

# Self-consistent modeling of accumulation layers and tunneling currents through very thin oxides

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Poisson and Schrödinger equations are solved self-consistently for accumulated layers in metal-oxide-semiconductor devices and applied to the calculation of tunneling currents at 300 K and 77 K and extraction of parameters for very thin oxides. Calculations at 300 K show strong agreement with measured tunneling currents and also point out the sources of inaccuracies in extracting thicknesses of oxides by electrical methods such as through measurement of capacitance. Direct tunneling current in thin oxides (1.5–2.0 nm) are shown to achieve larger than 1 A/cm<sup>2</sup> current density for applied voltages smaller than 3 V, pointing to possibilities of achieving high endurance injection across thin oxides. Comparison of calculations using a classical approach and self-consistent approach shows fortuitous agreements in tunneling currents despite large differences in the physical models. Appropriate methods for calculating tunneling currents from bound and extended quantum states are also described. © 1996 American Institute of Physics. [S0003-6951(96)00834-0]

An accurate description of metal-oxide-semiconductor devices requires careful modeling of inversion and accumulation layers at the semiconductor-oxide interface. Importance of quantum effects in inversion and accumulation layers are well known<sup>1</sup> and have been extensively studied for inversion layers<sup>2,3</sup>. Self-consistent modeling of accumulation layers has received less attention<sup>4–6</sup> even though determination of device parameters such as oxide thicknesses from capacitance measurements require an accurate description of accumulation layers. Self-consistent description is also necessary for any model which describes tunnel injection from accumulation layers. Some forms of electrically erasable programmable memories<sup>5</sup> employ such tunneling. Also, some recent demonstrations of memory structures employ charge storage in small silicon quantum dots by low field tunnel injection of electrons through very thin oxide layers.<sup>7</sup> With the continuing reduction in oxide thicknesses in transistors, the errors due to inaccuracies in modeling and extraction are becoming increasingly serious.

Self-consistent calculations of accumulation layers are more complex than those of inversion layers due to the absence of a separation region between the bulk extended states and the quasibound states near the interface. In case of inversion layers this separation is provided by the depletion region. The solution to this problem is to treat both extended and bound states equally. For the *n*-Si/SiO<sub>2</sub>/*n*<sup>+</sup>-polycrystalline silicon structure of Fig. 1, the self-consistent calculation starts using a question of the electrostatic potential in the form

$$\phi(x) = A \exp\left(-\frac{x}{\alpha l_D}\right) + B \exp\left(-\frac{x}{\beta l_D}\right) \quad (1)$$

for  $0 \leq x \leq L$ ,

$$\phi(x) = \phi(0) - F_{ox}x \quad \text{for } -t_{ox} \leq x \leq 0, \quad (2)$$

where  $F_{ox}$  is the field strength in the oxide and is related to the parameters  $A, B, \alpha$ , and  $\beta$ . The values of these parameters are chosen empirically to give the best results.  $l_D$  is the Debye length ( $\sqrt{e^2 N_D / \epsilon_{Si} k T}$ ) of bulk silicon. The Schrödinger equation in the effective mass approximation is solved in the region  $-t_{ox} \leq x \leq L$  by using the finite difference method with the boundary conditions on the electron wave function:

$$\psi(-t_{ox}) = \psi(L) = 0$$

and

$$\frac{1}{m_{Si}} \frac{d\psi(x=0^+)}{dx} = \frac{1}{m_{SiO_2}} \frac{d\psi(x=0^-)}{dx}. \quad (3)$$

Eigenvalues of the Hamiltonian are computed using Sturm sequencing and bisection and the eigenvectors are found by performing inverse iteration. For a (100) silicon surface, the total charge density,  $\rho(x)$ , is

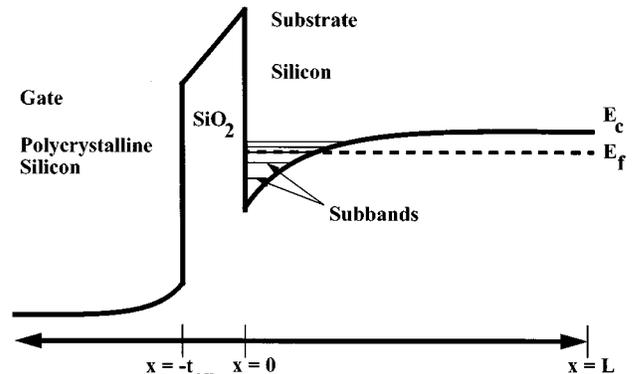


FIG. 1. Schematic band profile for the structure used in self-consistent calculations defining some of the structural parameters.

