the wire are taken as L_1=30nm and L_2=400nm. Fig. 3 shows the variations of the subband energies of the three conduction valleys due to the gate bias voltage for $T = 4.5K$, where all energies are measured from the Fermi energy E_F . The number of eigenmodes propagating in the wire increases with the gate bias voltage though there is no channel in the quantum wire for V_g=0V. This is due to the fact that the potential energy inside the wire region is lowered by applying the positive bias voltage to the gate electrode.

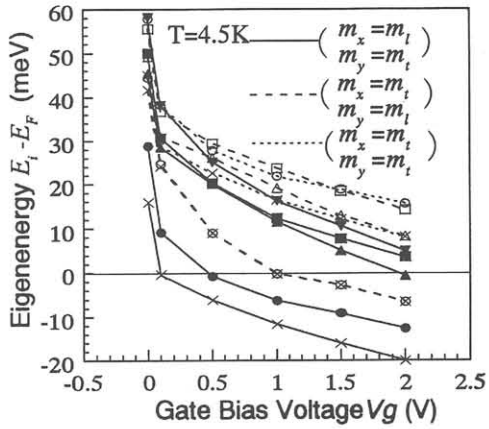

Fig. 3 Variations of subband energies due to gate bias voltage.

The representative conduction band energy is shown in Fig. 4(a) for V_g=1V. Note that a very large conduction band discontinuity(~3.25eV) is assumed at the Si-SiO_2 interface. The electron density distributions of the guided modes are shown in Fig. 4(b)-(e). In Fig. 4(b), the electron distribution has a double peak in the y direction regardless of the fundamental mode. The electron wave is pushed out toward the both sides of the wire due to the convex potential profile as shown in Fig. 4(a). It is found that the third and the forth eigenmodes, that are originally the first and the second eigenmodes for $m_x = m_t$, $m_y = m_l$, are also strongly affected by the convex potential profile.

Next, the two-terminal conductance of the Si-quantum wire is simulated as a function of V_g as shown in Fig. 5, where the source-drain voltage V_{SD} is given as 2μV. The quantized conductance in the unit of $4e^2/h$ are clearly found to the second step. However, the quantized value of the third step indicates $8e^2/h$, because the eigenenergies of the third and the fourth subbands are almost equal as shown in Fig. 3.

4. CONCLUSION

The guided modes of electron waves in Si-quantum wire are analyzed by self-consistent calculations of the two-dimensional Schrödinger and Poisson's equations. The higher order modes are included exactly by considering anisotropic effective mass in the six conduction band valleys. As a result, the eigenenergies of electron waves and the electron density distributions are found to be greatly affected by the electron-electron interaction. Further, it is demonstrated that the number of guided modes in the wire can be controlled by applying the positive bias voltage to the gate electrode. Hereafter, we will extend our self-consistent calculation model to the analysis of arbitrarily oriented Si-quantum wires with arbitrary cross-sectional shapes.

References

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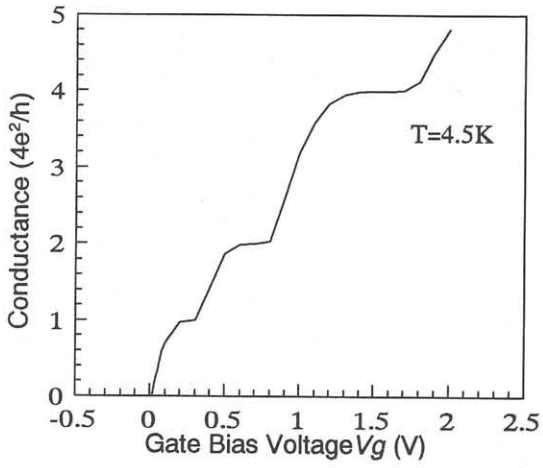

Fig. 5 Variations of quantized conductance due to gate bias voltage.

