

Incorporation of quantum mechanical effects in compact models of bulk MOSFETs

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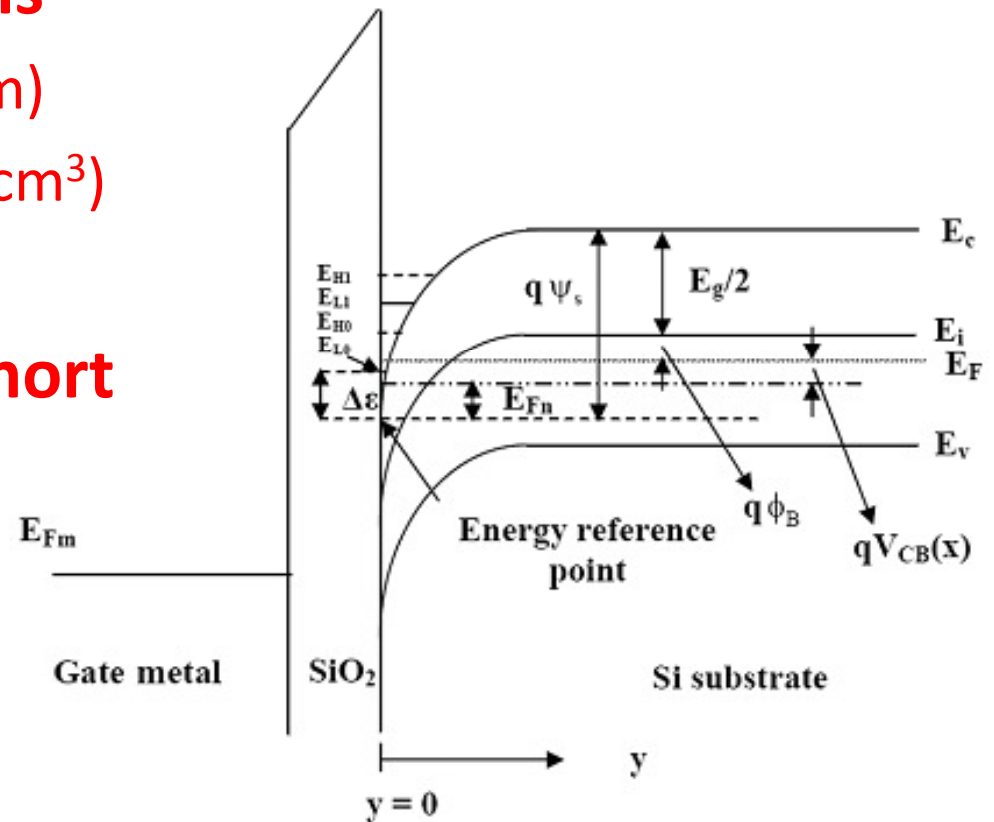
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Organization of talk

- **Quantum mechanical effects**
 - What & Why?
 - Effect on device parameters
- **Modification of parameters**
 - Bandgap
 - Intrinsic carrier concentration
 - Oxide thickness
 - Threshold voltage
 - Surface potential
- **Proposed surface potential based model**

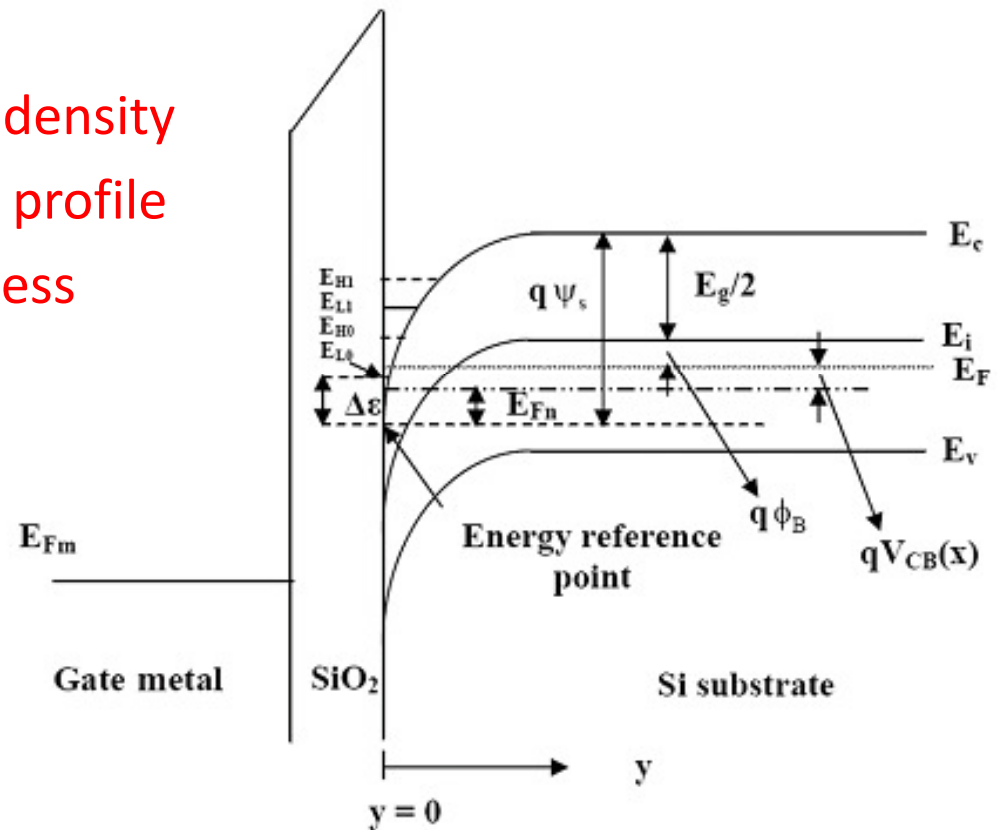
QM effect - Why & What?

- **Scaling of device dimensions**
 - Lower oxide thickness ($< 2 \text{ nm}$)
 - Higher doping conc. ($> 10^{18} / \text{cm}^3$)
 - **Higher electric field**
- **Carriers are confined in a short distance from the Si/SiO₂ interface**
 - **Creation of sub-bands**
- **Classical theory no longer sufficient for modelling**



What is the result of QM effect?

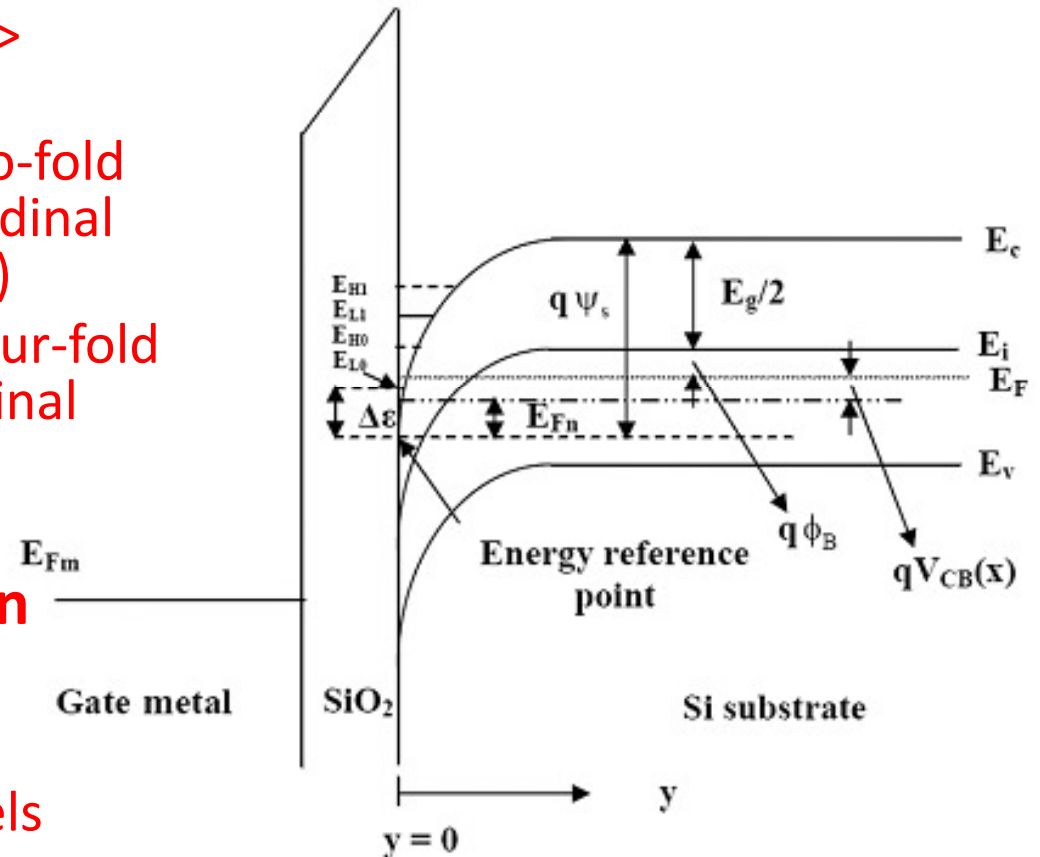
- QM effects result in
 - Increased effective bandgap
 - Reduced inversion layer charge density
 - Modified inversion layer charge profile
 - Increased effective oxide thickness
 - Reduced gate capacitance
 - Modified surface potential
 - Increased threshold voltage
 - Modified carrier mobility
 - Lower drain current
 - Modified gate current



G.S. Jayadeva & A. DasGupta, "Quantum mechanical effects in bulk MOSFETs from a compact modelling perspective: A review", IETE Technical Review, vol. 29, no.1, pp. 3 – 28, Jan-Feb 2012

Calculation of inversion charge

- **Consider formation of sub-bands**
 - Two set of sub-bands for $\langle 100 \rangle$ silicon surface
 - Lower ladder (E_{L0}, E_{L1}, \dots) is two-fold degenerate with heavy longitudinal effective mass ($m_{yL} = 0.916 m_0$)
 - Higher ladder (E_{H0}, E_{H1}, \dots) is four-fold degenerate with light longitudinal effective mass ($m_{yL} = 0.19 m_0$)
- **Solve Schrödinger and Poisson equations self-consistently**
 - computationally very intensive
 - not suitable for compact models
 - benchmark for simpler models



F. Stern and W.E. Howard, "Properties of semiconductor surface inversion layer in the electric quantum limit", Phys. Rev., vol. 163, pp. 816-835, 1967.