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$$\rho(x) = eN_D - \frac{4e\sqrt{m^t m^l} kT}{\pi \hbar^2} \times \sum_n \log \left[ 1 + \exp\left(\frac{E_f - E_n^t}{kT}\right) \right] |\psi_n^t(x)|^2 - \frac{2em^l kT}{\pi \hbar^2} \times \sum_n \log \left[ 1 + \exp\left(\frac{E_f - E_n^l}{kT}\right) \right] |\psi_n^l(x)|^2. \quad (4)$$

The superscript  $t(l)$  on the wave function indicate that they belong to the valley where the electron mass perpendicular to the interface is  $m^t(m^l)$ . Charge density obtained from Eq. (4) is used to solve the Poisson equation using the finite difference method with boundary conditions

$$\phi(x = -t_{\text{ox}}) = V_{\text{gate}} - V_{\text{flat band}}, \quad \phi(x = L) = 0, \quad \text{and} \quad \epsilon_{\text{Si}} \frac{d\phi(x=0^+)}{dx} = \epsilon_{\text{SiO}_2} \frac{d\phi(x=0^-)}{dx}. \quad (5)$$

The potential obtained from the Poisson equation is compared with the potential used in the Schrödinger equation with the  $(n+1)$ th iteration derived from the  $n$ th iteration using

$$\phi^{n+1}(x) = \phi^n(x) + r^{n+1}(x) [\phi_{\text{poisson}}^n(x) - \phi^n(x)]. \quad (6)$$

The function  $r^n(x)$  ( $0 < |r^n(x)| < 0.1$ ) is empirically chosen to speed up convergence. The boundary condition  $\psi(x=L)=0$ , produces a net positive charge density near  $x \approx L$ . As long as the length  $L$  of the region is chosen long enough so that there exists a quasineutral region between the accumulation layer and the artificial pile-up region near  $x \approx L$ , the calculation is realistic and accurate.

In case of extended states, transmission probability through the SiO<sub>2</sub> barrier is a well defined concept and has a value equal to the ratio of transmitted and incident flux. Total current from the extended states is

$$J_{\text{extended}} = e \int \frac{\hbar k_x}{m_x} T(k) \{ f[E(k) - E_{fL}] - f[E(k) - E_{fR}] \} \frac{d^3 \mathbf{k}}{(2\pi)^3}, \quad (7)$$

where the integral is taken over all extended states in the accumulation layer. Transmission probability is not a meaningful concept for quasibound states. For a quasibound state, lifetime (or the decay time) of the state is well defined provided that the state of the particle is decaying into a large number of possible final states. This lifetime can be calculated by various techniques such as a path integral expansion of the resolvent operator<sup>8</sup> or using the transfer Hamiltonian approach. The lifetime is approximately given by<sup>9</sup>

$$\frac{1}{\tau_n(E_t)} = \frac{T(E_t)}{\int_0^{x_n} \sqrt{2m_x} / [E_n - E_c(x)] dx}. \quad (8)$$

$T(E_t)$  is the transmission probability of a particle and depends on its total energy  $E_t$  ( $E_t = E_n + E_{\parallel}$ ).  $E_n$  is the subband energy for the quasibound state,  $E_c(x)$  is the bottom of the conduction band, and  $x_n$  is the classical turning point for the  $n$ th bound state. Lifetimes calculated this way turn out to be much greater than energy relaxation times in the accumula-

tion layer even for very thin oxides. Thus, it is justifiable to assume that the quasi-Fermi level for the bound states has a well defined value. We also assume that this value is equal to that in the bulk even when tunneling current is not zero. This latter assumption may not be justified at large gate voltages under conditions of high injection. With these approximations, the total tunneling current from bound states is

