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Quantum Simulation of Silicon Nanowire FETs: Ballistic Transport and Corner Effects

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In this work, the device characteristics of silicon nanowire eld-effect transistor (SNWFET) have been investigated by solving the three-dimensional (3D) Poisson equation and the quantum ballistic transport equation self-consistently, using an ef ci ent numerical algorithm to solve the 2D Schrödinger equations in the cross-sectional planes. The dependence of the device performance on the gate number, con gur ation, and shape has been examined in conjunction with the effect of the wave function con nement .

The simulated device is a three-dimensional (3D) structure which can have multiple gates around the silicon channel (Fig. 1). The source/drain doping concentration is heavily n-doped and the channel region is lightly p-doped or undoped. To simulate the device, we have adopted the uncoupled mode-space NEGF method, where the original 3D problem is split into 2D Schrödinger equation in the plane perpendicular to the transport direction and 1D NEGF equation in the transport direction (x)[1], [2]. In such numerical simulations, most of the computing time is spent on solving the 2D Schrödinger equation in the cross-sectional planes, whether they are solved in the real-space or k-space.

In this work, we have developed an ef cient way to solve the 2D Schrödinger equations in the cross-sectional planes, by transforming them into the “mode-space”, as follows. We expand the wavefunction $\Psi(y,z)$ by a product of two 1D wavefunctions $\chi_i(y)$ and $\zeta_j(z)$ that are chosen appropriately: $\Psi(y,z) = \sum_K a_K|K\rangle$, where $|K\rangle \equiv \chi_i(y)\zeta_j(z)$. Then the problem reduces to solving $M \times M$ eigenvalue problem of $\sum_L \langle K|H_{2D}|L\rangle a_L = \epsilon_K a_K$, where H_{2D} is the 2D Hamiltonian, ϵ_K its K-th eigenvalue, and M the number of modes participating in the transport. Since M is $10 \sim 200$ for the nanowire transistors with a cross-sectional area $S \lesssim 20\text{nm} \times 20\text{nm}$, the computational burden can be greatly lifted.

Using the ef ci ent numerical scheme, we have studied the scaling issues of the SNWFETs with the rectangular cross-section. Also we have investigated the effect of the corner rounding, starting with the rectangular cross-section and gradually rounding the corners until the cross-section becomes a circular one (Fig. 2).

Fig. 3 shows the I-V characteristics when the silicon channel of the transistor of the gate-all-around (GAA) structure shrinks three-dimensionally: starting with $L = T_{si} = W_{si} = 25$ nm, L is reduced gradually until $L = 5$ nm (T_{si} and W_{si} are reduced by the same ratio). It can be seen in the gure that almost the same I-V characteristics are maintained until $L = 10$ nm.

Fig. 4 shows the effect of the corner rounding of a GAA transistor with $L = T_{si} = W_{si} = 5$ nm; the degree of the corner rounding is given by $2R/W_{si}$ where R is the radius of the curvature as shown in Fig. 2. The effect of the corner rounding becomes pronounced as the cross-section becomes closer to a circular shape. In Fig. 5, the dependence of the subthreshold swing (SS) on the curvature radius is shown for various transistor dimensions and gate con gur ations. It can be seen in the gure that, if the device performance of the transistor with the rectangular-shaped cross section is poor with greater SS values, the corner-rounding improves the device performance more greatly, and as the SS value approaches 60 mV/decade, the effect of the corner rounding becomes negligible. This can be understood by examining the quantum charge distributions in the cross-sectional planes, as shown in Fig. 6, where the current conduction

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channels formed at the corners of the rectangular cross-section move toward the center as the corner rounding proceeds.

References

[1] P.S. Damle et. al., in Molecular Electronics (ed. M. Reed and T. Lee, Amer. Sci. Pub., 2003.)

[2] J. Wang, E. Polizzi, and M. Lundstrom, J. of Applied Physics, vol. 96, pp. 2192 - 2203, 2004.

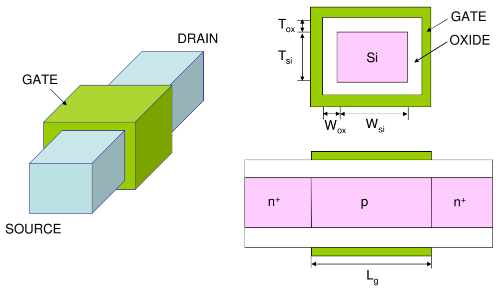

Fig. 1. Silicon nanowire eld effect transistor

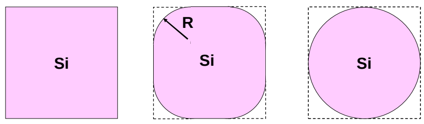

Fig. 2. Cross sections of SNWFETs with different radius of the curvature at the corners.

