Finite element analysis of guided modes in a silicon-quantum wire

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Abstract

The eigenmodes of electron wave propagating through a physically confined Si-quantum wire by a SiO$_2$ barrier are analyzed self-consistently by using a finite element method. The anisotropic effective mass tensor corresponding to the three inequivalent alignments of conduction band valleys in Si and the continuity of the probability current densities at the Si-SiO$_2$ interface are duly taken into account. As a result, the eigenenergies of electron wave and the electron density distribution are found to be greatly affected by the electron-electron interaction. It is also demonstrated that the number of guided modes in the Si-quantum wire is controlled by the gate bias voltage.

1 Introduction

A Si-quantum wire on a SOI(silicon on insulator) substrate is a promising quantum device, because it is possible to fabricate nanoscale wire structures through the use of its established technologies, and quantized conductance is observed at temperatures over 100 K [1] [2]. In this paper, the eigenmodes of electron waves propagating through a physically confined Si-quantum wire by a SiO$_2$ barrier are studied. In particular, a finite-element method is developed for the analysis of an arbitrarily oriented Si-wire with an arbitrary cross-section. The electron-electron interaction is incorporated within the limits of the Hartree approximation by solving the Poisson equation with the Schrödinger equations self-consistently. As a result, the eigenenergies of electron waves and the electron density distribution are found to be greatly affected by the electron-electron interaction. It is also demonstrated that the number of guided modes in the Si-quantum wire is controlled by the
gate bias voltage.

2 Simulation Model

The eigenmodes of electron waves propagating through a Si-quantum wire oriented in the $z$ direction are analyzed by solving the lateral two-dimensional Schrödinger equation in the effective mass approximation

$$-\frac{\hbar^2}{2} \left[ w_{xx} \frac{\partial^2 \xi}{\partial x^2} + 2w_{xy} \frac{\partial^2 \xi}{\partial x \partial y} + w_{yy} \frac{\partial^2 \xi}{\partial y^2} \right] + V(x,y) \xi(x,y) = E' \xi(x,y), \quad (1)$$

where $\xi(x,y)$ is a transverse envelope function which is related to the original wave function $\psi$ as

$$\psi(x,y,z) = \xi(x,y) \exp(i k_z z) \exp[i k_z (\alpha x + \beta y)], \quad (2)$$

$$\alpha = \frac{w_{xy}w_{yz} - w_{yy}w_{xz}}{w_{xx}w_{yy} - w_{xy}^2}, \quad (3)$$

$$\beta = \frac{w_{xy}w_{xz} - w_{xx}w_{yz}}{w_{xx}w_{yy} - w_{xy}^2}. \quad (4)$$

where $w_{ij}$ is a component of the reciprocal effective mass tensor. $E'$ is a transverse eigenenergy related to the total energy $E$ as

$$E = E' + \frac{\hbar^2 k_z^2}{2m_z}, \quad (5)$$

where $m_z$ is the effective mass in the $z$ direction given by

$$\frac{1}{m_z} = w_{zz} + w_{xz} \alpha + w_{yz} \beta. \quad (6)$$

The potential energy of the conduction band $V(x,y)$ is given by

$$V(x,y) = -e\phi(x,y) + \Delta E_c(x,y), \quad (7)$$

where $\phi(x,y)$ is the electrostatic potential and $\Delta E_c(x,y)$ denotes the conduction-band offset. The functional of Schrödinger equation (1) used for the finite-element analysis is given by

$$I_z(\xi, \xi^*, \nabla \xi, \nabla \xi^*) = \int \int \left[ \frac{\hbar^2}{2} \left( w_{xx} \frac{\partial \xi}{\partial x} \frac{\partial \xi^*}{\partial x} + w_{xy} \frac{\partial \xi}{\partial x} \frac{\partial \xi^*}{\partial y} + w_{yy} \frac{\partial \xi}{\partial y} \frac{\partial \xi^*}{\partial y} \right) + (V - E') \xi \xi^* \right] dx dy. \quad (8)$$

Note that the Euler equation of the functional with respect to $\xi^*$ corresponds to the Schrödinger equation (1), while the one with respect to $\xi$ gives the
complex conjugate equation of (1). Further, it is inherently included in (8) that the continuity of the following probability current densities is satisfied on the boundary if the envelope function $\xi$ is continuous on the boundary of each element.

$$J_x = -\hbar \text{Im} \left[ w_{xx} \xi^* \frac{\partial \xi}{\partial x} + w_{xy} \xi^* \frac{\partial \xi}{\partial y} \right],$$

$$J_y = -\hbar \text{Im} \left[ w_{xy} \xi^* \frac{\partial \xi}{\partial x} + w_{yy} \xi^* \frac{\partial \xi}{\partial y} \right].$$

Using the normalized envelope function $\xi_i$ for the $i$-th guided mode, the electron density distribution in the quantum wire is defined as

$$n_0(x, y) = \sum_i \xi_i(x, y) \xi_i^*(x, y) \frac{g(2m_e k_B T)^{1/2}}{\pi \hbar} F_{-1/2}(\eta),$$