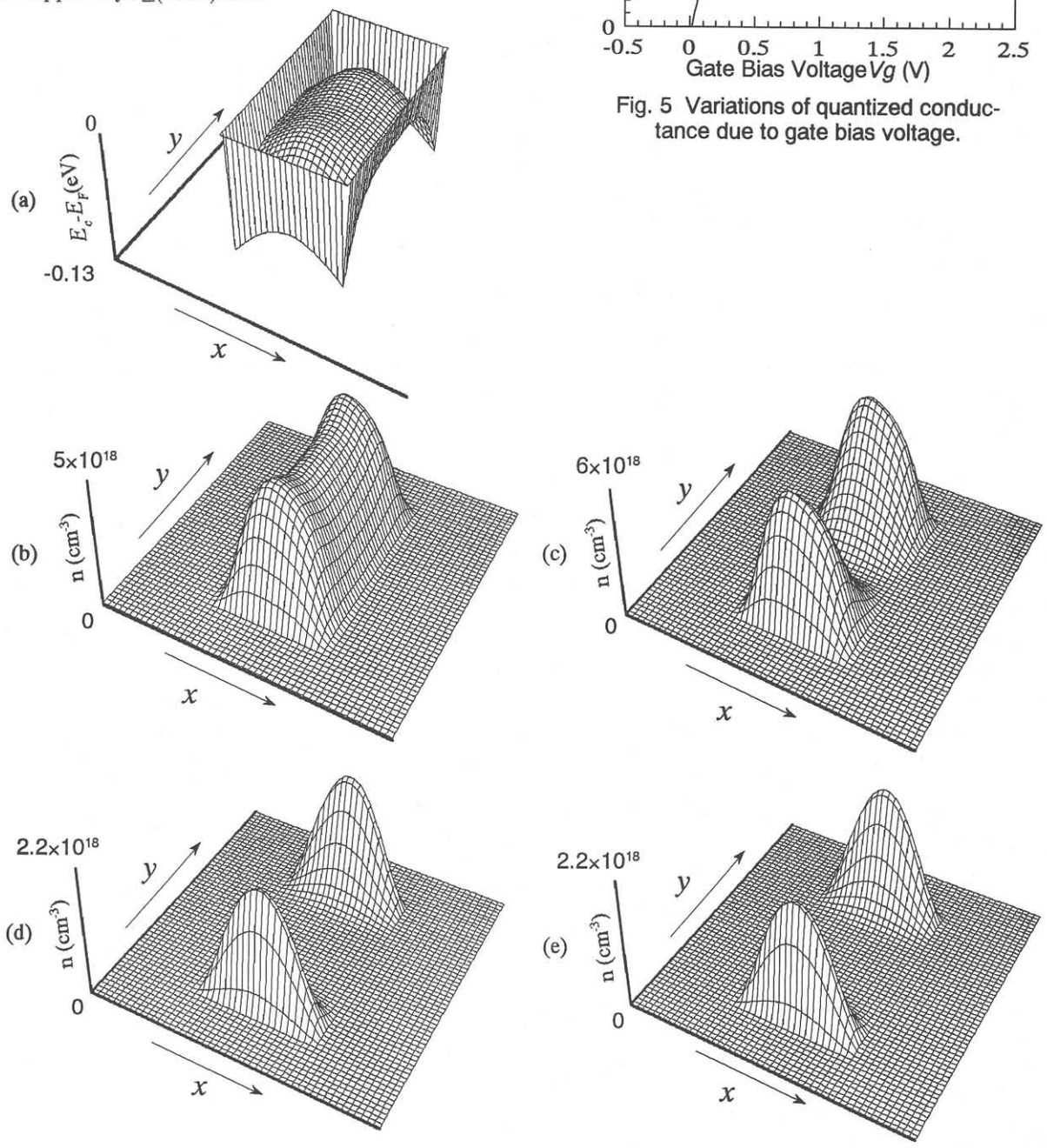

Fig. 4 (a) conduction band distribution. (b) electron density distribution of the fundamental mode ,and (c) the second, (d) the third, and (e) the forth eigenmodes.