Self Consistent Poisson-Schrödinger equation solution

- **Poisson equation (polysilicon, oxide and silicon region)**
 - **Boundary condition : $\phi(z) = V_G$ at the gate contact $\phi(z) = 0$ and at the bulk**

$$\frac{d}{dz} \left[\epsilon(z) \frac{d\phi(z)}{dz} \right] = q \left[N_D^+(z) - N_A^-(z) - n(z) + p(z) \right]$$

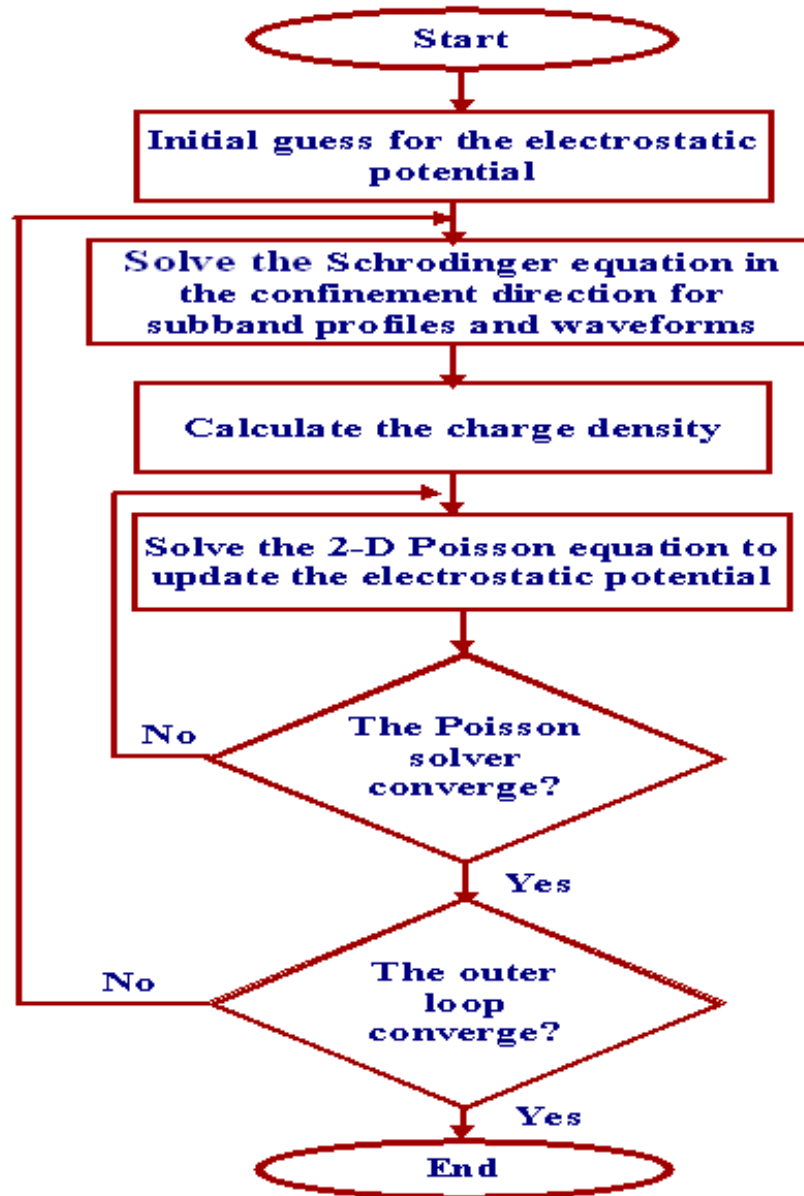
- **Schrodinger equation (dielectric and silicon regions)**
 - **Boundary condition : $\psi_{ij} = 0$ at the gate dielectric interface**

$$\left[-\frac{\hbar^2}{2} \frac{d}{dz} \frac{1}{m_{di}^*} \frac{d}{dz} + V(z) \right] \psi_{ij}(z) = E_{ij} \psi_{ij}(z)$$

- **Electron concentration**

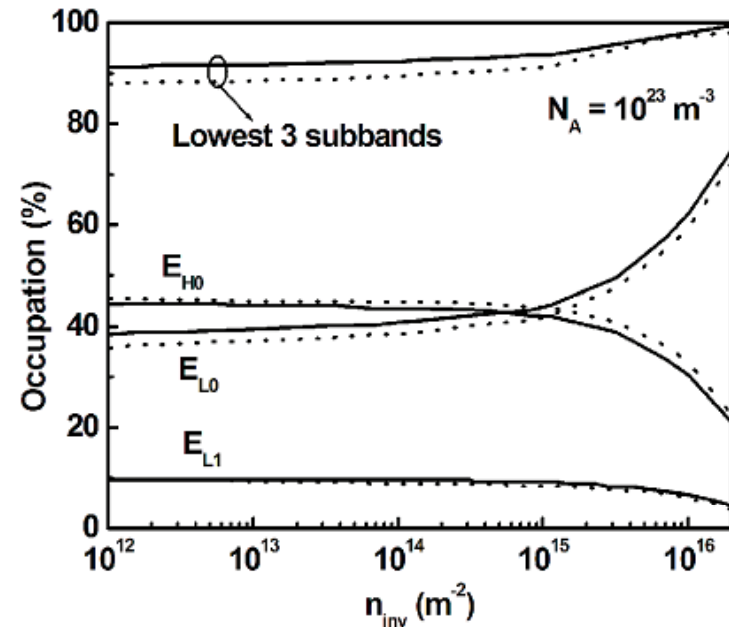
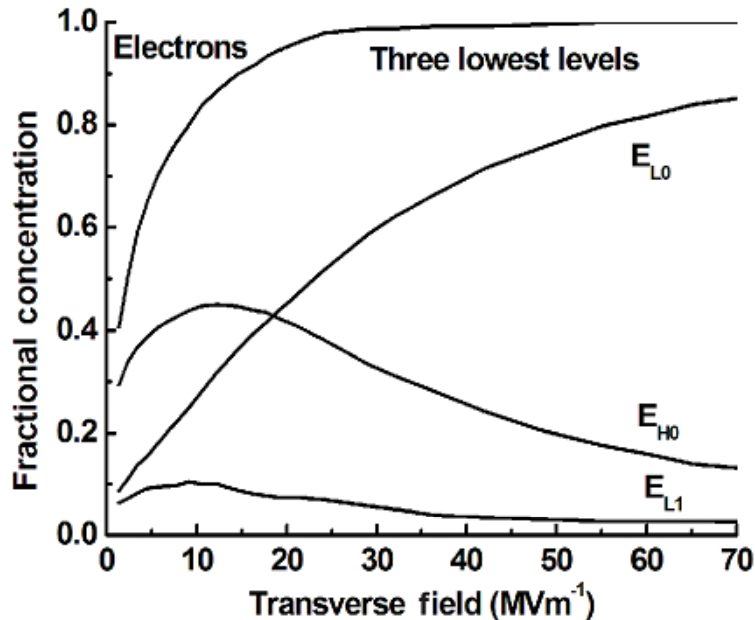
$$n(z) = \frac{k_B T}{\pi \hbar^2} \sum_i g_i m_{di}^* \sum_j \ln \left[1 + \exp \left(\frac{E_F - E_{ij}}{k_B T} \right) \right] |\psi_{ij}|^2$$

Flowchart for self-consistent solution



Some results from self-consistent solution of Schrödinger and Poisson equations

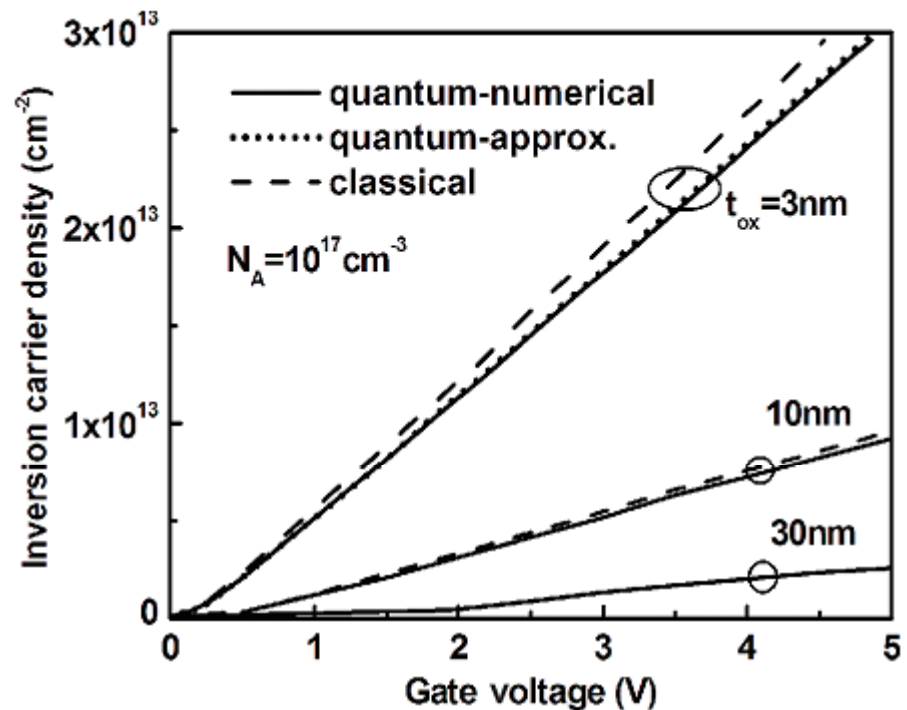
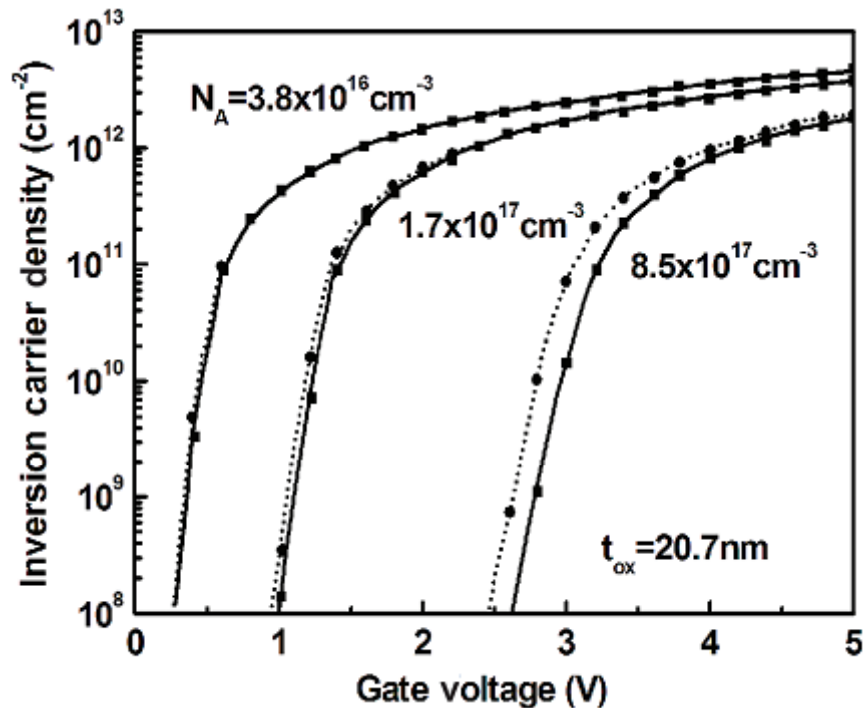
Occupation of sub-bands



