# A Compact model to Predict Quantized Sub-Band Energy Levels and Inversion Layer Centroid of MOSFET with the Parabolic Potential Well Approximation

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## **1. Introduction**

Scaling of MOSFETs into nano-scale requires use of ultra-thin gate oxide layer and high substrate doping concentration in the substrate. This results in a high transverse field. Such a strong interfacial field gives rise to the significant quantization mechanical effects (QME) [1-2]. Traditionally, the triangular well approximation has been widely used for MOSFET compact modeling[1,3]. However, the real MOSFET always operates in the inversion region where the potential in the semiconductor retains one parabolic well distribution as shown by the numerical analysis and theoretical prediction [4,5]. In this case, the triangular well approximation leads to large error in calculating both the inversion layer centriod and the sub-band energy levels.

A novel compact model to predict the inversion-layer centroid and the QME sub-band energy levels has been developed in this paper based on a parabolic potential well approximation. From the WKB method, a simplified coupled solution of Poisson and Schrodinger equations is obtained. Then, the analytical expressions of quantized sub-band energy levels and the inversion layer centroid are derived and their predictions show a good agreement with the numerical results.

#### 2. Compact model derivation

The MOSFET with the uniformly doped substrate and (100) oriented p-type silicon is considered here. Following the semiconductor device physics, the semiconductor energy band bending creates a potential well support by depletion charge and inversion layer electrons. Since electrons present in this well occupy a set of energy sub-bands, which distribution energy and wave function should follow the Schrodinger equation

$$\left[-\frac{h^2}{2m^*}\Delta + eV(z)\right]\psi_{ij}(x, y, z) = E_{ij}(x, y)\psi_{ij}(x, y, z)$$
(1)

where  $m^*$  is the mass tensor, V(z) is the electrostatic potential, and  $E_{ij}$  and  $\Psi_{ij}$  are energy eigenvalue of and wave function, respectively, of jth sub-band in ith valley.

The potential V(z) is defined with respect to the potential at the interface and varies with the space charge due to depletion of hole and, if present, also by the inversion layer electrons. The potential can be calculated from Poisson equation

$$\frac{d^{2}V(z)}{dz^{2}} = \frac{e\sum_{ij}\int_{-\infty} dz \,\psi_{ij}(z)\psi_{ij}^{*}(z)n_{ij} + eN_{a}}{\varepsilon_{si}}$$
(2)

the potential at z = 0 or semiconductor surface is defined to be zero and the gradient is taken to be  $-F_s$ , the electrical

field at the interface. Here  $N_a$  represents the background depletion charge density.

Although there are several ways to approach the numerical solution of Schrodinger equation, we will look at the WKB(Wentzel-Kramer-Brillouin) method of finding the approximate eigenvalues. To solve explicitly Schordinger equation, one important classical assumption, the effective mass approximation (EMA), is firstly applied to de-coupe 3-D Schordinger equation into 1-D case that describes the wave function perpendicular to the interface,  $\Psi_{ii}(z)$ , that constrains the Bloch waves traveling parallel to the interface (x-y plane). And then, the Schordinger Eq.(1) is solved approximately by the use of WKB( Wentzel-Kramer-Brillouin) method. This approach, which is quite accurate, is based on the Bohr theory of quantization of action and is conceptually simple. The Bohr theory postulated that for stable quantum states, the electron motion must have quantized " action", defined as the integral of the momentum over the orbit. In the case of vibration motion bounded on the left conduct edge bottom and right eigenvalue level, or the semiconductor surface inversion layer thickness, which meaning the inversion layer centroid, the action is defined by the integral of the momentum being those quantized eigenvaue levels from WKB method.

In solving Poisson equation, a corrected parabolic potential well approximation (CPPWA) is used, which assuming that a parabolic potential well is always available either in depletion or inversion states and the quantum effect of non-zero inversion layer charge thickness does not change the substrate depletion depth and charge, as shown in Fig.1. In traditional parabolic potential well case, the surface field is determined by the depletion charges. In CPPWA, the surface field is determined by the combination of depletion charges and inversion layer charges. As a result, the traditional surface field is corrected by adding inversion charge effects so as to result in an effective surface field. Such a treatment great simplifies solving the Poisson equation. In the following discussion, an effective surface field expression is followed in order to avoid complex integral:

$$E_{eff} = (Q_B + \eta Q_{inv}) / \varepsilon_{si}$$
(3)

where  $\eta$  is often treated as a constant, being 0.5 for electrons and 0.3 for holes in mobility extraction and characterization. In fact, this parameter has a quantum effect characteristic, which will be discussed later.