$$J_{\text{bound}} = \frac{4e\sqrt{m^t m^l} kT}{\pi \hbar^2} \sum_n \log \left\{ \frac{(1 + \exp[(E_{fL} - E_n^t)/kT])}{(1 + \exp[(E_{fR} - E_n^t)/kT])} \right\} \times \frac{1}{\tau_n(E_n^t)} + \frac{2em^l kT}{\pi \hbar^2} \times \sum_n \log \left\{ \frac{1 + \exp[(E_f - E_n^l)/kT]}{1 + \exp[(E_{fR} - E_n^l)/kT]} \right\} \frac{1}{\tau_n(E_n^l)}. \quad (9)$$

Total tunneling current is the sum of  $J_{\text{extended}}$  and  $J_{\text{bound}}$ . We have assumed here that transmission probability depends only on the energy component perpendicular to the interface. Expression for transmission probability in terms of Airy functions is given by Gundlach<sup>10</sup>. We assume that the energy dispersion relation in the midgap region of SiO<sub>2</sub> is described by effective mass  $m_{\text{ox}} = 0.5m_0$ . The barrier height due to conduction band discontinuity at the Si/SiO<sub>2</sub> interface is taken to be 3.15 eV. Effects due to image forces are ignored.

Figure 2 shows the calculated tunneling currents at 300 K for oxides of thicknesses 1.5, 2.0, 2.5, 3.0, and 3.5 nm. Experimental results are shown by the shaded regions in the plot with the thickness indicated adjacent to the shading. These shaded regions correspond to measurements made on different samples with the same oxide thickness. The large width of the distribution at small thickness are representative of the current state of art. The measurements at larger thicknesses are performed on larger areas (nearly 1 cm<sup>2</sup>) resulting in possible excess current from defect currents. All samples had an  $n$ -Si substrate with a doping concentration of  $\sim 10^{17}$  cm<sup>-3</sup>. The  $n^+$  polysilicon gates had a doping concentration of about  $5 \times 10^{19}$  cm<sup>-3</sup>. For the voltage range shown, tunneling occurs in the direct regime. The agreement with experimental results is good **without the use of fitting parameters!**

The classical and self-consistent models yield almost the same tunneling currents. The reason for this can be understood from Fig. 3 which shows the potential drop in the semiconductor as a function of gate voltage for the classical and self-consistent solutions. Self-consistent solution gives a greater potential drop in the semiconductor than that given by the classical solution. Consequently, the electric field in oxide is larger in the classical case. Tunneling rates from both bound and extended states depend exponentially on the electrons' energy perpendicular to the barrier and the field strength in the barrier. Although, the classical model gives a higher field inside the SiO<sub>2</sub> barrier, the electrons have, on average, higher energy in the self-consistent model as a result of energy quantization. As the gate voltage increases, the difference in oxide fields predicted by the classical and self-consistent models increases, but at the same time the energies of quasi-subbands in the self-consistent model also increase, making the tunneling currents predicted by both

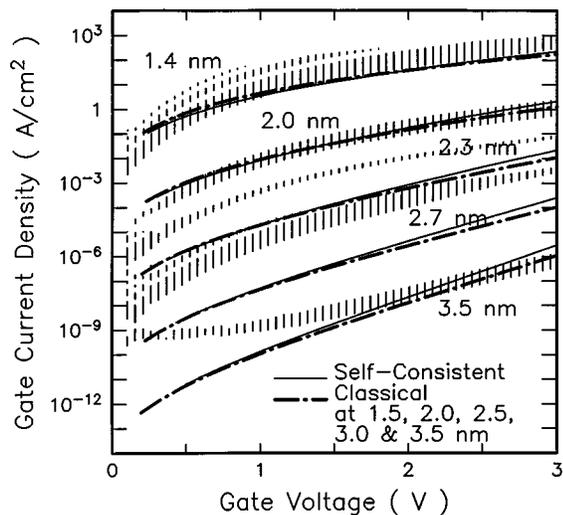


FIG. 2. Calculated and experimental results for tunneling currents at 300 K. The  $n$ -type substrate doping for each case is  $\approx 10^{17} \text{ cm}^{-3}$  and the doping of the  $n$ -type polycrystalline silicon gate is  $\approx 5 \times 10^{19} \text{ cm}^{-3}$ . The thicknesses of the calculated curves are marked on the left while the ellipsometric thickness of experimental measurements, whose lower and upper bound defines the shaded region, are marked on the right. Calculations include depletion in the polysilicon gate.

models almost the same over a wide range of gate voltages. Tunnel injection from inversion layers should behave similarly.