- With increase in electric field (or inversion charge)
 - Separation between sub-bands increases
 - Occupation of lowest three sub-bands increases (>98% for $E > 3 \times 10^4$ V/cm or $n_s > 2 \times 10^{12}$ /cm²)
- **Considering lowest three sub-bands is sufficient for above threshold operation**

C. Moglestue, "Self-consistent calculation of electron and hole inversion charges at silicon-silicon dioxide interfaces", J. Appl. Physics, vol. 59, pp. 3175-3183, 1986

Effect of substrate doping concentration and oxide thickness

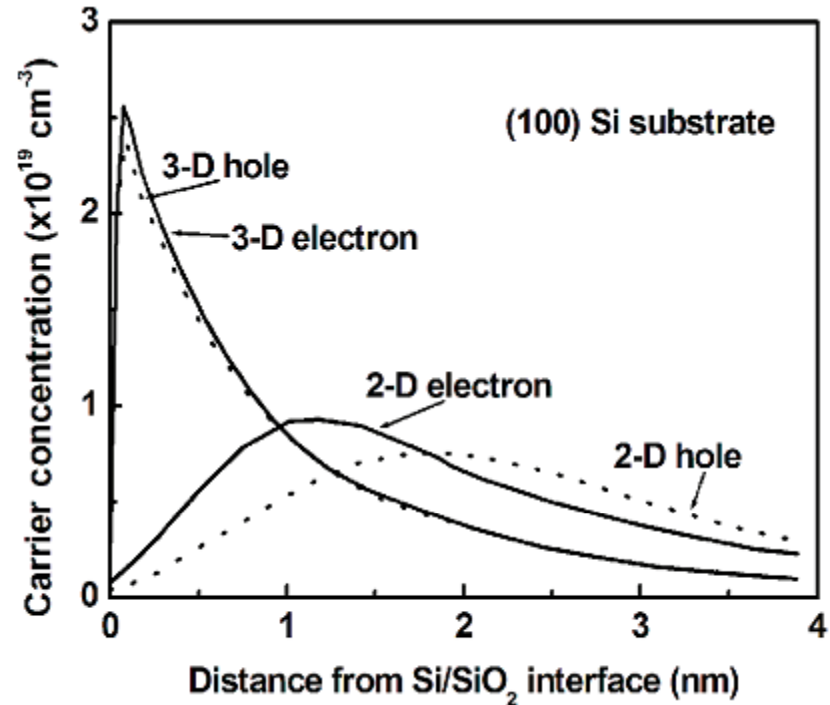
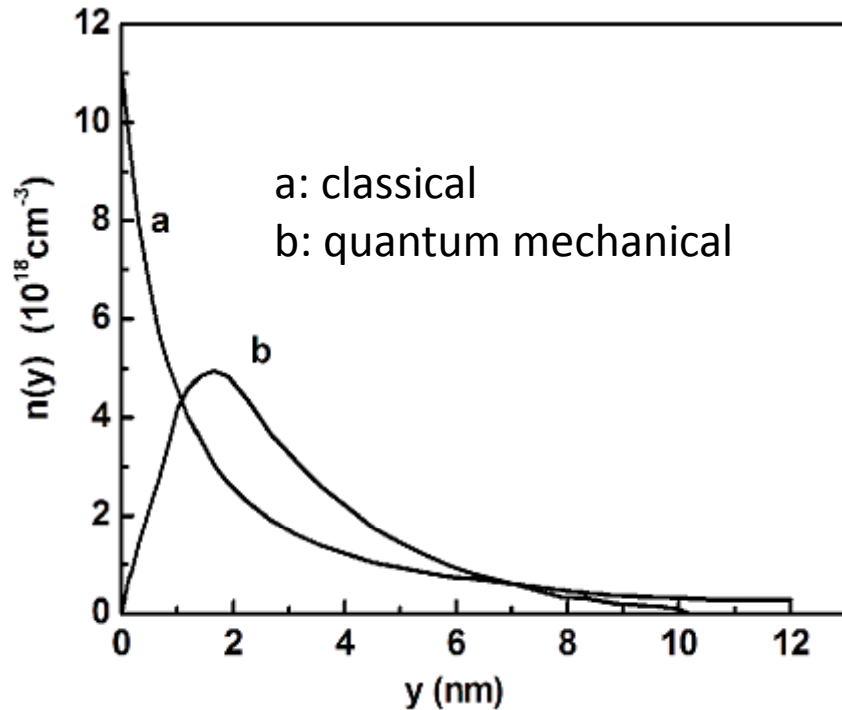


- **QM effects become more important with increasing E-field**
 - increase in substrate doping concentration
 - decrease in oxide thickness

Y. Ohkura, "Quantum effects in Si n-MOS inversion layer at high substrate concentration", Solid-State Electron., vol. 33, pp. 1581-5, 1990

T. Janik and B. Majkusiak, "Analysis of the MOS transistor based on the self-consistent solution to the Schrodinger and Poisson equations and on the local mobility model", IEEE Trans. Electron Devices, vol. 45, pp. 1263-71, 1998

Inversion charge concentration profile



- **Due to QM effects, peak carrier concentration occurs away from Si/SiO₂ interface**
 - The depth is more for holes than electrons

A.P. Gnädinger and H.E. Talley, "Quantum mechanical calculation of the carrier distribution and thickness of inversion layer of a MOS field-effect transistor", Solid-State Electron, vol. 13, pp. 1301-1309, 1970

C.Y. Hu, S. Banerjee, K. Sadra, B.G. Streetman and R. Sivan, "Quantization effects in inversion layers of PMOSFET's on Si (100) substrates", IEEE Electron Dev. Letter, Vol. 17, pp. 276-278, 1996

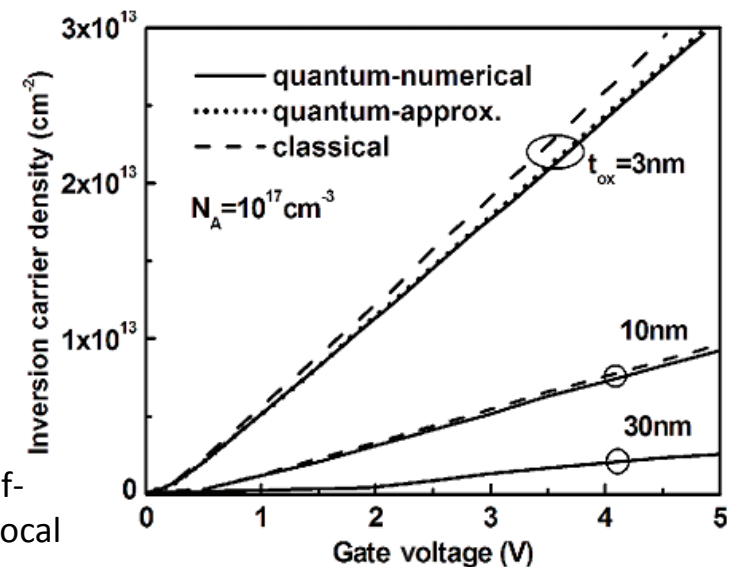
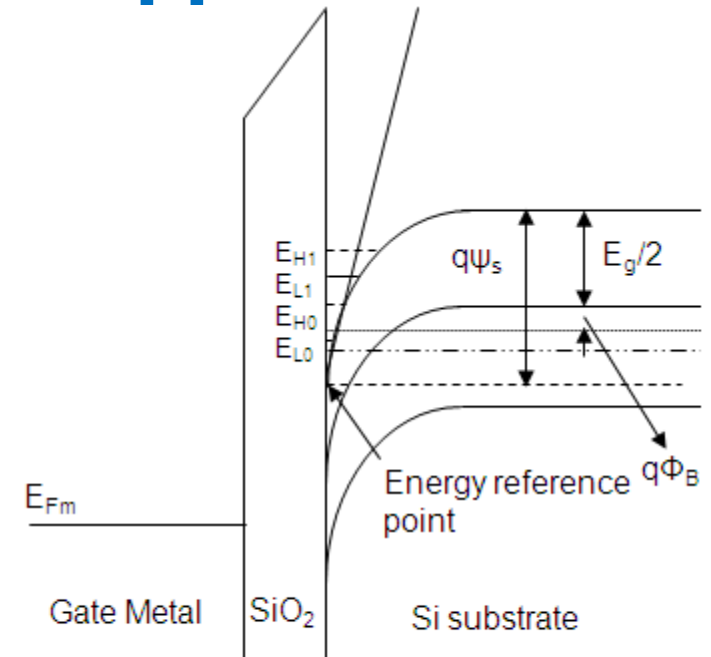
Triangular potential well approximation

- **Constant electric field**

$$\psi(y) = -\mathcal{E}_s y$$

$$\mathcal{E}_s = \frac{q(n_{inv} + N_{dep})}{\epsilon_{si}}$$

- Standard form of solution of Schrödinger equation involving Airy functions
- Simplifies self-consistent solution, although iteration is not avoided
- **Very good match obtained with exact solution** \Rightarrow