Inversion charge centroid is commonly defined as

$$z_I = \int zndz / \int ndz \tag{4}$$

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This definition features the statistical meaning, it is, however, very difficult in computing due to integral involving infinite edge. In our treatment, a new physics based inversion charge centroid definition, originally coming from WKB method, which means the inversion layer centroid is a potential well depth at which electron eigenvalue is equal to the parabolic potential this depth corresponds to is used

$$z_{I} = z_{0} \Big|_{U^{'}(z_{0}) = E_{ij}}$$
(5)

This new definition is easy determined and demonstrates the quite same magnitude with the statistics definition to first order approximation. More importantly, the definition coincides well with the WKB method.

All assumptions above are demonstrated in Fig.1, where classical parabolic well approximation, corrected parabolic potential well approximation due to quantum effect and its resulting in subband levels and corresponding inversion layer centroids, and quantum effect contribution to surface potential are all figured.

Considering a 1-Dimensional MOS capacitance case, in general parabolic case, the electrostatic potential under the gate can be written from the depletion approximation

$$\frac{d^2\phi(z)}{dz^2} = \frac{eN_a}{\varepsilon_{si}} \tag{6}$$

where z is the distance in cm of the semiconductor bulk form the semiconductor surface.

Integrating (6) gives

$$\frac{d\phi(z)}{dz} = \frac{eN_a}{\varepsilon_{si}} \left( z - d_{\max} \right) \tag{7}$$

$$\phi(z) = -\frac{eN_a}{2\varepsilon_{si}} \left( 2zd_{\max} - z^2 \right) = \frac{E_s}{2d_{\max}} \left( z^2 - 2zd_{\max} \right) \tag{8}$$

where  $d_{\text{max}}$  is the maximum depletion depth in the semiconductor bulk of MOS, which is given

$$d_{\max} = \frac{Q_B}{N_a} = \sqrt{\frac{4\phi_F \varepsilon_{si}}{eN_a}}$$
(9)

and  $E_s$  is surface maximum field, which is expressed as

$$E_s = \frac{eN_a}{\varepsilon_{si}} d_{\max} = \frac{Q_B}{\varepsilon_{si}}$$
(10)

If we define the carrier energy  $U(x) = -e\phi(z)$ , combining Eqs.(7) and (8) gives

$$U(z) = -\frac{eE_s}{2d_{\max}} \left( z^2 - 2zd_{\max} \right) \tag{11}$$

Eqs. (8) gives the magnitude of the maximum electrostatic potential

$$\phi_{\max} = \frac{eN_a d_{\max}^2}{2\varepsilon_{si}} \tag{12}$$

where  $\phi_{\text{max}}$  is the maximum surface potential without including the effect of non-zero thickness of the inversion charges.

Since the inversion charge effect on the surface field is added to that determined by the depletion charges, under CPPWA case, an effective surface field  $E_{eff}$  as defined by Sabnis and Clemens, which is the average transverse electrical

field in the inversion layer, is used replacing the surface field determined by depletion charges in electrostatic potential and carrier energy expressions for considering the effect of the inversion charges

$$\phi'(z) = -\frac{E_{eff}}{2d_{\max}} \left( 2zd_{\max} - z^2 \right)$$
(13)

$$U'(z) = -\frac{eE_{eff}}{2d_{\max}} \left( z^2 - 2zd_{\max} \right)$$
(14)

where  $\phi'(z)$  and U'(z) are the electrostatic potential and carrier energy distribution including the effect of non-zero thickness of inversion charges, respectively.

Eqs. (13) and (14) imply a parabolic potential well in MOSFET's surface layer, which being in contrast with the previous triangular potential well, as shown in Fig.2. Many numerical analyses revealed a parabolic potential well is more realistic to the practical case of MOSFETs compared with a triangular potential well approximation.

