

# Analytical Solutions to Quantum Drift-Diffusion Equations for Quantum Mechanical Modeling of MOS Structures

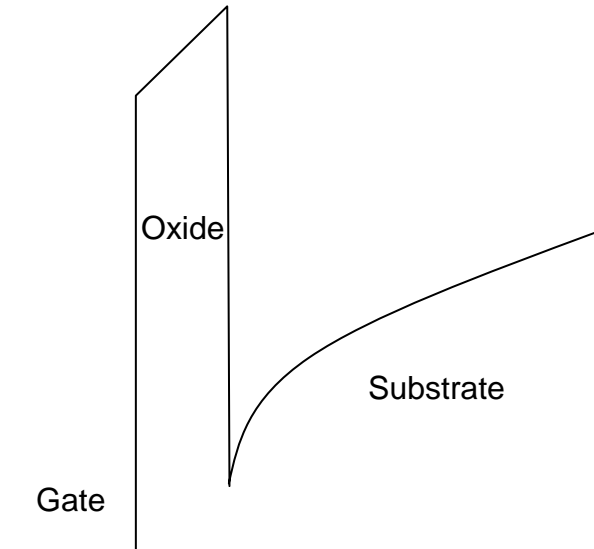
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# Modeling Quantum Effects in Inversion Layer

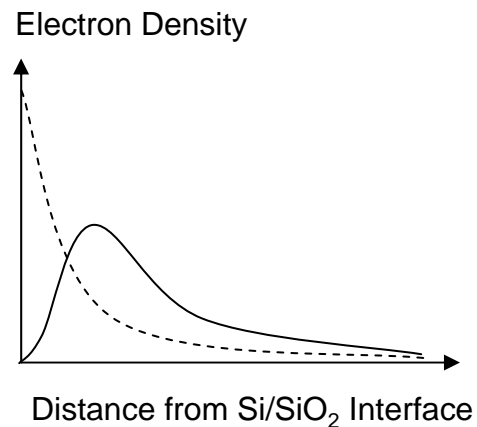


## Schrödinger-Poisson Self-consistent Calculation

- Numerical
- Exact solution
- Expensive computation time

## Hänsch Model, Van Dort Model

- Analytical
- Coarse approximation (bad accuracy)
- Cheap & Fast



## Density Gradient Model

- Numerical
- Approximate but excellent accuracy
- Not too fast, not too bad

We **ANALYTICALLY** solve equations from **density gradient model** using perturbation methods.

# Density Gradient Model

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In this work, the following assumptions are used to simplify the problem.

- Holes are treated as classical particles.
- Electron and hole quasi Fermi levels are constant.
- No tunneling current occurs through the oxide.
- Poly gate depletion is neglected.
- Doping concentration is constant.
- Electron mobility is constant.
- Carrier generation-recombination is neglected.

Then Poisson and carrier density equations (quantum drift-diffusion equation) in density gradient model read

$$\left\{ \begin{array}{l} \frac{d}{dx} \left[ \varepsilon(x) \frac{d}{dx} \psi(x) \right] = -e \left[ n_i e^{\frac{e}{k_B T} (\phi_p - \psi(x))} - n(x) - N_A \right] \\ \phi_n = \psi(x) - \frac{k_B T}{e} \ln \left[ \frac{n(x)}{n_i} \right] + 2b_n \left( \frac{\frac{d^2}{dx^2} \sqrt{n(x)}}{\sqrt{n(x)}} \right) \end{array} \right.$$

, where  $b_n = \frac{\gamma_n \hbar^2}{12em_e^*}$  Quantum Correction Term

Note that these are the standard equations in drift-diffusion, amended by the quantum correction term.

# Perturbation Method

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1 Solutions are expanded by small parameter in the equations

$$\begin{cases} \psi(x) = \psi_0(x) + \delta\psi_1(x) + \dots \\ n(x) = n_0(x) + \delta n_1(x) + \dots \end{cases}$$

2 They are substituted to the original equations, and then sorted in terms of order of the small parameter.

$$F_0[\psi_i(x), n_i(x), x] + \delta F_1[\psi_i(x), n_i(x), x] + \dots = 0 \quad i = 0, 1, \dots$$