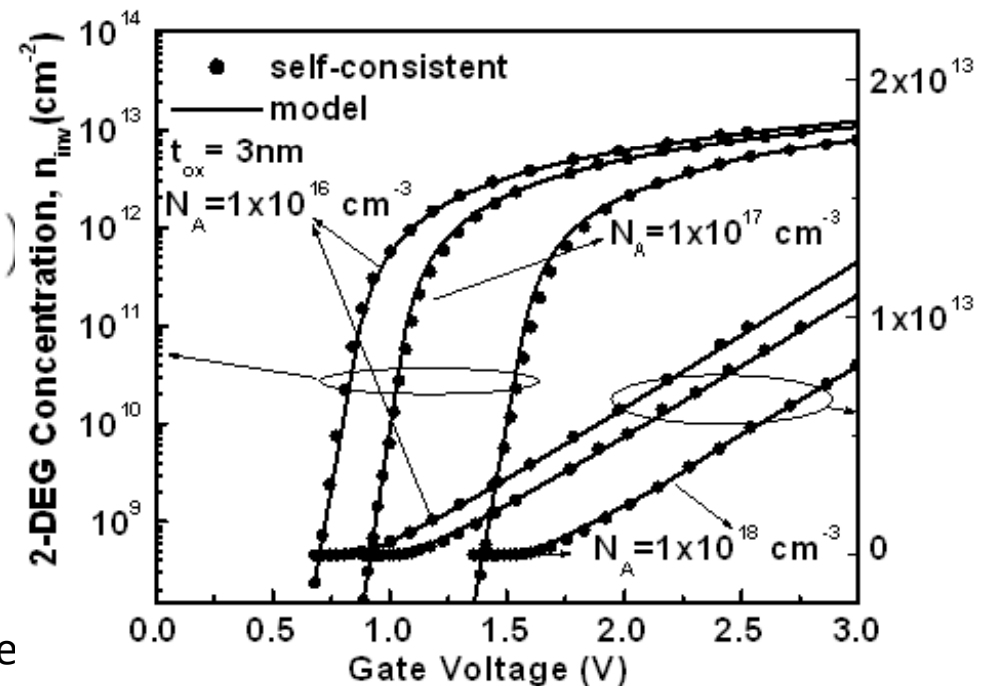
T. Janik and B. Majkusiak, "Analysis of the MOS transistor based on the self-consistent solution to the Schrodinger and Poisson equations and on the local mobility model", IEEE Trans. Electron Devices, vol. 45, pp. 1263-71, 1998

Triangular potential well approximation

- Possible to obtain closed-form expression for inversion electron concentration
- Further assumption: relation between Fermi level and inversion charge

$$n_{\text{inv}} = \left(\left(\sqrt{k_2^2 + 4k_4 V_{\text{GI}}} - k_2 \right)^2 / 4k_4^2 \right) (1 + \delta_n)$$

k_2 , k_4 , δ_n are constants for a particular device at a given temperature and are calculated from input parameters



G.S. Jayadeva and A. DasGupta, "Compact mode of short-channel MOSFETs considering quantum mechanical effects", Solid State Electron, vol. 53, pp. 649-657, 2009

Compact models

Modelling QM effects through
modification of parameters
within classical model
framework

Effective increase in oxide thickness

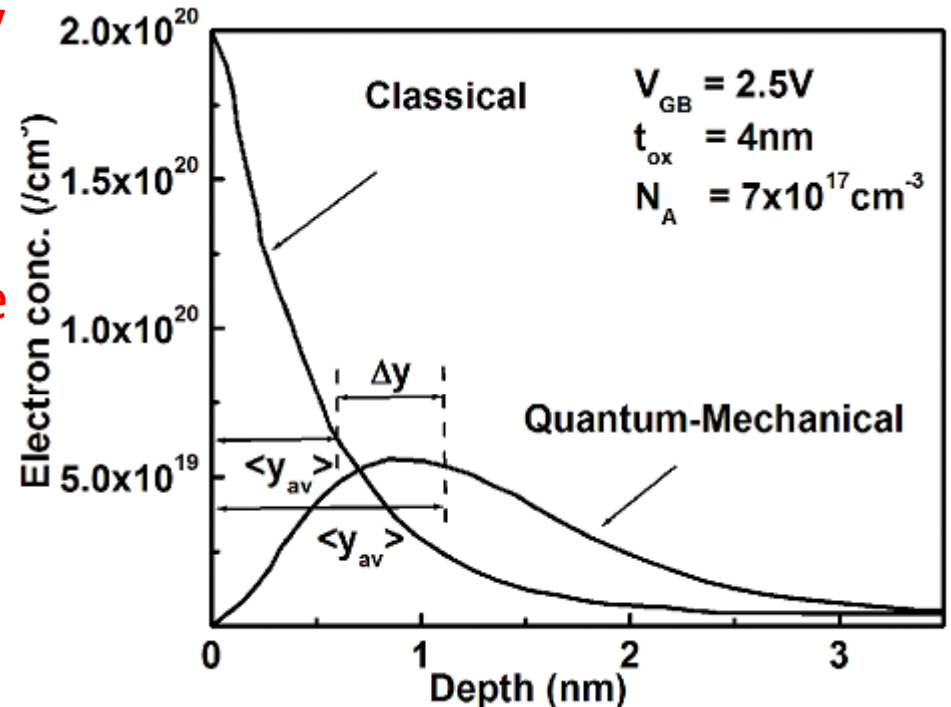
- The peak of the inversion layer charge is located away from Si/SiO₂ interface by a few nm
 - equivalent to increased oxide thickness (Δy) and reduced capacitance
 - Δy reduces with increased electric field (gate voltage)

$$t_{oxeff} = t_{ox} + (\epsilon_{ox} / \epsilon_{Si}) \Delta y$$

$$t_{oxeff} = t_{ox} + \alpha \left(Q_b + \frac{11}{32} Q_{inv} \right)^{-\frac{1}{3}}$$

$$\alpha = 3.5 \times 10^{-10} (Ccm)^{1/3}$$

F. Stern, "Quantum properties of surface space-charge layers", CRC Crit. Rev., vol 4, pp. 499-514, 1974



S. A. Hareland, S. Krishnamurthy, S. Jallepalli, C.F. Yeap, K. Hasnat and A.F. Tasch, "A computationally efficient model for inversion layer quantization effects in deep submicron n-channel MOSFETs", IEEE Trans. Electron Devices, vol. 43, pp. 90-96, 1996

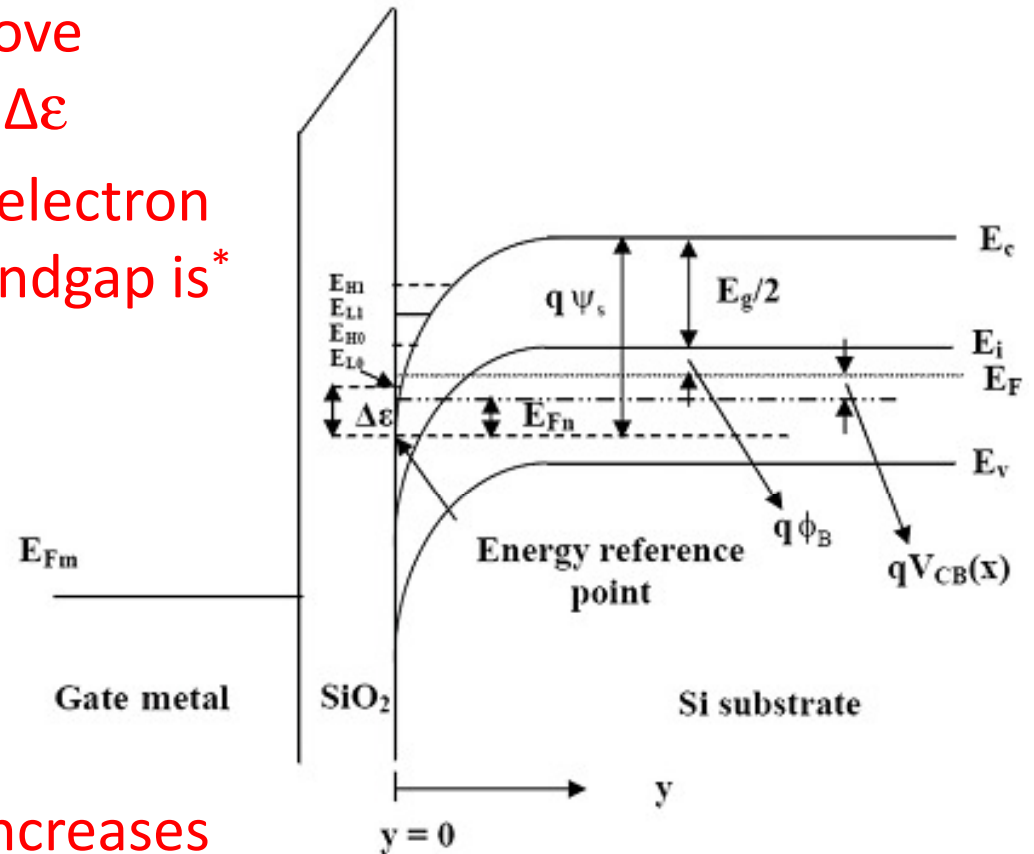
Effective increase in bandgap

- First allowed energy level is above bottom of conduction band by $\Delta\varepsilon$
- Considering TPWA and shift in electron profile, effective increase in bandgap is*

$$\Delta E_g = \frac{13}{9} \Delta\varepsilon$$

$$\Delta\varepsilon = \beta \left(\frac{\varepsilon_{si}}{4qkT} \right)^{1/3} \varepsilon_s^{2/3} \text{ for } \varepsilon_s > 0$$

$$\beta = 4.1 \times 10^{-8} \text{ eV.cm}$$



- Effective increase in bandgap increases with increase in surface electric field (ε_s)
- Models use empirical relations for ε_s
- BSIM 3v3 $\varepsilon_s = (V_{GS} + V_{th}) / 6t_{ox}$

* M.J. van Dort *et al*, "Influence of high substrate doping levels on the threshold voltage and the mobility of deep-submicrometer MOSFET's", IEEE Trans. Electron Devices, vol. 39, pp. 932-938, 1992

Effective increase in bandgap (contd.)