Comparing the classical depletion approximation and CPPWA, it is easy found that the magnitude of the maximum electrostatic potential of CDA slightly increases by  $\eta Q_{in}d_{max}$ 

 $\frac{\eta Q_{in} d_{\max}}{2}$  due to adding the effect of the inversion charges,

which is just the quantum effect, as given by Eq.(13)

$$\phi_{\max}^{\prime} = \frac{E_{eff} d_{\max}}{2} = \frac{e N_a d_{\max}^2}{2\varepsilon_{si}} + \frac{\eta Q_{in} d_{\max}}{2} = \phi_{\max} + \frac{\eta Q_{in} d_{\max}}{2\varepsilon_{si}}$$
(15)

Comparing Eq.(15) and the pioneering paper on influence of the inversion layer centroid on the total band bending on a MOS capacitor [7] gives

$$\eta = \frac{2z}{d_{\max}} \tag{16}$$

This expression will be used to determine parameter  $\eta$ .

According to concept of WKB method, solving Eqs.(5) and (14) gives the inversion layer centroid:

$$z_{I} = d_{\max} \left[ 1 - \sqrt{1 - \frac{2E_{ij}}{eE_{eff}d_{\max}}} \right] = d_{\max} \left[ 1 - \sqrt{1 - \frac{E_{ij}}{e\phi_{\max}}} \right]$$
(17)

The physical key of the quantum mechanical effects lies in that energy levels of electrons present in the quantized form. According to WKB method, the electron wave function in the inversion layer can be expressed in the following way

$$\psi_{ij}(z) = \frac{A}{\sqrt{k_{ij}(z)}} \sin\left(\int k_{ij}(z)dz + \frac{\pi}{4}\right)$$
(18)

where A is a normalization constant and

$$k_{ij} = \frac{P}{h} = \sqrt{\frac{2m_z (E_{ij} - U'(z))}{h^2}}$$
(19)

where h is Planck constant and P is the electron quantized momentum.

Since assuming that the inversion electrons are localized in the infinite inversion layer, which should imply that the electron wave function at the semiconductor surface and the maximum inversion layer vanishes, thus electron wave function is limited only in the parabolic potential well under WKB approximation. It requires  $\sin\left(\int k_{ij}(z)dz + \frac{\pi}{4}\right) = 0$  in two classical turning

points, thus  $\left(\int k_{ij}(z)dz + \frac{\pi}{4}\right) = n\pi$  if the integral range is from

the semiconductor surface to the maximum inversion layer, namely, from zero to  $z_I$ .

After substituting Eq.(19) into this condition, the following expression is obtained:

$$\int_{0}^{z_{l}} \frac{P}{h} dz = n\pi - \frac{\pi}{4}$$
(20)

where *n* is the quantum level number, n=1,2,3...6.

Substitution of Eqs. (17) and (19) to perform the integral of Eq. (20) gives

$$d_{\max}\sqrt{\frac{2d_{\max}E_{ij}}{eE_{eff}}} + \left(d_{\max}^2 - \frac{2d_{\max}E_{ij}}{eE_{eff}}\right) \left[\ln\sqrt{d_{\max}^2 - \frac{2d_{\max}E_{ij}}{eE_{eff}}} - \ln\left(d_{\max} + \sqrt{\frac{2d_{\max}E_{ij}}{2E_{eff}}}\right)\right] = 2\pi h \left(n - \frac{1}{4}\right) \sqrt{\frac{d_{\max}}{m_e e_{eff}}}$$
(21)

The expression is a transcendental equation that the inversion electrons in silicon MOS surface layer satisfied. It is evident that  $E_{ij}$  is related with the quantum number *n*, e.g.,  $E_{ij} = E(n)$ . It is very interesting that the inversion thickness can be exactly determined from Eq. (17) as long as sub-band energy levels are known. However, an analytical solution of Eq. (21) is hardly to be found.