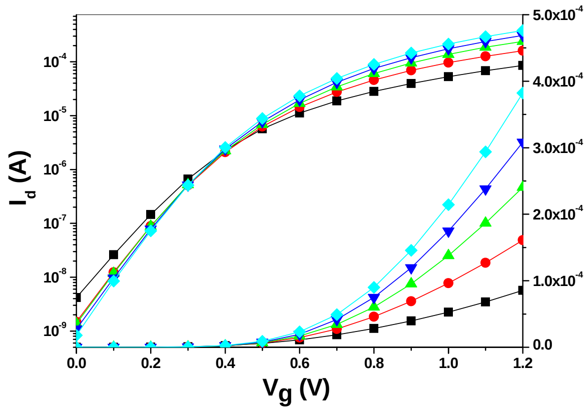

Fig. 3. I-V characteristics for L= 25 (diamonds), 20 (inverse triangles), 15 (triangles), 10 (circles), and 5 nm (squares), respectively (W_{si} = T_{si} = L) .

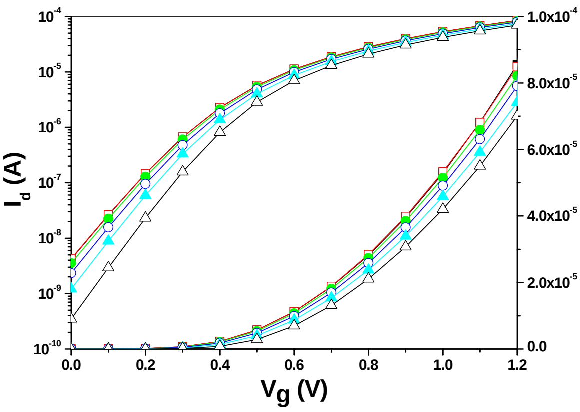

Fig. 4. Corner rounding effect for L = T_{si} = W_{si} = 5 nm, for $2R/W$ = 0.0 (solid squares), 0.2 (open squares), 0.4 (solid circles), 0.6 (open diamonds), 0.8 (solid triangles), and 1.0 (open triangles).

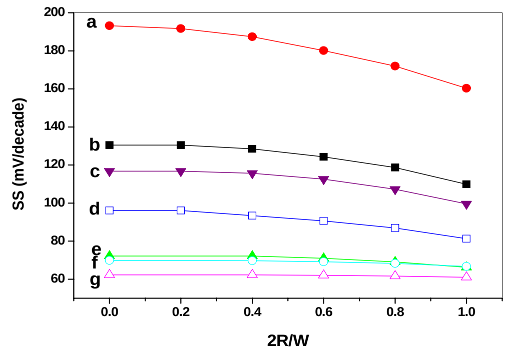

Fig. 5. Subthreshold swing values for different channel dimensions: GA (b,c,e,f,g), Tri (a,d), $L = 5$ (a,b,d,e), $L = 10$ (c,f,g), $L_g = 5$ (a,b), $L_g = 10$ (c,f), $L_g = 15$ (d,e), $L_g = 20$ (g), $W = 5$ (a,b,d,e,f,g), $W = 10$ (c) nm.

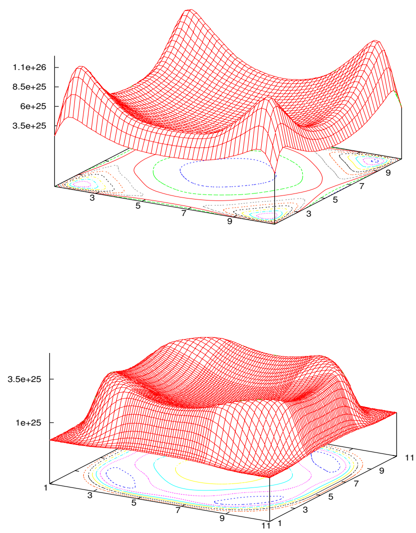

Fig. 6. Electron distributions in a cross-sectional plane of 10nm x 10nm : $2R/W$ = 0.0 (top) and $2R/W$ = 0.6 (bottom).