3 Each term is set to zero to obtain separate differential equations.

$$F_0[\psi_i(x), n_i(x), x] = 0, F_1[\psi_i(x), n_i(x), x] = 0, \dots$$

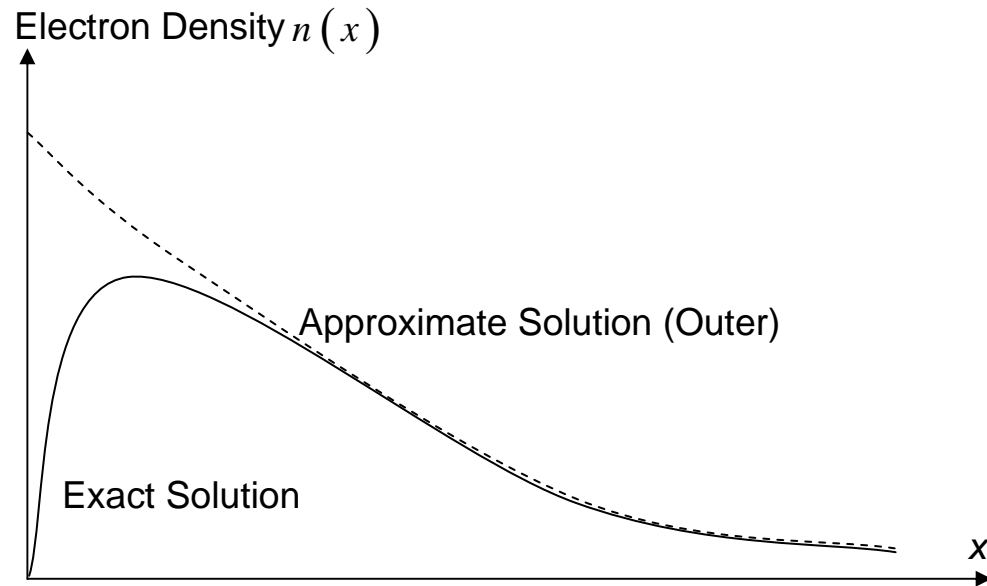
4 Each equations are solved to obtain solutions

$$\psi_0(x), \psi_1(x), \dots, n_0(x), n_1(x), \dots$$

5 Approximate solutions are obtained by ignoring higher order terms

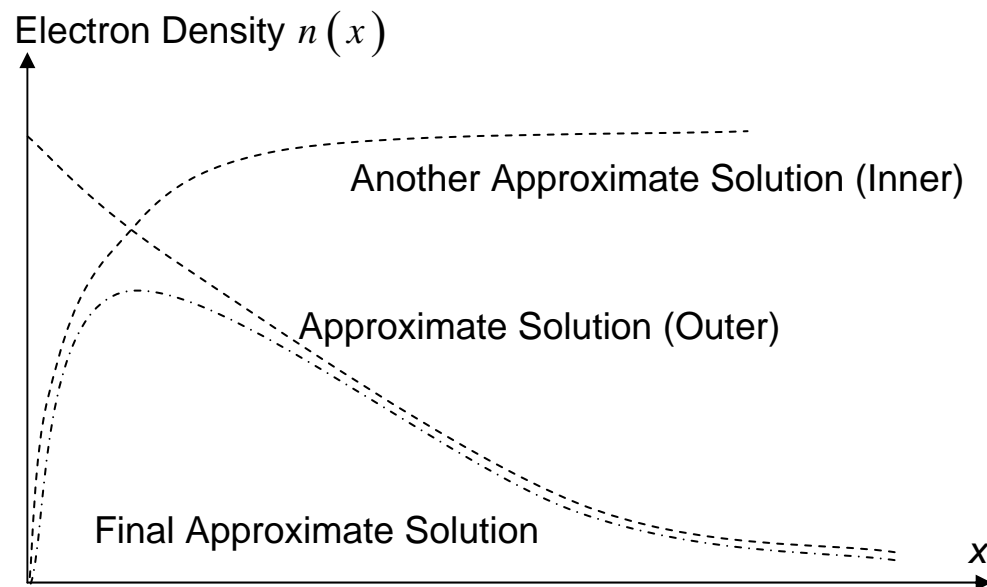
$$\psi(x) \simeq \psi_0(x) + \delta\psi_1(x), n(x) \simeq n_0(x) + \delta n_1(x)$$

# Singular Perturbation Method



The expansion fails to reproduce the carrier density near the Si/SiO<sub>2</sub> interface because it implicitly assumes that the approximate solution has characteristics similar to the exact solution obtained by setting  $\delta = 0$ , that is, the classical solution. Therefore, it neglects the quantum mechanical carrier reduction near the interface no matter how many higher order terms are taken into account. In order to reproduce the solutions in the inner region, this region is re-scaled. A new variable  $X$  is introduced as follows

$$X \equiv \frac{x}{\delta}$$



Then the functions  $\psi(X)$  and  $n(X)$  are expanded in terms of  $\delta$ , and the approximate solutions are obtained.