- In PSP and MOS11

$$\Delta\mathcal{E}_g = \Delta\mathcal{E} + q \cdot E_{Si} \cdot \Delta y$$

- Assuming only first sub-band is occupied

$$\Delta y \approx \frac{2}{3} \cdot \frac{\Delta\mathcal{E}}{q \cdot E_{Si}}$$

$$\Delta\mathcal{E} \approx \frac{3}{2} \cdot \left(\frac{3 \cdot q \cdot \hbar \cdot E_{\text{eff}}}{2 \cdot \sqrt{m_{Si}}} \right)^{2/3} = q \cdot \frac{3}{5} \cdot QM \cdot (\epsilon_{Si} \cdot E_{\text{eff}})^{2/3}$$

$$QM_N = 5.951993 \text{ V}\cdot\text{m}^{4/3}/\text{C}^{2/3} \text{ for electrons}$$

$$QM_P = 7.448711 \text{ V}\cdot\text{m}^{4/3}/\text{C}^{2/3} \text{ for holes}$$

$$E_{\text{eff}} = -\frac{Q_b + \frac{1}{3} \cdot Q_{\text{inv}}}{\epsilon_{Si}}$$

M.J. van Dort, P.H. Woerlee and A.J. Walker, "A simple model for quantization effects in heavily-doped silicon MOSFET's at inversion conditions" Solid State Electron, vol. 37, pp. 411-414, 1994.

Effective reduction in intrinsic carrier concentration

- The effective intrinsic carrier concentration (n_i^{QM}) is

$$n_i^{QM} = n_i^{cl} e^{(-\Delta E_G / 2KT)}$$

- To ensure smooth transition between the value of n_i at the Si/SiO₂ interface (n_i^{QM}) and in the bulk (n_i^{cl})

$$n_{ieff} = n_i^{cl} \{1 - F(a)\} + F(a)n_i^{QM}$$

$$a = y / y_{ref} \quad F(a) = \frac{2 \exp(-a^2)}{1 + \exp(-2a^2)}$$

M.J. van Dort, P.H. Woerlee and A.J. Walker, "A simple model for quantization effects in heavily-doped silicon MOSFET's at inversion conditions" Solid State Electron, vol. 37, pp. 411-414, 1994.

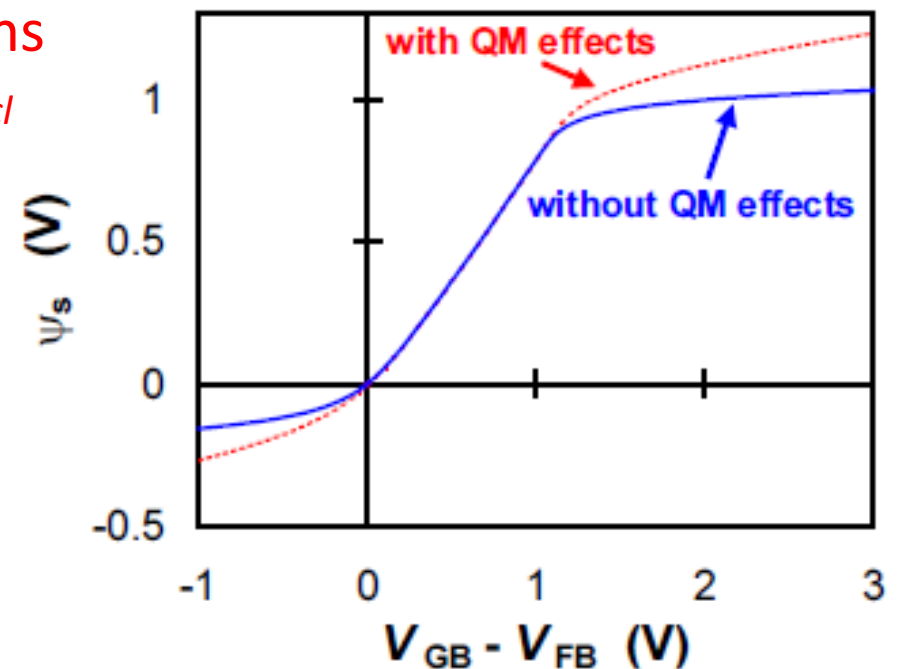
Modification in surface potential

- Surface potential calculated classically (ψ_s^{cl}) deviates from that calculated quantum mechanically (ψ_s^{qm}) in accumulation and inversion regions
 - In inversion region, $\psi_s^{qm} > \psi_s^{cl}$

- From Gauss Law

$$V_{GB} - V_{FB} = \psi_s^{qm} + \frac{Q_s^{qm}}{C_{ox}}$$

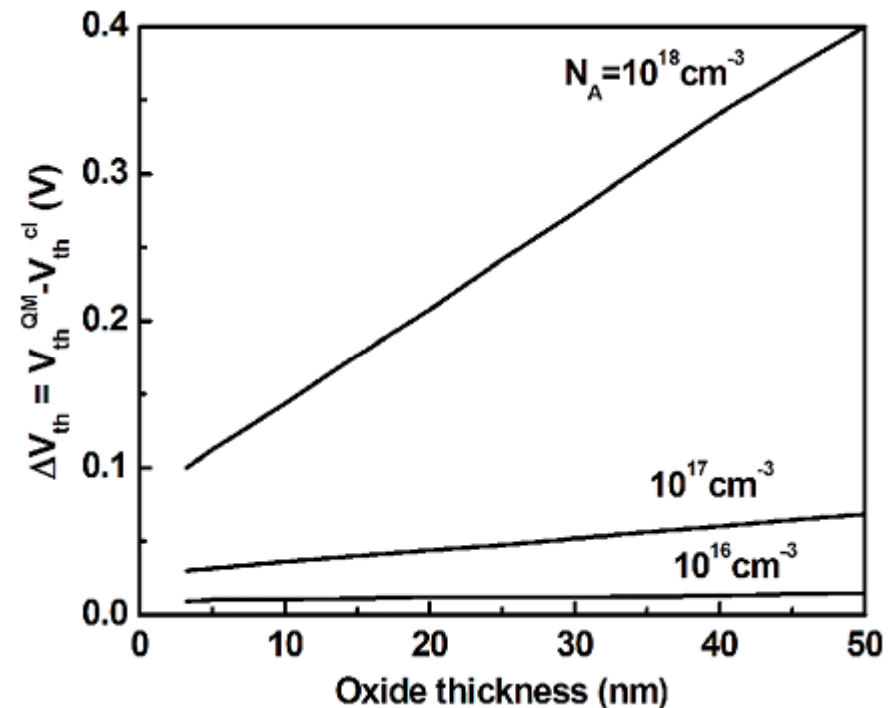
- Higher ψ_s^{qm} implies
 - Lower semiconductor charge (Q_s^{qm})
 - Higher bulk charge (Q_B)
 - Lower electron charge ($Q_n = Q_s - Q_B$)
 - Lower drain current



Increase in threshold voltage

- Threshold voltage difference increases with increase in
 - Substrate doping (increased bulk charge)
 - Oxide thickness

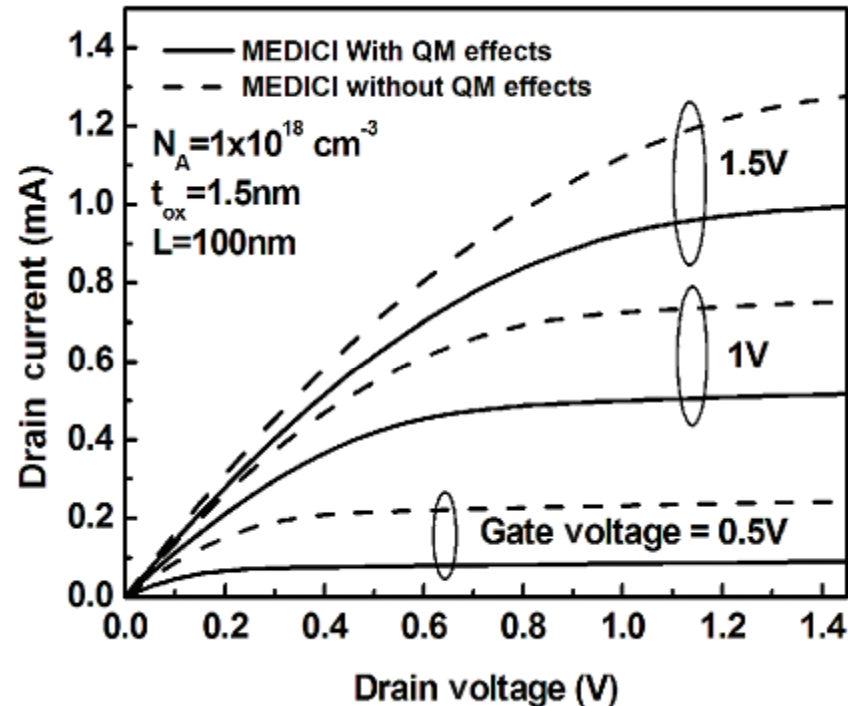
$$V_{th} \approx V_{th}^{sim} + \Delta\psi_s \left(1 + \frac{1}{2C_{ox}} \sqrt{\frac{\epsilon_{si} q N_A}{\phi_B}} \right)$$



*M.J. van Dort *et al*, "Influence of high substrate doping levels on the threshold voltage and the mobility of deep-submicrometer MOSFET's", IEEE Trans. Electron Devices, vol. 39, pp. 932-938, 1992

T. Janik and B. Majkusiak, "Analysis of the MOS transistor based on the self-consistent solution to the Schrodinger and Poisson equations and on the local mobility model", IEEE Trans. Electron Devices, vol. 45, pp. 1263-71, 1998

Effect on drain current



- Drain current calculated considering QM effects is lesser than that obtained using classical method
 - Lower inversion layer charge

Existing surface potential based models

- Do not calculate surface potential from QM considerations (e.g. formation of sub-bands)
- Include QM effect through modification of parameters
 - PSP uses modified oxide thickness and intrinsic carrier concentration
 - needs additional model parameters

A proposed model

- Objective
 - Develop an expression for the surface potential considering quantum mechanical effects (ψ_s^{qm})
 - Obtain analytical approximations to calculate ψ_s^{qm}
 - Use ψ_s^{qm} to model the MOSFET characteristics without any additional model parameter

