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A Simplified Quantum Mechanical Model for the Electron Distribution in a Si Nanowire

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Abstract

In order to investigate the technological potential ascribed to semiconductor nanowires, it is paramount to include quantum effects into the models used to simulate carrier transport as well as optical and excitonic features of various nanowire layouts.
In particular, one needs to determine the energy eigenvalues and eigenfunctions of the charge carriers in terms of material parameters and tunable parameters, such as the external voltages and the wire radius. As the latter may be running from a few nanometers up to a few tens of nanometers, the number of occupied subbands may substantially increase. Consequently, a flexible Poisson–Schrödinger solver needs to be invoked to minimize the computational burden, especially when it is to be integrated into another simulation program.

1 Introduction

In this paper we present a robust Poisson–Schrödinger solver that can be used as a basic building block for simulation programs addressing electrical transport characteristics [1, 2] as well as optical properties [3] of semiconductor nanowires. We summarize the theoretical background and the numerical approach underlying the simulation program and show some typical transport related results obtained for a Si nanofet. Though being developed for a cylindrical quantum wire, as shown in Fig. 1, the theoretical framework can straightforwardly be extended to other geometries.

2 Theory

Consider a cylindrical Si nanowire with radius R consisting of two heavily n^+doped source and drain regions, separated by an unintentionally doped p-type channel region with length L_{CH}. Choosing the z-axis along the symmetry axis of the wire (assumed to be a <0,0,1> direction), we introduce cylindrical coordinates r, ϕ, z. Applying gate and drain voltages generally induces an electrostatic potential profile $V(r,z)$ which, together with the oxide barrier $U_B(r,z)$, is part of the potential energy $U(r,z) = U_B(r,z) - eV(r,z)$

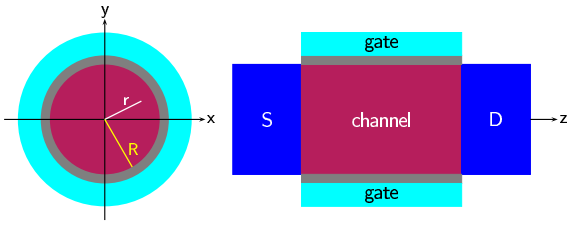

Figure 1: Si nanowire with cylindrical symmetry

entering the one-electron Schrödinger equation

$$-\frac{\hbar^2}{2}\left[\frac{1}{m_{\alpha\perp}}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}\right)+\frac{1}{m_{\alpha z}}\frac{\partial^2}{\partial z^2}\right]\psi_{\alpha mlk}(r,\phi,z)+ \\ \big(U(r,z)-E_{\alpha mlk}\big)\psi_{\alpha mlk}(r,\phi,z)=0 \quad (1)$$

with $m_{\alpha\perp}=2m_{\alpha x}m_{\alpha y}/(m_{\alpha x}+m_{\alpha y})$. $m_{\alpha x},m_{\alpha y},m_{\alpha z}$ are the effective masses at the bottom of the α-th valley, and m,l,k are quantum numbers labeling the electron eigenstates. Then the electron concentration inside the channel may be extracted from

$$n(r,z)=2\sum_{m,l,k}|\psi_{\alpha mlk}(r,\phi,z)|^2F(E_{\alpha mlk}),\ F(E)\equiv(1+\exp(E-E_{\mathrm{F}})/k_{\mathrm{B}}T)^{-1} \quad (2)$$

Adopting a classical treatment for holes, we evaluate the hole concentration as

$$p(r,z)=N_{\mathrm{V}}\exp\left(\frac{E_{\mathrm{g}}+E_{\mathrm{F}}+U(r,z)}{k_{\mathrm{B}}T}\right) \quad (3)$$

where N_{V} is the effective valence band concentration (bulk) and E_{g} denotes the bandgap. Assigning a uniform donor profile N_{D}^+ to the source and drain regions, the total charge density in the nanowire is obtained from

$$\rho=e\big(p(r,z)-n(r,z)+N_{\mathrm{D}}^+\big) \quad (4)$$

A conventional Schrödinger–Poisson solver now combines Eqs. (2), (3) and (4) to solve them self-consistently with Poisson's equation

$$\frac{\partial^2V(r,z)}{\partial r^2}+\frac{1}{r}\frac{\partial V(r,z)}{\partial r}+\frac{\partial^2V(r,z)}{\partial z^2}=-\frac{1}{\varepsilon_{\mathrm{s}}}\rho(r,z),\qquad \varepsilon_{\mathrm{s}}=\text{Si permittivity} \quad (5)$$

Consequently, the Schrödinger equation needs to be solved each time when a new iteration of the potential profile is being imposed which is a CPU-intensive task. On the other hand, the local density approach giving rise to classical, local relations between potentials and carrier densities such as Eq. (3) is computationally less expensive but entirely ignores quantum mechanical reflections and confinement effects. As a trade-off we have adapted the generalized local density approach introduced by Paasch and Uebensee [4] for studying planar structures and quantum wells to the case of a nanowire