Figure 4 emphasizes the relative errors inherent in measuring oxide thickness if the classical model is used in electrical characterization of very thin oxides. The relative error increases with a decrease in oxide thickness. In the classical model the peak of accumulation layer charge density occurs right at the oxide-semiconductor interface. In the self-consistent model the centroid of charge density is always a few angstroms away from the oxide-semiconductor interface.

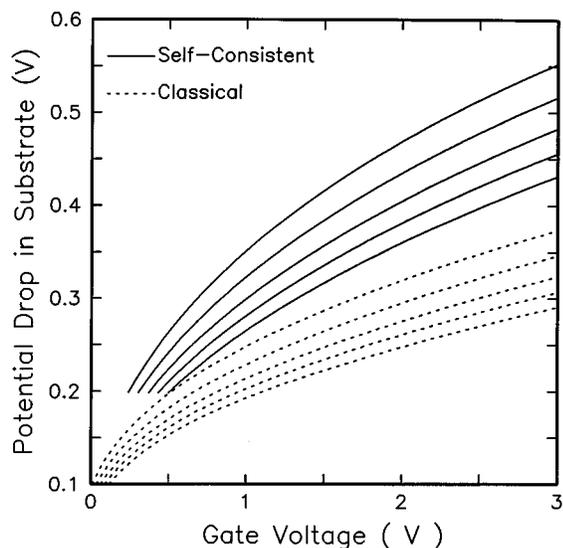


FIG. 3. Potential drop in bulk semiconductor obtained from self-consistent and classical models as a function of the difference between gate voltage and flat-band voltage. The top curve for each set is for 1.5 nm oxide with successive curves for 2.0, 2.5, 3.0, and 3.5 nm. The substrate is  $n$ -type with a doping of  $10^{17} \text{ cm}^{-3}$ .

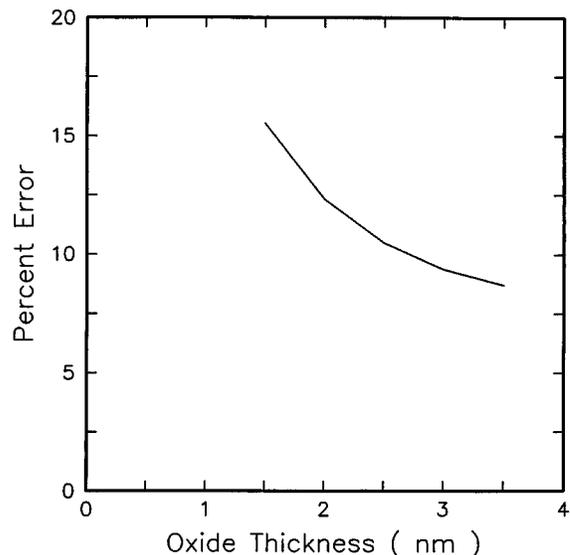


FIG. 4. Relative (%) error in extraction of oxide thickness with the classical model at 300 K for an  $n$ -type substrate with a doping of  $10^{17} \text{ cm}^{-3}$ .

This distance becomes a larger fraction of the actual oxide thickness as the oxide thickness decreases. Thus, the classical model yields a larger relative error for thinner oxides and should be carefully utilized in fitting device models for currently researched structures such as those of Rodder *et al.*<sup>11</sup>

We have presented a method to obtain self-consistent results for accumulation layers. A method to calculate tunneling currents from bound states is also described which is free from conceptual problems associated with the usual approaches. We conclude that electron tunneling in the direct regime can be reasonably well described by effective mass theory even for very thin oxides. However, it remains a mystery whether the good agreement is by chance or that crystalline effective mass theory really captures the essential physics for describing tunneling through amorphous thin films.

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