Expression for ψ_s^{qm}

- Normalized implicit expression of surface potential
 - Considering QM effects in a triangular potential well

$$U_{GFB} - u_s = q_n + \gamma_1 \sqrt{\left[e^{-u_s} - 1 + u_s \left(1 - e^{-u_n} \right) \right]}$$

$$q_n = \sum_i a_i \sum_j \ln \left[1 + e^{u_s - u_u - e_{ij}} - e^{-u_u} \right]_{i=L,H \quad j=0,1,2,\dots}$$

$$u_s = \psi_s^{qm} / V_t \quad u_n = \phi_n / V_t$$

$$a_i = \left(\frac{q^2 n_{vi} m_{di}}{C_{ox} \pi \hbar^2} \right) \quad e_{ij} = E_{ij} / qV_t$$

$$u_u = \frac{E_g / 2q + \phi_B + \xi}{V_t} \quad \phi_n = 2\phi_B + \xi$$

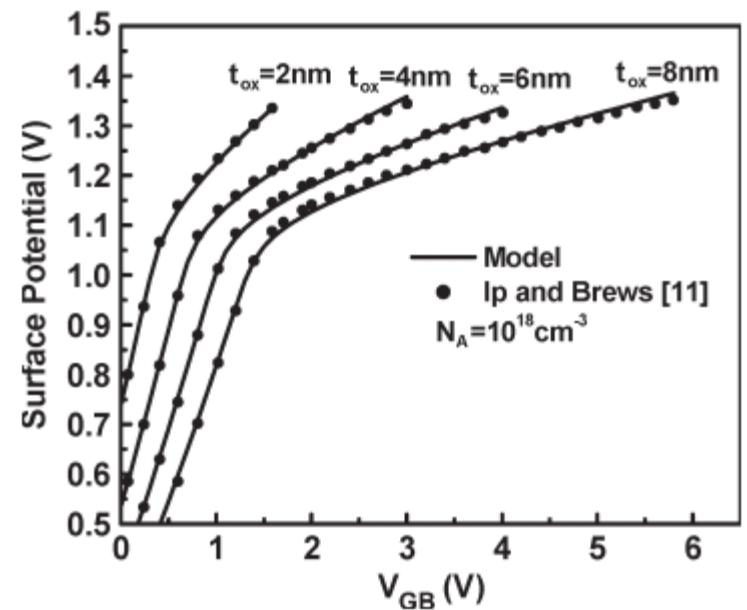
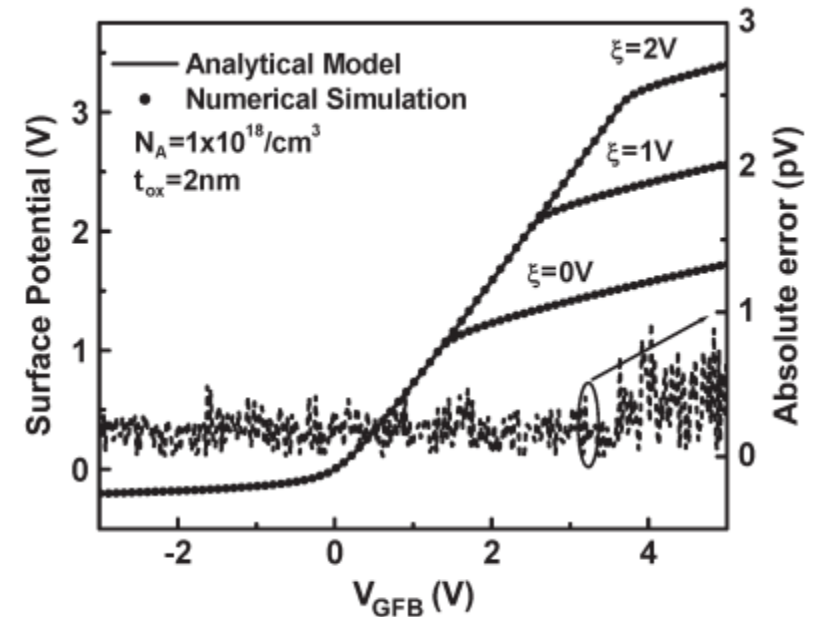
– Classical

$$(U_{GFB} - u_s) = \gamma_1 \sqrt{\left[e^{-u_s} - 1 + u_s \left(1 - e^{-u_n} \right) + e^{-u_n} \left(e^{u_s} - 1 \right) \right]} \quad u_s = \psi_s^{cl} / V_t$$

G.S. Jayadeva and Amitava DasGupta, “Analytical approximation for the surface potential in n-channel MOSFETs considering quantum mechanical effects”, IEEE Trans. Electron Devices, vol. 57, pp. 1820-1828, 2010

Analytical calculation of surface potential

- The surface potential (ψ_s^{qm}), as well as the first and second derivatives are smooth and continuous
 - no smoothing function or fitting parameter required
 - Excellent match for wide range of N_A and t_{ox}
- ψ_s^{qm} and inversion layer charge obtained from the analytical calculation shows excellent match with self-consistent solution of Schrödinger and Poisson equations



Gate voltage shift model

- **Objective of Gate Voltage shift model**
 - incorporate QM effects in the classical framework
 - first proposed by Ip & Brews*
 - empirical model requiring fitting parameters
- **What is Gate Voltage shift model?**
 - QM effect is incorporated by reducing the gate voltage by ΔV_{GB} to account for reduced charge and drain current
- **Objective of proposed model is to obtain ΔV_{GB} physically without any additional parameter**

*B. K. Ip and J. R. Brews, "Quantum effects upon drain current in a biased MOSFET", 26 IEEE Trans. Electron Devices, vol. 45, No. 10, pp 2213-2221, October 1998.

Theory of Gate voltage shift model

- From Gauss Law (valid for both classical and QM considerations)

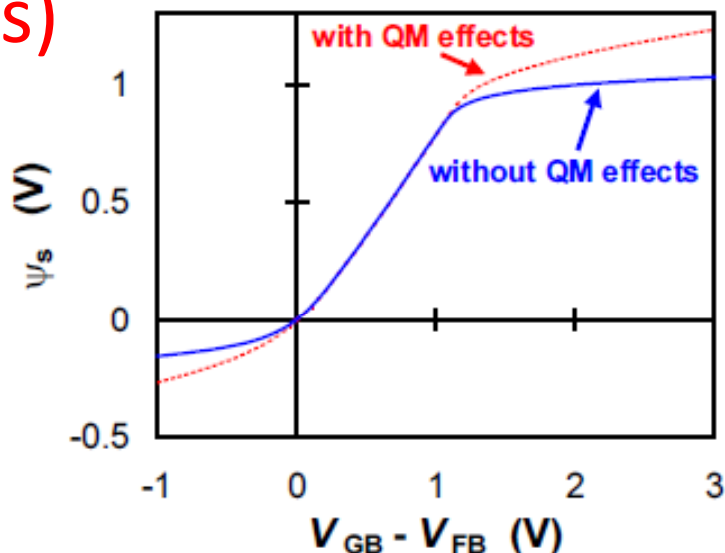
$$V_{GB} - V_{FB} = \psi_s^{qm} + \frac{Q_s^{qm}}{C_{ox}} = \psi_s^{cl} + \frac{Q_s^{cl}}{C_{ox}}$$

- Let $\Delta V_{GB} = \psi_s^{qm} - \psi_s^{cl} = \Delta\psi$

- Hence $(V_{GB} - \Delta V_{GB}) - V_{FB} = \frac{Q_s^{qm}}{C_{ox}} + \psi_s^{cl}$

- ψ_s^{cl} can be used to calculate Q_s^{qm}

- ψ_s^{cl} calculated at $(V_{GB} - \Delta V_{GB})$ and ψ_s^{qm} calculated at V_{GB} result in same Q_s^{qm}



Calculation of ΔV_{GB}

- In the figure, ψ_s calculated quantum mechanically at V_{GB}^{app} and calculated classically at V_{GB}^{eff} result in same Q_s
- Thus $\Delta V_{GB} = V_{GB}^{app} - V_{GB}^{eff}$
- From the figure

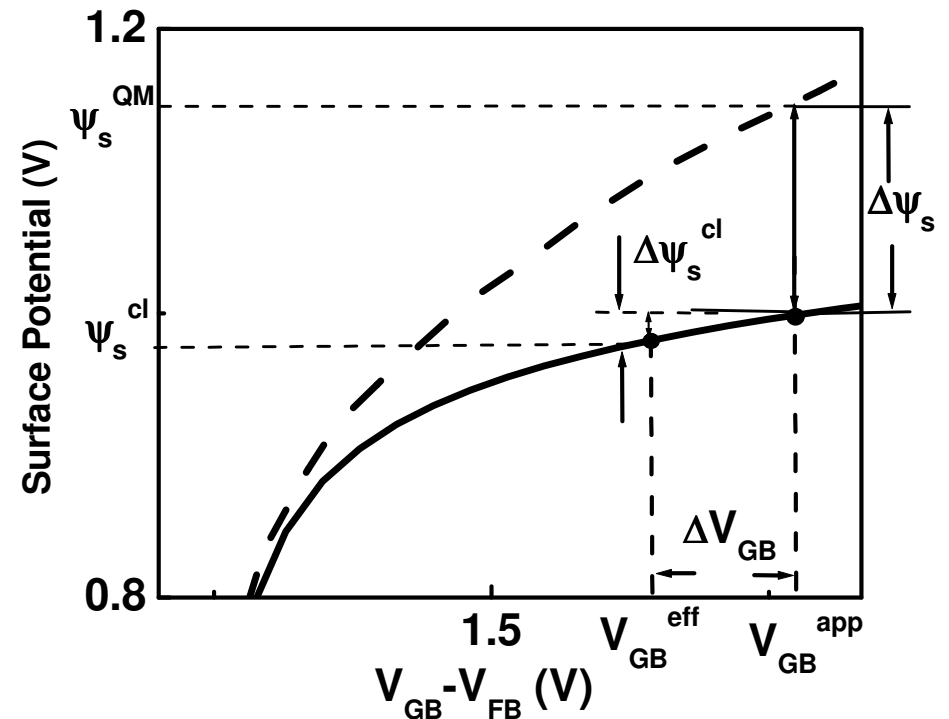
$$\Delta V_{GB} = \Delta\psi_s^{cl} + \Delta\psi_s$$

- Considering

$$d\psi_s^{cl} / dV_{GB} \approx \Delta\psi_s^{cl} / \Delta V_{GB}$$

$$\Delta V_{GB} = \Delta\psi_s / \left(1 - d\psi_s^{cl} / dV_{GB}\right)$$

$$\text{where } \left(1 - \frac{d\psi_s^{cl}}{dV_{GB}}\right) = \frac{\gamma_1^2 \left[-e^{-u_s} + 1 - e^{-u_n} + e^{-u_n} e^{u_s}\right]}{\left\{2(U_{GFB} - u_s) + \gamma_1^2 \left[-e^{-u_s} + 1 - e^{-u_n} + e^{-u_n} e^{u_s}\right]\right\}}$$

