Improved Compact Model of Quantum Sub-band Energy Levels for MOSFET Device Application

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Abstract

Compact models for quantum mechanical behavior of transistors are becoming increasingly important as shrinking transistor sizes bring the oxide thickness to below four nanometers. Analytic solutions to Schrödinger's equation are available only for a limited class of energy potential profiles. Much use has been made of the Stern, [1], triangular approximation for the energy well close to the gate oxide. Here an exponential approximation for the silicon potential is used to derive an improved approximation to the energy band levels. The exact analytical solution to Schrödinger's equation is known for this type of potential. Asymptotic approximations to the wave functions are used to find accurate compact formulae for the exact energy levels. These formulae agree more closely with exact numerical results (from SCHRED [2]) for the energy band levels than Stern's results.

Keywords: quantum effect, mosfet, spice, device modeling

1 Introduction

With silicon-oxide dielectric thickness for MOSFET devices shrinking below 4 nm increasing quantum mechanical effects perturb the device characteristics significantly from the predictions of classical models [3]. Quantum effects reduce source-to-drain current from their classical estimates, and tunneling current in the gate region can cause battery run-down. In the quantum mechanical regime the average inversion charge density is no longer at a maximum at the dielectric boundary. With zero charge density at the dielectric-semiconductor surface the effective oxide thickness and the semiconductor band gap are increased over the predictions of the classical model. In order to effectively simulate these nanoscale chips using SPICE, accurate compact models are needed for these quantum effects.

We develop a model for the potential in the semiconductor, previously studied by [4], which approximates the asymptotic model of [5]. This develops previous work of the authors from [3]. In this approximation we have a potential which approximates the behavior of the true potential both near the dielectric-semiconductor boundary, and in the bulk region. Moreover, it yields a version of the Schrödinger equation with a known analytic solution. We use this solution to develop new approximations to the energy levels. Furthermore, such a model may be used in various approximations to the tunneling current.

2 Approximations to the Potential

The quantum mechanical electrostatic potential ψ in the MOSFET is modeled by solving in the quasi-one-dimensional approximation the coupled Schrödinger-Poisson differential equations. The Poisson equation,

$$\epsilon_s \frac{d^2\psi}{dx^2} = q(p - n + N), \qquad (1)$$

requires hole and electron densities from the Schrödinger equation,

$$E\zeta(x) = -\frac{\hbar^2}{2m^*}\frac{d^2\zeta}{dx^2} + V(x)\zeta(x). \qquad (2)$$

In order to derive a compact model for application to the n-channel MOSFET we estimate the potential $V = -q\psi$ using an approximation to equation (1).

2.1 Triangular Approximation

A first approximation for the potential near the barrier between the semiconductor and the gate region is to take the first term of the Taylor Series expansion at $x = 0$. This leads to approximation called the triangular-potential in the literature [1], [3]. Note that the potential is shifted by the surface potential so that it is zero at the surface $x = 0$.

$$V = q\mathbb{E}_s x. \qquad (3)$$

This approximation with reference to inversion layers is due to Stern [1]. The linear potential yields a Schrödinger equation with a known analytic solution in terms of Airy Functions. With boundary conditions on the wave function $\zeta(0) = \zeta(\infty) = 0$ and using asymptotics of the Airy functions for large argument the energy levels are given by

$$E_j^{\text{triangular}} = \left[\frac{\hbar^2}{2m^*}\right]^{1/3}\left[\frac{3}{2}q\pi\mathbb{E}_s(j+3/4)\right]^{2/3} \qquad (4)$$

with $j = 0, 1, 2, ...$

2.2 Exponential Approximation

We model the potential energy in the semiconductor as an exponential,

$$V = \alpha(1 - e^{-x/d}). \qquad (5)$$

This approximation has been used previously in [4]. The parameters α and d are chosen to approximate the potential obtained from [5]. That is

$$\begin{aligned} \alpha &= \lim_{x\to\infty} V(x) \\ d &= \frac{\alpha}{q\mathbb{E}_s}. \end{aligned}$$

Expressions for these values in terms of gate voltage, doping level, and other device parameters are given by explicit formulas in [5]. The time independent Schrödinger Equation (2) is solvable with this exponential potential. Calling $\mu^2 = \frac{\hbar^2}{2m}$ and substituting in the approximated form of the potential, (2) becomes:

$$\frac{d^2\zeta}{dx^2} + \frac{1}{\mu^2}(E - \alpha(1 - e^{-x/d}))\zeta = 0 \qquad (6)$$

Making the substitution

$$\tau = \frac{2d}{\mu}\sqrt{\alpha}e^{-x/2d}$$

(6) is transformed to become Bessel's Equation:

$$\tau^2\frac{d^2\zeta}{d\tau^2} + \tau\frac{d\zeta}{d\tau} + \left[\tau^2 - \left(\frac{2d}{\mu}\sqrt{\alpha - E}\right)^2\right]\zeta = 0. \qquad (7)$$

The solution to (7) can be written in terms of Bessel functions of the first kind with $\nu = \frac{2d}{\mu}\sqrt{\alpha - E}$:

$$\zeta(\tau) = C_1\ J_\nu(\tau) + C_2\ J_{-\nu}(\tau)$$

J_ν and $J_{-\nu}$ constitute the two linearly independent solutions to the second order ODE. Since ν is not an integer, this is a general solution.