Generally, the quantized energy is always less than that in the whole depletion region. In this case, assumption  $E_p \leq \frac{1}{2}eE_{eff}d_{max}$  can give a trial solution of Eq.(21). The use

of this condition simplifies the exponential part of Eq. (21) via the Taylor expansion:

$$\left[\ln\sqrt{d_{\max}^2 - \frac{2d_{\max}E_{ij}}{eE_{eff}}} - \ln\left(d_{\max} + \sqrt{\frac{2d_{\max}E_{ij}}{eE_{eff}}}\right)\right] \approx -\sqrt{\frac{2E_{ij}}{eE_{eff}d_{\max}}}$$
(22)

Substitution of Eq. (22) into Eq.(21) gives  $\frac{1}{2}$ 

$$E_{ij} = \left(\frac{e^2 E_{eff}^2 h^2}{2m_z}\right)^{\frac{1}{3}} \left[\pi \left(n - \frac{1}{4}\right)\right]^{\frac{2}{3}}$$
(23)

Eqn. (23) is an analytical solution of the sub-band energy levels of 2-D electrons in MOS surface layer with the corrected parabolic potential well.

Combining Eqs.(17) and (23) gives the final expression of the inversion layer centroid

$$z_{I} = d_{\max} \left[ 1 - \sqrt{1 - \frac{\left[ \pi h (2n - 1/2) \right]^{2/3}}{(em_{z} E_{off})^{1/3} d_{\max}}} \right] = d_{\max} \left[ 1 - \sqrt{1 - \frac{E_{ij}}{e\phi_{\max}}} \right]$$
(24)

Moreover, the parameter  $\eta$  is given by solving Eqs.(5) and (24)

$$\eta = 2 \left[ 1 - \sqrt{1 - \frac{\left[\pi h (2n - 1/2)\right]^{2/3}}{(em_z E_{eff})^{1/3} d_{\max}}} \right] = 2 \left[ 1 - \sqrt{1 - \frac{E_{ij}}{e\phi_{\max}}} \right]$$
(25)

## 3. Result and discussion

Fig.2 shows the difference between the triangular well and the parabolic approximations. Fig.3 shows the QM subband energy level comparisons between the result of the triangular well and the parabolic approximation and the numerical result [1, 7-8] for the substrate doping 1e17cm-3. It is evident that the parabolic result is more close to the numerical.

More interesting is that (24) can degrade into the inversion layer centriod expression derived by the variation method [6] if the Taylor expansion is used. The numerical calculation has demonstrated existence of such multiple inversion charge centroids. Fig.4 shows the comparison of the inversion layer centroids of the different sub-band energy level for the substrate doping concentration 1e18 cm-3. It is found the higher of the sub-band energy level, the larger the inversion layer centroid is. For device and circuit compact modeling, an average inversion charge centroid can be evaluated from this analytical model via the maserjian ruler of the inversion charge centroid. The result comparison with the numerical solution [5,9] is shown in Fig.5. Fig.5 also demonstrates the effect of the different substrate doping concentration on the inversion centroid, which indicates the higher the substrate doping, the smaller the inversion centroid.

More importantly, this compact model predicts the dependence of the inversion charge weight factor of (1) on the effective field, as shown in Fig.6.

## 4. Conclusions

A compact model to predict the sub-band energy levels and inversion charge centroid in MOS surface inversion layer has been presented for the parabolic potential well approximation. Based on coupled solution of Schrodinger equation and Poisson equation from the WKB method, one transcendental equation of sub-band energy level has been rigorously derived and then the approximate analytical solutions for the subband energy levels and inversion charge centroid have been obtained. Analytical results are compared with the numerical result and good agreement between the analytical and numerical is found.

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Fig.1 Diagram of definition of inversion charge centroid of different energy levels and effect of quantum effect on the potential distribution.



Fig.2 Diagram of difference between triangular well potential approximation and the parabolic approximation.



Fig.3 Comparison of quantized sub-band energy levels predicted by the triangular well approximation, the parabolic approximation and the self-consistent solution [7,8].



Fig.4 Inversion layer centroid of the different sub-band energy levels versus the effective field.



Fig.5 Average inversion layer centroid comparison between the analytical and the numerical result[5,9].



Fig.6 Inversion charge weight factor versus the effective field.