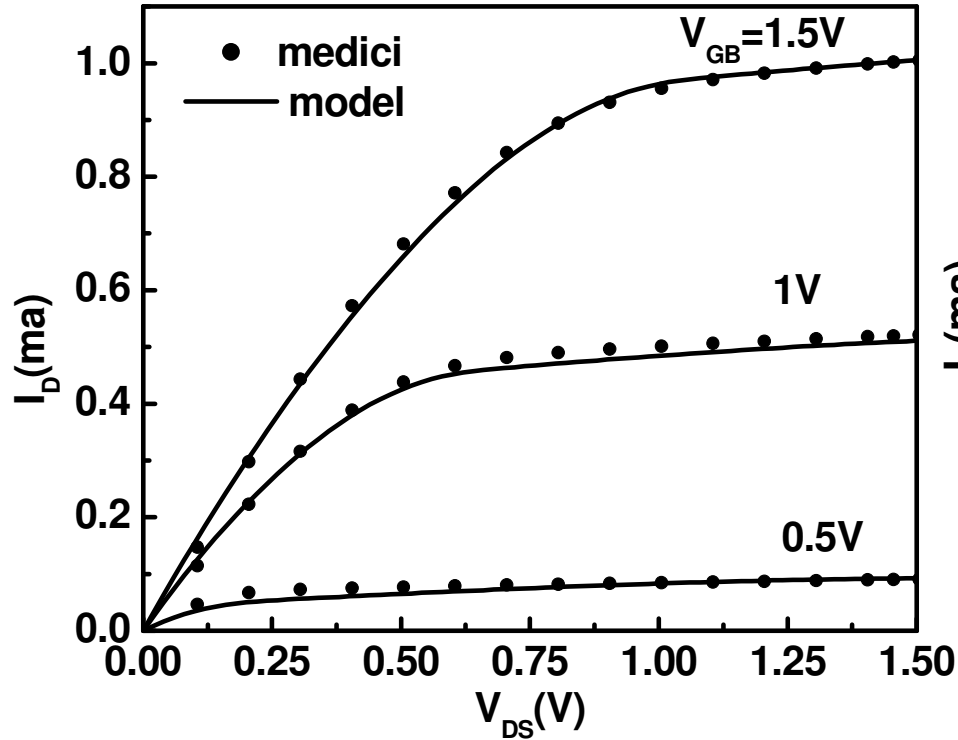


ΔV_{GB} can be calculated analytically

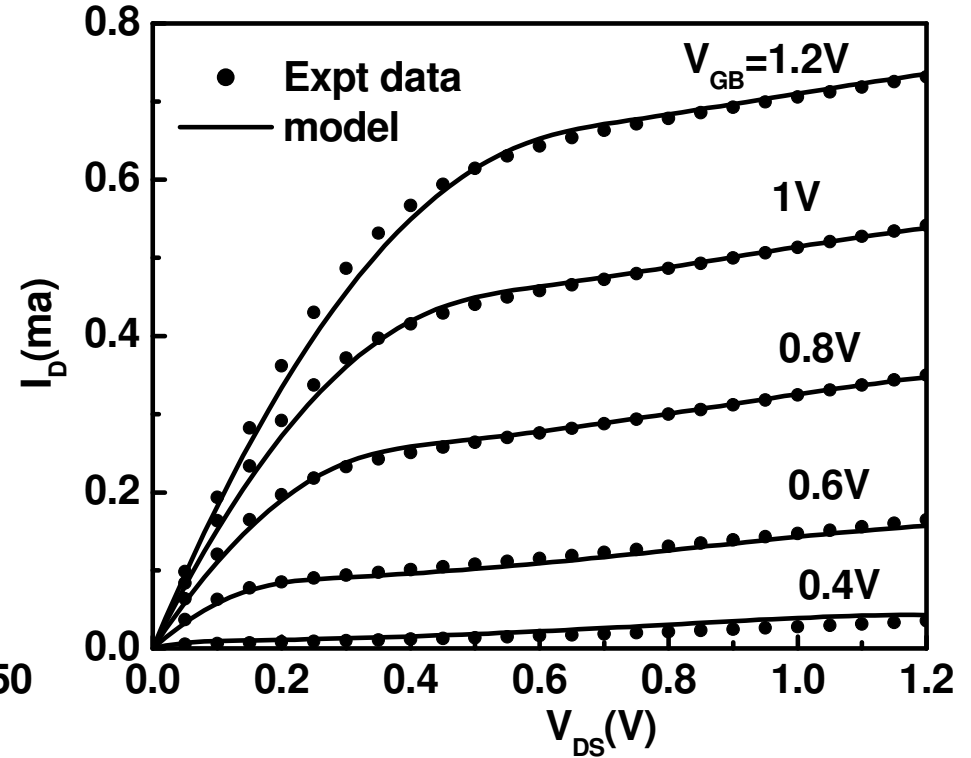
Gate voltage shift model

- Calculate ψ_s^{cl} at V_{GB}^{app} (as in PSP)
- Calculate ψ_s^{qm} at V_{GB}^{app} (using analytical method)
- Calculate $\Delta\psi_s = \psi_s^{qm} - \psi_s^{cl}$
- Calculate ΔV_{GB} from $\Delta V_{GB} = \Delta\psi_s / (1 - d\psi_s^{cl} / dV_{GB})$
- Calculate $V_{GB}^{eff} = V_{GB}^{app} - \Delta V_{GB}$
- Use bulk charge linearization model (as PSP) at $V_{GB} = V_{GB}^{eff}$ to calculate drain current and capacitance

Results



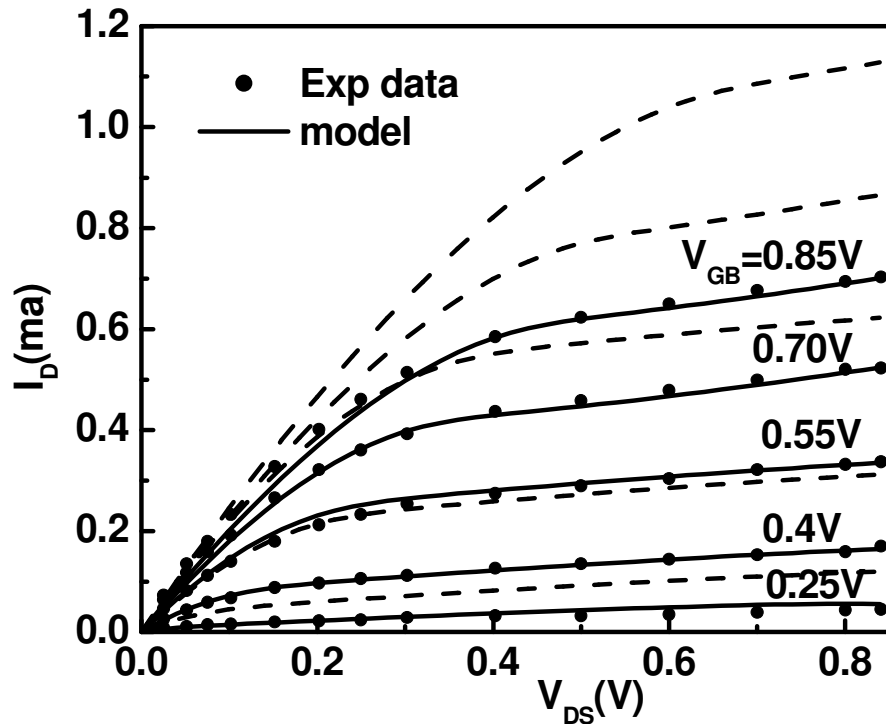
Comparison of the I-V characteristics obtained from the present model (solid line) with MEDICI simulated data (dots) for $L=100\text{nm}$, $t_{\text{ox}} = 1.5\text{nm}$, $N_A=10^{18}\text{cm}^{-3}$.



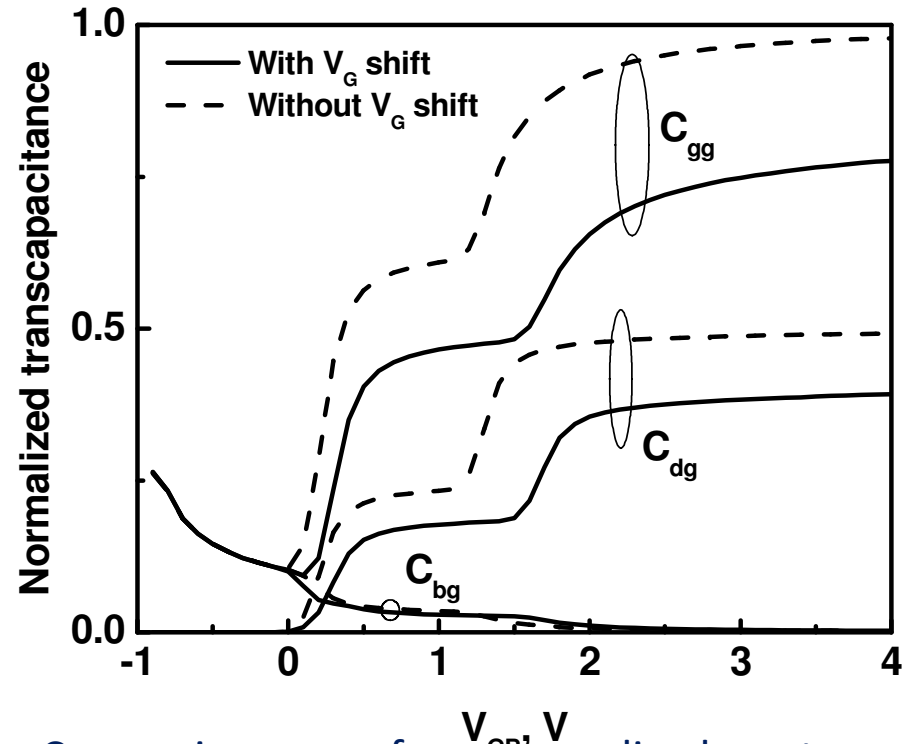
Comparison of the I-V characteristics obtained from the present model (solid line) with experimental data (dots) obtained from [1] for $L=70\text{nm}$, $t_{\text{ox}}=1.9\text{nm}$, $N_A=10^{18}\text{cm}^{-3}$.

[1] K. Miyashita, T. N. Nakayama, et al., Symp. on VLSI Tech., pp. 11-12, 2001.