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

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

$$\eta = \frac{E_F - E_i'}{k_B T}.$$
When we use the approximate representation of $F_{-1/2}(\eta)$ [4], the derivative of $F_{-1/2}(\eta)$ with respect to $\eta$ is given as

$$\frac{dF_{-1/2}(\eta)}{d\eta} = F_{-1/2}(\eta)^2 \left\{ 2^d d^2 \frac{1}{\Gamma(d)} \frac{1}{\left[b + \eta + (|\eta - b|^c + a^c)\right]^{\frac{1}{2}}} + \exp\left(-\eta\right) \right\},$$

where $+$ and $-$ in eq.(17) correspond to the cases of $\eta > b$ and $\eta \leq b$, respectively. The functional of eq.(14) used in the finite-element analysis is given by

$$I_p(\phi_1, \nabla \phi_1) = \iint \left[ \left( \frac{\partial \phi_1}{\partial x} \right)^2 + \left( \frac{\partial \phi_1}{\partial y} \right)^2 + \frac{e}{\varepsilon \varepsilon_0} n_1 \phi_1 - 2\phi_1 \left\{ \frac{\partial^2 \phi_0}{\partial x^2} + \frac{\partial^2 \phi_0}{\partial y^2} + \frac{e}{\varepsilon \varepsilon_0} (N_d - n_0) \right\} \right] dx dy.$$ 

In the above expression, the continuity of electric flux density is inherently satisfied on the boundary.

The iterative procedure to obtain self-consistent solution is summarized in the flow chart of Fig. 1.

![Flow chart for the self-consistent calculation](image-url)
3 Simulation Results

Gate Electrode

As an example, the n-type Si-wire with a trapezoidal cross-section on the (100) n-type Si substrate as shown in Fig. 2 [1] is analyzed. The (011) axis is chosen as a propagation direction. In this case, the electronic states are divided into two classes as shown in Table 1. 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 0.5\( m_0 \) is assumed in SiO\(_2\) [5]. Here, \( m_0 \) denotes the mass of a free electron, \( m_t \) and \( m_l \) are the transverse and longitudinal effective mass of a bulk Si, respectively. The static dielectric constant \( \varepsilon \) is given as 11.9 and 3.8 for Si and SiO\(_2\) regions, respectively. The conduction band offset \( \Delta E_c \) at the Si-SiO\(_2\) interface is assumed to be 3.25eV [6].

Due to the symmetry of the structure with respect to the \( x-z \) plane, the half area of Fig. 2 is analyzed. Further, the Schrödinger equation is solved only inside a smaller area including the Si-wire as shown in Fig. 3 because the most of electron wave of a guided mode is confined in the wire region. On the other hand, the whole area is analyzed for the Poisson equation. The boundary conditions for the Poisson equation are \( \varphi = V_g \), \( \varphi = 0 \), and \( \partial \varphi / \partial y = 0 \) on the boundaries C\(_1\), C\(_2\) and C\(_3\), respectively. As for the Schrödinger equation, \( \psi = 0 \) for odd mode and \( \partial \psi / \partial y = 0 \) for even mode are used on the symmetrical plane. On the rest of the boundary, \( \psi = 0 \) is assumed. For simplicity, it is assumed that no surface charge exists at the Si-SiO\(_2\) interface. The first-order triangular elements are used for discretization.

In the simulation, the Schrödinger equation (1) and the Poisson equation (14) 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 0.01 meV everywhere.

<table>
<thead>
<tr>
<th>Table 1: Classification of electronic states.</th>
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<tbody>
<tr>
<td>degeneracy</td>
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<tr>
<td>( w_{xx} )</td>
</tr>
<tr>
<td>( w_{yy} )</td>
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<tr>
<td>( m_t )</td>
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Figure 2: Schematic diagram of Si-quantum wire.
Figure 3: Simulation region of the Poisson equation and Schrödinger equation.

It needs about 20 times iterative calculation for convergence. Using HP9000 series model 735, it takes about 2 minutes for one iteration when 194×166 elements for Poisson equation and 92×64 elements for Schrödinger equation are used.
For $L_h=6$ nm, $L_w=20$ nm, $L_1=30$ nm, $L_2=400$ nm, $N_d=10^{14}$ cm$^{-3}$, and $T=4.5$ K the variation of the subband energies $E'_i$ as a function of the gate bias voltage $V_g$ is shown in Fig. 4, where all energies are measured from the Fermi energy $E_F$. The eigenmode with $E'_i$ becomes a guided mode when $E'_i<E_F$. The number of eigenmodes propagating in the wire increases with gate bias voltage though there is no channel in the quantum wire for $V_g=0$ V. 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. The representative conduction band energy is shown in Fig. 5(a) for $V_g=2.0$ V. Note that a very large conduction band discontinuity ($\sim 3.25$ eV) is assumed at the Si-SiO$_2$ interface. The electron density distributions of the guided modes are shown in Figs. 5(b)-5(d). At this gate voltage, electron wave belonging to class (a) in Table 1 is mainly excited in the wire. The electron distribution has a double peak in the $y$ direction even for the fundamental mode. The electron wave is strongly pushed out toward the sides of the wire due to the convex potential profile as shown in Fig. 5(a).
The above results show that the n-type Si-quantum wire operates in an electron accumulation mode. Our further investigation on the inversion operation in a p-type Si-wire reveals that an extra positive gate voltage (about 1 V for the same structure) is required to obtain the same properties as those shown in Figs. 4 and 5.

4 Conclusions

We have analyzed the guided modes of electron wave in an arbitrarily oriented n-type Si-quantum wire self-consistently by a finite element method. The higher-order modes were 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 were found to be greatly affected by the electron-electron interaction. Furthermore, it was demonstrated that the number of guided modes in the wire can be controlled by applying the positive bias voltage to the gate electrode. Such a gate bias control of guided modes in a Si-quantum wire, taking anisotropic effective mass into consideration, has been discussed for the first time by performing the self-consistent calculation for the potential.

Acknowledgement

This work was partially supported by the Grant-in-Aid for Scientific Research on Priority Area “Quantum Coherent Electronics” from the Ministry of Education, Science, Sports and Culture.
References