MOSFET. Their approach basically amounts to providing a quantum mechanical treatment of all abrupt potential barriers, such as the Si/insulator barrier while retaining a classical description for the smoother parts of the potential profile in both the radial and z-direction. Practically, we solve the Schrödinger equation for a flat profile $V(r,z)=0$ but accounting for an infinite Si/insulator barrier confining the electrons to the wire, yielding the one-electron spectrum

$$E_{\alpha mlk} = \frac{\hbar^2 k^2}{2m_{\alpha z}} + \frac{\hbar^2 x_{ml}^2}{2m_{\alpha\perp}R^2}, \quad m=0,\pm1,\pm2,\ldots, \quad l=1,2,\ldots, \tag{6}$$

$$\psi_{\alpha mlk}(r,\phi,z) = C_{ml}\,J_m\!\left(\frac{x_{ml}r}{R}\right)\mathrm{e}^{\mathrm{i}m\phi}\,\mathrm{e}^{\mathrm{i}kz}, \quad C_{ml} = \frac{1}{\sqrt{2}\,\pi R|J_{m+1}(x_{ml})|} \tag{7}$$

where x_{ml} is the l-th zero of the m-th Bessel function $J_m(x)$. Next, we impose the profile $V(r,z)$ as a local perturbation of the energy eigenvalues, thereby rewriting Eq. (2) as

$$n(r,z) = \left(\frac{2}{\pi R}\right)^2 \sum_{m=0}^{\infty}\sum_{l=1}^{\infty}\left(\frac{J_m(x_{ml}r/R)}{J_{m+1}(x_{ml})}\right)^2 \sum_{\alpha}\int_0^{\infty} F(E_{\alpha mlk}+U(r,z))\,\mathrm{d}k \tag{8}$$

Defining a two-dimensional grid of (r_i,z_j) points and providing an educated initial guess for the potential profile $V(r_i,z_j)$ into Eqs. (8) and (3), we extract a charge density profile from Eq. (4). Substituting the latter into the discretized Poisson equation, we recalculate the potential using a Gauss-Seidel iteration scheme until convergence is reached.

3 Results

As a typical result, we have shown in Fig. (2) the electron density and the potential profile for a $R=10$ nm nanowire with a $L_{\mathrm{CH}}=20$ nm channel length for three different

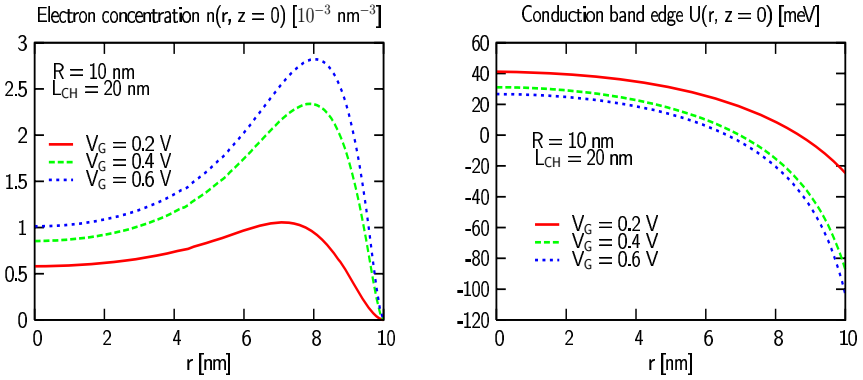

Figure 2: Electron concentration (*left*) and potential energy profile (*right*) in the middle of the channel versus r for various gate voltages V_{G}.

values of the gate voltage V_G. The lateral size quantization is clearly reflected in the electron concentration tending to zero when $r \rightarrow R$. Note also the occurrence of volume inversion emerging from the significant portion of electrons residing in the central part of the wire.
Finally, as a mere illustration, Fig. (3) compares longitudinal potential energy profile at the wire center ($r = 0$) for various channel lengths at zero drain and gate voltages.

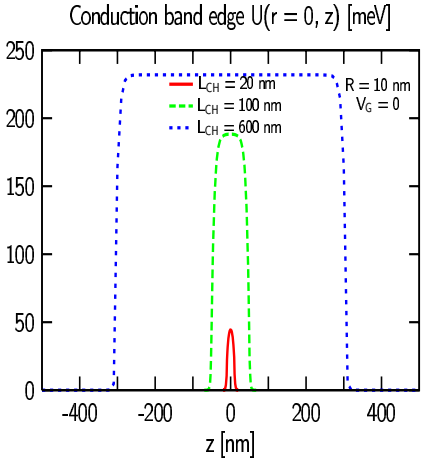

Figure 3: Potential profile (built-in potential) along the z-direction for various channel lengths.

4 Conclusion

Offering a trade-off between quantum mechanical rigor and speed, the above presented Poisson–Schrödinger solver is a promising candidate for implementation in numerical programs that need to rely on a fast evaluation of quantum mechanical charge density profiles in semiconductor quantum wires.

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