Results (contd.)



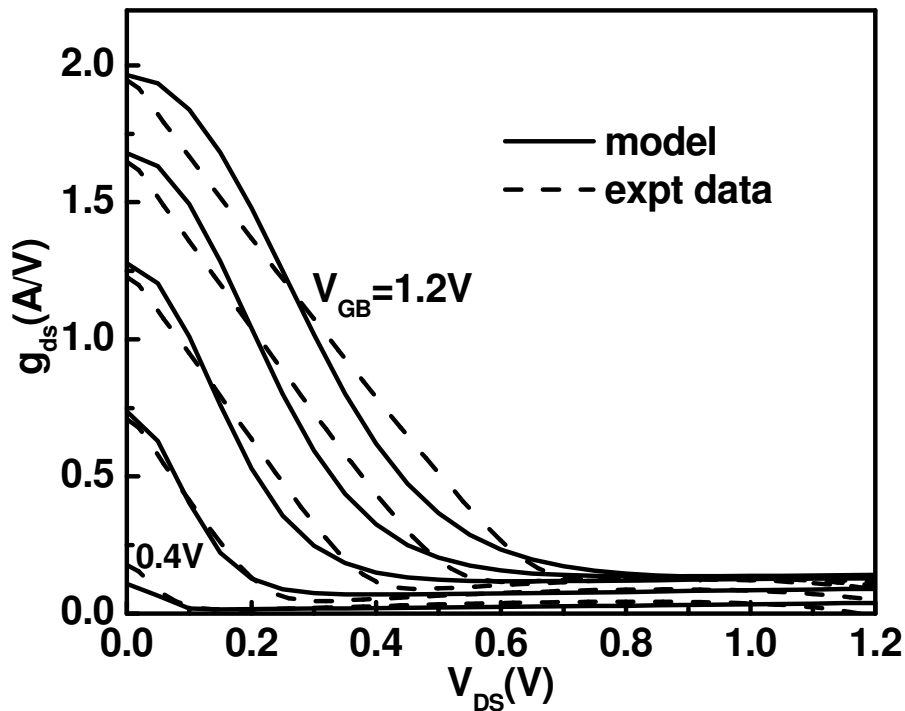
Comparison of I-V characteristics obtained from proposed model (solid line) with experimental data (dots) obtained from [2] for $L=30\text{nm}$, $t_{\text{ox}}=1\text{nm}$, $N_A=1.5 \times 10^{18} \text{cm}^{-3}$. Figure also shows I-V characteristics obtained without considering QM effects (dotted line).



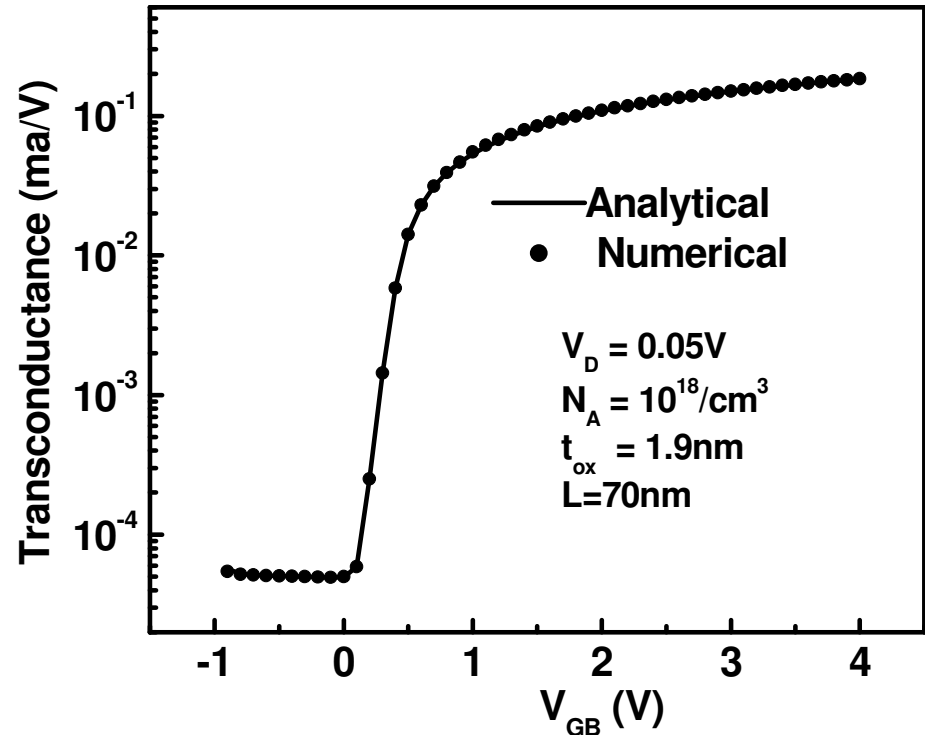
Comparison of normalized transcapacitances obtained from the present model considering QM effects (solid line) with the one obtained without considering QM effects (dotted line) [2] for $L=30\text{nm}$, $t_{\text{ox}}=1\text{nm}$, $N_A=1.5 \times 10^{18} \text{cm}^{-3}$.

[2] N. Yanagiya, S. Matsuda et. al, IEDM Tech. Dig., pp. 57-60, 2002.

Results (contd.)



Comparison of the channel conductance obtained from the present model (solid line) with experimental data (dots) obtained from [1] for $L=70\text{nm}$, $t_{ox}=1.9\text{nm}$, $N_A=10^{18}\text{cm}^{-3}$.



Comparison of transconductance versus gate voltage obtained from the analytical model (solid line) with surface potential calculated numerically (dot) for $L=70\text{nm}$, $t_{ox}=1.9\text{nm}$, $N_A=10^{18}\text{cm}^{-3}$ [1]

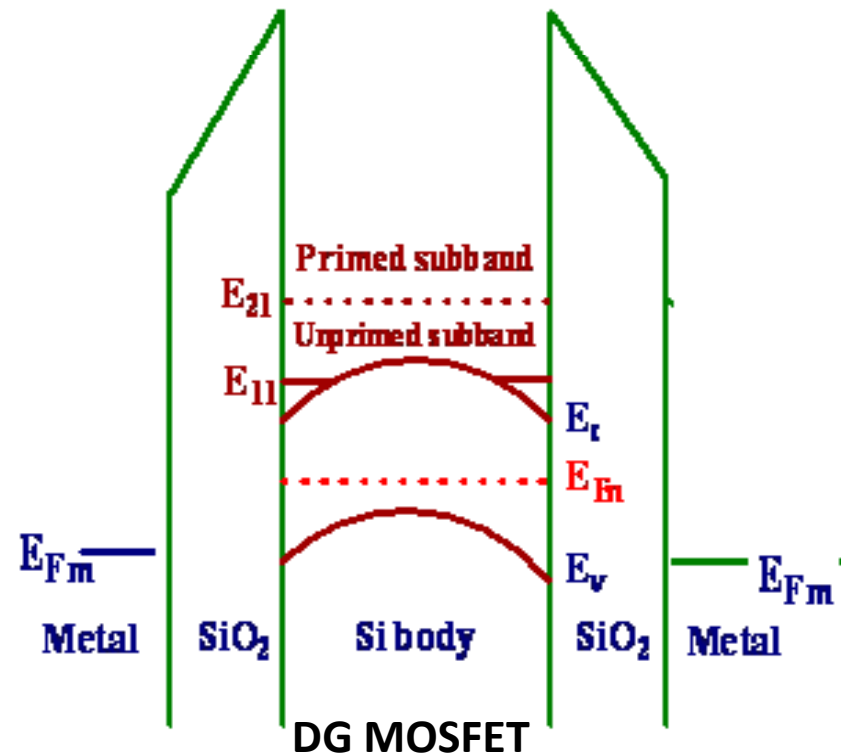
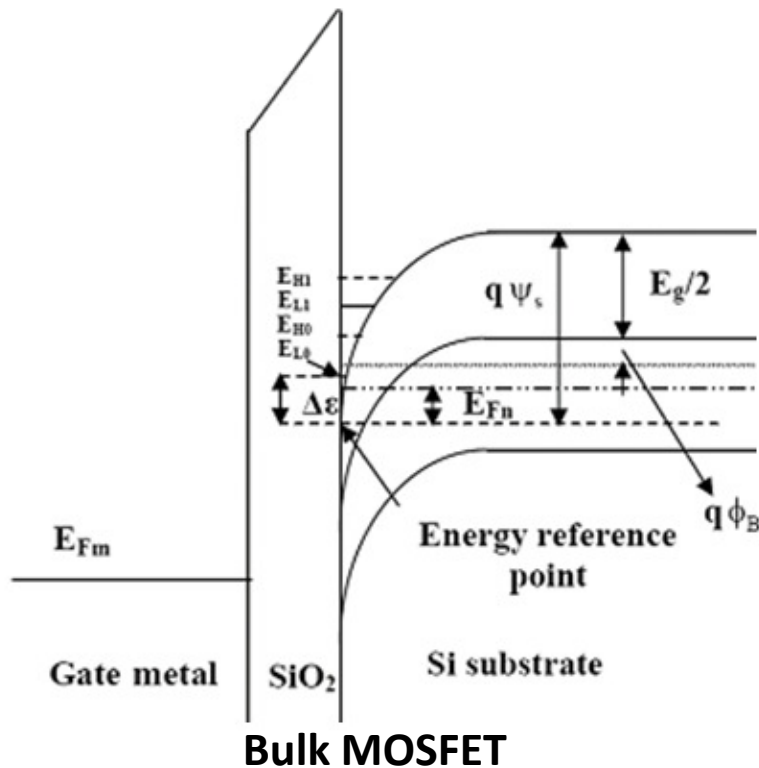
[1] K. Miyashita, T. N. Nakayama, et al., Symp. on VLSI Tech., pp. 11-12, 2001.

Summary & Conclusions

- What is QM effect?
- Some interesting effects
 - Shift in the inversion charge concentration profile
- Triangular potential well approximation
- Modelling using modification of parameters
- V_G shift model
- A proposed model
 - Incorporates QM effects without any additional model parameter

Summary & Conclusions (contd.)

- Can the models for bulk MOSFETs be replicated for Multiple Gate MOSFETs (MuGFETs)?
 - No, the effects are different
 - In MuGFETs,
 - the confinement is due to a thin (< 10 nm) Si layer sandwiched between SiO₂ /dielectric layers
 - electric field is low



Thank you