These approximate solutions are blended in a well-established way, and the final approximate solutions are valid everywhere.

# We Successfully Obtained Analytical Solutions

We finally successfully obtained analytical solutions to the equations as follows:

## Potential $\psi(x)$ and quantum-mechanical carrier density $n(x)$

$$\left\{ \begin{array}{l} \psi(x) = \frac{k_B T}{e} \ln \lambda + \phi_n + \frac{k_B T}{e} \left( \ln [\alpha_0^2 \ln \lambda] - 2 \ln \left[ \sinh \left[ \frac{1}{2} \alpha_0 \sqrt{\lambda \ln \lambda} \frac{x}{L_D} + \gamma \right] \right] + \frac{1}{4} \lambda \left( \frac{x}{L_D} \right)^2 + \delta (\ln \lambda) C_1 \coth \left[ \frac{1}{2} \alpha_0 \sqrt{\lambda \ln \lambda} \frac{x}{L_D} + \gamma \right] \right) \\ n(x) = n_i \exp \left[ \frac{e(\psi_s - \phi_n)}{k_B T} + 2 \ln \left[ S \left( \frac{x}{\delta L_D} \sqrt{\frac{\lambda}{2 \ln \lambda}} \right) \right] + \left\{ 2 \ln \left[ \frac{\sinh \gamma}{\sinh \left[ \frac{\alpha_0}{2} \sqrt{\lambda \ln \lambda} \frac{x}{L_D} + \gamma \right]} \right] + \delta (\ln \lambda) C_1 \left( 1 - \exp \left[ -\frac{13}{10} \frac{x}{\delta L_D} \sqrt{\frac{\lambda}{2 \ln \lambda}} \right] \right) \coth \left[ \frac{\alpha_0}{2} \sqrt{\lambda \ln \lambda} \frac{x}{L_D} + \gamma \right] \right\} \left( \exp \left[ -3 \left( \frac{x}{\delta L_D} \sqrt{\frac{\lambda}{2 \ln \lambda}} - \frac{1}{2} \right) \right] + 1 \right)^{-1} \right. \end{array} \right.$$

**Constants  $\lambda$  and  $\delta$**   $\left\{ \begin{array}{l} \lambda \equiv N_A / n_i \\ \delta \equiv \sqrt{\frac{\lambda}{2 \ln [\lambda]} \frac{e b_n}{k_B T L_D^2}}, \text{ where } L_D = \sqrt{\varepsilon_{si} k_B T / 2 e^2 n_i} \end{array} \right.$

**Function S(X)**  $\left\{ X = \int_0^s d\xi \left[ \frac{1}{2} + \xi^2 \left( \ln [\xi] - \frac{1}{2} \right) \right]^{-1/2} \leftrightarrow S(X) = 1 + a e^{-X} + \frac{1}{6} a^2 e^{-2X} + \frac{1}{1080} a^4 e^{-4X}, \text{ where } a = -1.2722 \right.$