$J_{-\nu}(\tau)$ blows up as $\tau \to 0$, so imposing the boundary condition $\zeta = 0$ as $x \to \infty$ requires $C_2 = 0$, leaving us with the solution

$$\zeta(x) = C_1 J_{\frac{2d}{\mu}\sqrt{\alpha-E}}\left(\frac{2d}{\mu}\sqrt{\alpha}e^{-x/2d}\right). \qquad (8)$$

To determine the energy band levels we enforce the approximate boundary condition of no tunneling, $\zeta(0) = 0$. The energy band levels $E < \alpha$ must satisfy:

$$\zeta(0) = J_{\frac{2d}{\mu}\sqrt{\alpha - E}}\left(\frac{2d}{\mu}\sqrt{\alpha}\right) = 0. \qquad (9)$$

The boundary conditions $\zeta(0) = \zeta(\infty) = 0$ result in an eigenvalue problem for the energy level E similar to the one for the triangular potential. That eigenvalue problem is expressed in the equation for E which we obtain from (9) by substituting $a = \sqrt{\frac{\alpha}{\alpha - E}} = \sec\beta$

$$J_\nu(\nu \sec\beta) = 0. \qquad (10)$$

For $\nu \gg 1$ there is an asymptotic expansion [7]
,

$$0 = J_\nu(\nu\sec\beta) \sim \frac{\cos\left[\nu(\tan\beta - \beta) - \frac{1}{4}\pi\right]}{\sqrt{\frac{1}{2}\nu\pi\tan\beta}}. \qquad (11)$$

or

$$\tan\beta - \beta = \frac{(j + \frac{3}{4})\pi}{\nu} = \frac{(j + \frac{3}{4})\pi}{\frac{2d}{\mu}\sqrt{\alpha}} \frac{1}{\cos\beta}.$$

Calling $\kappa = \frac{(j+\frac{3}{4})\pi}{\frac{2d}{\mu}\sqrt{\alpha}}$,

$$\sin\beta - \beta\cos\beta = \kappa. \qquad (12)$$

For low energy levels it is expected that β will be small enough (on the order of 0.5) to make Taylor series expansions for $\sin\beta$ and $\cos\beta$ in (12) however not so small as to invalidate the asymptotic in equation (11). Making these approximations yields

$$\beta \approx (3\kappa)^{1/3}. \qquad (13)$$

When we take the first term of the Taylor series for $\sin\beta$ in $\frac{E}{\alpha} = \sin^2\beta$ this approximation for β (13) directly yields the Stern triangular result of (4). Using more sophisticated approximations and putting $\beta = (3\kappa)^{1/3}\varphi$ yields

$$\varphi^3 - 3\delta(3\kappa)^{2/3}\varphi^5 =$$
$$\left(1 - \gamma(3\kappa)^{2/3}\varphi^2 + \delta(3\kappa)^{4/3}\varphi^4\right)\left(1 - \frac{1}{3}(3\kappa)^{2/3}\varphi^2\right)^{-3/2},$$

where the constants δ and γ and the approximations used are defined in the appendix. Taking (13) or $\varphi_1 = 1$ as an initial guess, we get the improved approximation

$$\varphi_2^3 = \frac{1 - \gamma(3\kappa)^{2/3}}{1 - 3\delta(3\kappa)^{2/3}}\left(1 - \frac{1}{3}(3\kappa)^{2/3}\right)^{-3/2}. \qquad (14)$$

We now have an improved approximation for the energy level $\frac{E}{\alpha} = \sin^2\beta$ where $\beta = (3\kappa)^{1/3}\varphi_2$ and φ_2 is given by (14).

3 Results and Comparison

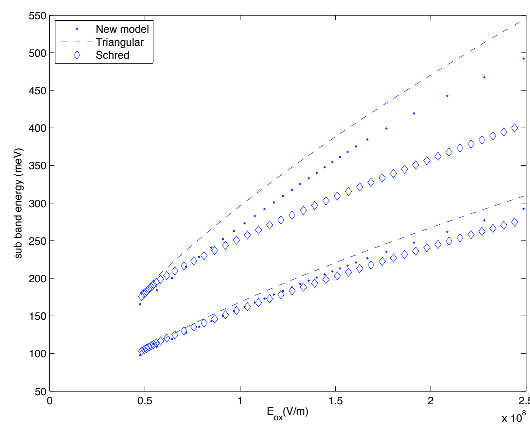

Figure 1: Energy band level for triangular and exponential approximations compared with numerical results from SCHRED at various $\mathbb{E}_{ox}$. The first two energy levels are shown.

The energy band levels derived from (14) is a very accurate approximation of the exact energy band levels of the exponential model potential (5). More importantly, it is an improved approximation to the ground level energy for a wide range of surface electric fields as can be seen in Figure 1.

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