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Nanoscale FinFET simulation: A quasi-3D quantum mechanical model using NEGF

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Abstract

In this paper, a numerical simulation of FinFET is carried out. This computational model is also applicable to nanowires. The non-equilibrium Green's function (NEGF) is used to handle the quantum transport along the channel, and 2-D Schrödinger equation is solved at the channel cross-section to obtain the electron density profile. With the 3-D Poisson's equation solved self-consistently, the model provides insights into the performance of FinFETs with ultra-small channel cross-dimension.
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1. Introduction

The development of silicon planar technology over the past half-century has been one of the most important achievements in modern engineering history. With the fundamental physics limits approached rapidly, however, the continuous MOS scaling is much more difficult especially when the device size becomes smaller than 50 nm. New structures must be developed to get over this challenge.

The double-gate FinFET is one of such promising structures, which improves the gate controllability and thus minimizes the short-channel effect through adoption of multiple gates. By using tri-gate, an FinFET structure is born, which is compatible with the planar CMOS process. Good performance for both NMOS [1] and PMOS [2,3] with sub-100 nm channel length have been reported.

In FinFET devices, quantum effects and non-equilibrium, ballistic or near-ballistic transport have large impact on device performance. Quantum mechanical modelling is important for many reasons, e.g., the tunnelling current through ultra-thin gate oxide adds to the low limit of the off-state current. For channel length comparable to the carrier scattering length, carriers transport ballistically. The inversion layer thickness along the channel can be treated as the same no longer. So more accurate 2-D (and 3-D) simulation of the device is needed.

For deep sub-micron bulk CMOS, solving the 1-D Schrödinger equation in the substrate at direction perpendicular to the substrate/gate oxide interface reveals the increase of the threshold voltage, or equivalently the increase of the effective gate oxide thickness. As the channel length is further reduced, however, the quantum mechanical effects along the channel, such as the tunnelling through the source/drain (S/D) barrier, becomes non-negligible. Moreover, with the quantum mechanical confinement on the channel cross-section in FinFET configuration, the carrier distribution is

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highly multi-dimensional. Thus, a 3-D quantum mechanical model is preferred. The NEGF provides the ability of solving Schrödinger equation with open boundary conditions (BC) [4–6], and with neglect of scattering the ballistic transport is modelled naturally. To save the computational cost, a hybrid method is proposed of solving 2-D Schrödinger equation in the channel cross-section with the confined BC, combined with the 1-D NEGF solution along the channel. These solutions to 3-D Schrödinger equation are obtained by solving Poisson's equation in 3-D device structure self-consistently using the Newton iteration method.

2. Model for quantum mechanical ballistic transport

In this section, we explain the quasi-3D quantum mechanical model which has been developed in details. The numerical simulation of the model is based on

- 2-D Schrödinger equation in channel cross-section,
- 1-D NEGF along the channel, and
- 3-D Poisson's equation in entire device structure.

The finite difference method (FDM) is used for the discretization with tensor-product mesh, and two iteration loops are involved in the simulation. Fig. 1 shows the schematic of the FinFET structure under study.

The 3-D effective mass Schrödinger equation is written as follows with x-direction along the channel:

$$-\left[\frac{\hbar^2}{2m_x^*}\frac{\partial^2}{\partial x^2}+\frac{\hbar^2}{2m_y^*}\frac{\partial^2}{\partial y^2}+\frac{\hbar^2}{2m_z^*}\frac{\partial^2}{\partial Z^2}+qV(x,y,z)\right]\Psi(x,y,z) = E\Psi(x,y,z) \tag{1}$$

Using the separation of variables for Ψ and applying WKB approximation for wavefunction in x [8], one obtains

$$\Psi(x,y,z) = X(x)\varphi(y,z) = \mathrm{e}^{jk_x x}\varphi(y,z) \tag{2}$$

where a plane wave solution in x-direction has been assumed, implying that the potential is flat along x-direction. Then one obtains the following 2-D Schrödinger equation for $\varphi(y, z)$,

$$\left[\frac{\hbar^2 K_2^2}{2m_x^*}-\frac{\hbar^2}{2m_y^*}\frac{\partial^2}{\partial y^2}-\frac{\hbar^2}{2m_z^*}\frac{\partial^2}{\partial z^2}-qV(x,y,z)\right]\varphi(y,z) = E\varphi(y,z) \tag{3}$$

The following notations are used to explicitly indicate the x-dependence, which acts as a parameter in 2-D functions: $\Psi_x(y, z) = \varphi(y, z)$, $V_x(y, z) = V(x, y, z)$, and the transverse eigen-energy $E_{t,x} = E - \hbar^2 k_x^2/2m_x^*$. Eq. (3) is then re-written as

$$\left(-\frac{\hbar^2}{2m_y^*}\frac{\partial^2}{\partial y^2}-\frac{\hbar^2}{2m_z^*}\frac{\partial^2}{\partial z^2}\right)\Psi_x^i(y,z) - qV_x(y,z)\Psi_x^i(y,z) = E_{t,x}^i\Psi_x^i(y,z) \tag{4}$$

In the above equations, m_y^* and m_z^* are the effective masses in the cross-section. $\Psi_x^i(y,z)$ and $E_{t,x}^i$ are the eigen-wavefunction and eigen-energy, respectively, for the cross-section located at x. The superscript i is the index of subbands. This 2-D effective mass Schrödinger equation is solved for every y–z section along the channel. For any cross-section at x, the solution region is the entire cross-section including the gate oxide. A zero-value BC is set for electron wavefunction at the gate electrode. The electron effective mass is different for Si and SiO_2 region. Although this zero boundary condition fails to model the tunnelling current through the gate oxide accurately, the effect of electron-wavefunction penetration into oxide region has nonetheless been included in the simulation.

Now we discuss the values of m_y^* and m_z^*. Assume the channel is along the [1 0 0] direction, there are three sets of energy valleys in the k_y–k_z plane with different combination of m_y^* and m_z^* and each set has two valleys.

For a square cross-section, i.e., $l_y = l_z$ where l represents the side length of the cross-section, the two sets of valleys are collapsed into one with four valleys. Thus, there are two (instead of three) sets of different combination for m_y^* and m_z^*.

In Fig. 3, profiles of subband edges along the channel are shown for a FinFET with cross-section 3×3 nm^2. Plotted are six lowest subband edges in two groups: group 1 for valley sets 2 and 3 in Fig. 2 and group 2 for set 1. For each group, the three lowest subbands are drawn. Note that because of the square shape for the channel cross-section, effective masses in sets 2 and 3 result in identical subbands. In Fig. 4, the density of states in cross-section at $x = 0$ for the lowest three subbands of valley set 3 is shown, in which the penetration of electron into oxide regions can be clearly observed (the thickness of the gate oxide is 1 nm).

Once the subband edge, $E_{t,x}$, as the function of x, $E_t(x)$, is obtained, the Schrödinger equation along the x-direction can be written as

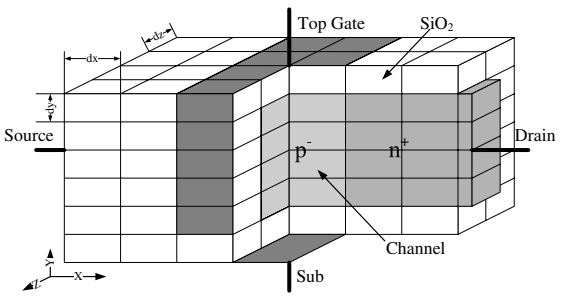

Fig. 1. Schematic of the FinFET structure.

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