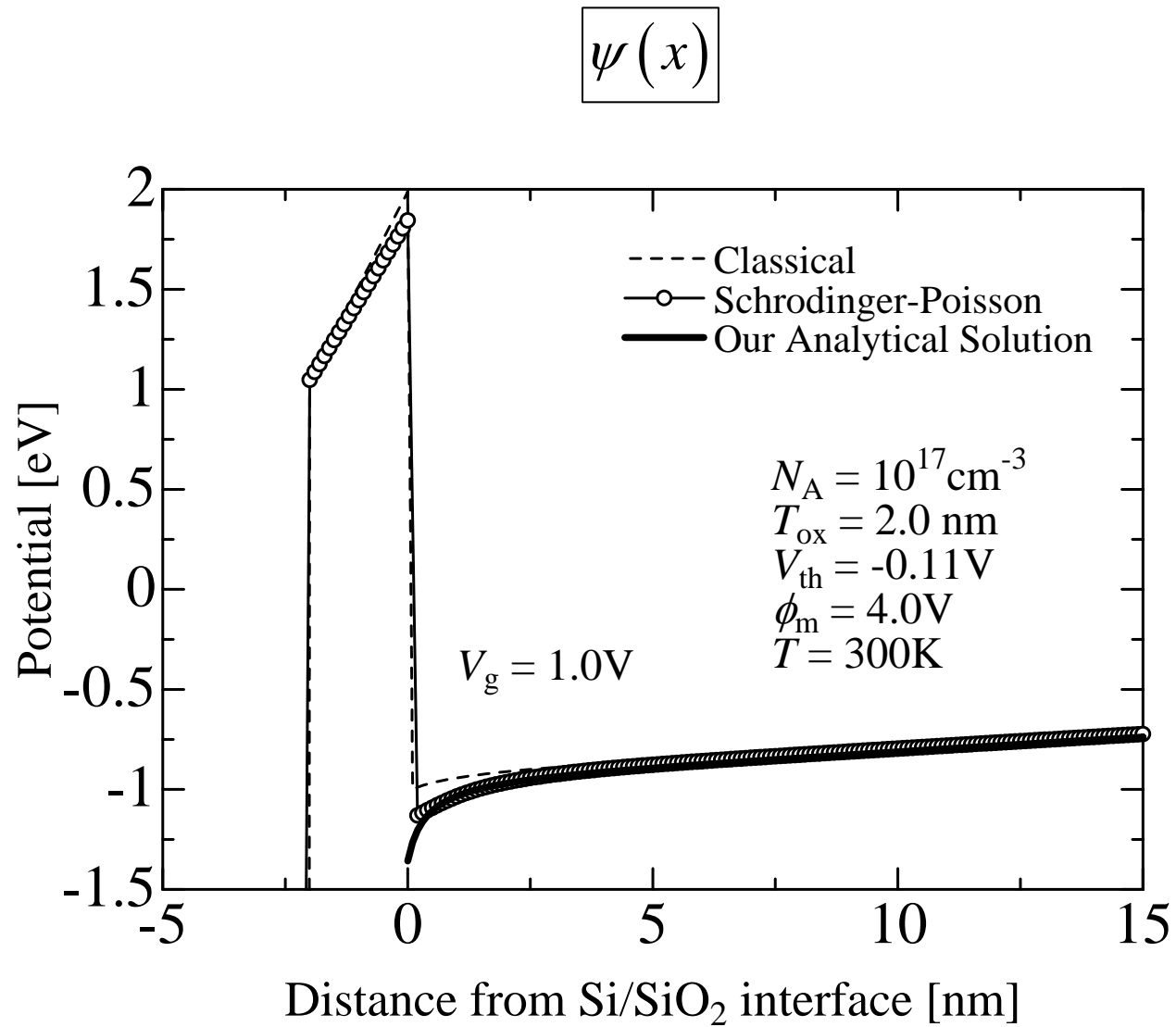
## Constants $\alpha_0$ and $\psi_0$

$$\left\{ \begin{array}{l} \alpha_0 \sqrt{\ln [\lambda]} = \sqrt{\frac{e \phi_n}{k_B T} + \ln [4 \alpha_0^2 \lambda \ln [\lambda]] - 2 \sinh^{-1} \left[ \alpha_0 \sqrt{\exp \left[ \frac{-e(\psi_s - \phi_n)}{k_B T} \right] \lambda \ln [\lambda]} \right] - 1} \\ \psi_s = V_G - V_{FB} - \frac{k_B T}{e} \frac{\varepsilon_{Si} T_{ox}}{\varepsilon_{ox} L_D} \sqrt{\alpha_0^2 \lambda \ln [\lambda] + \exp \left[ \frac{e(\psi_s - \phi_n)}{k_B T} \right]} \end{array} \right.$$

## $C_1$ and $\gamma$

$$\left\{ \begin{array}{l} C_1 = \left( 2r_1 - \frac{1}{2} r_1^2 - r_2 \right) \frac{\sqrt{2} T_{ox} \varepsilon_{Si} \exp \left[ \frac{e(\psi_s - \phi_n)}{k_B T} \right] \sinh [\gamma]^2}{L_D \varepsilon_{ox} \sqrt{\lambda \ln [\lambda]} \sinh [2\gamma] + T_{ox} \varepsilon_{Si} \alpha_0 \lambda \ln [\lambda]} \\ \gamma = \sinh^{-1} \left[ \alpha_0 \sqrt{\exp \left[ \frac{e(\phi_n - \psi_s)}{k_B T} \right] \lambda \ln [\lambda]} \right] \end{array} \right.$$

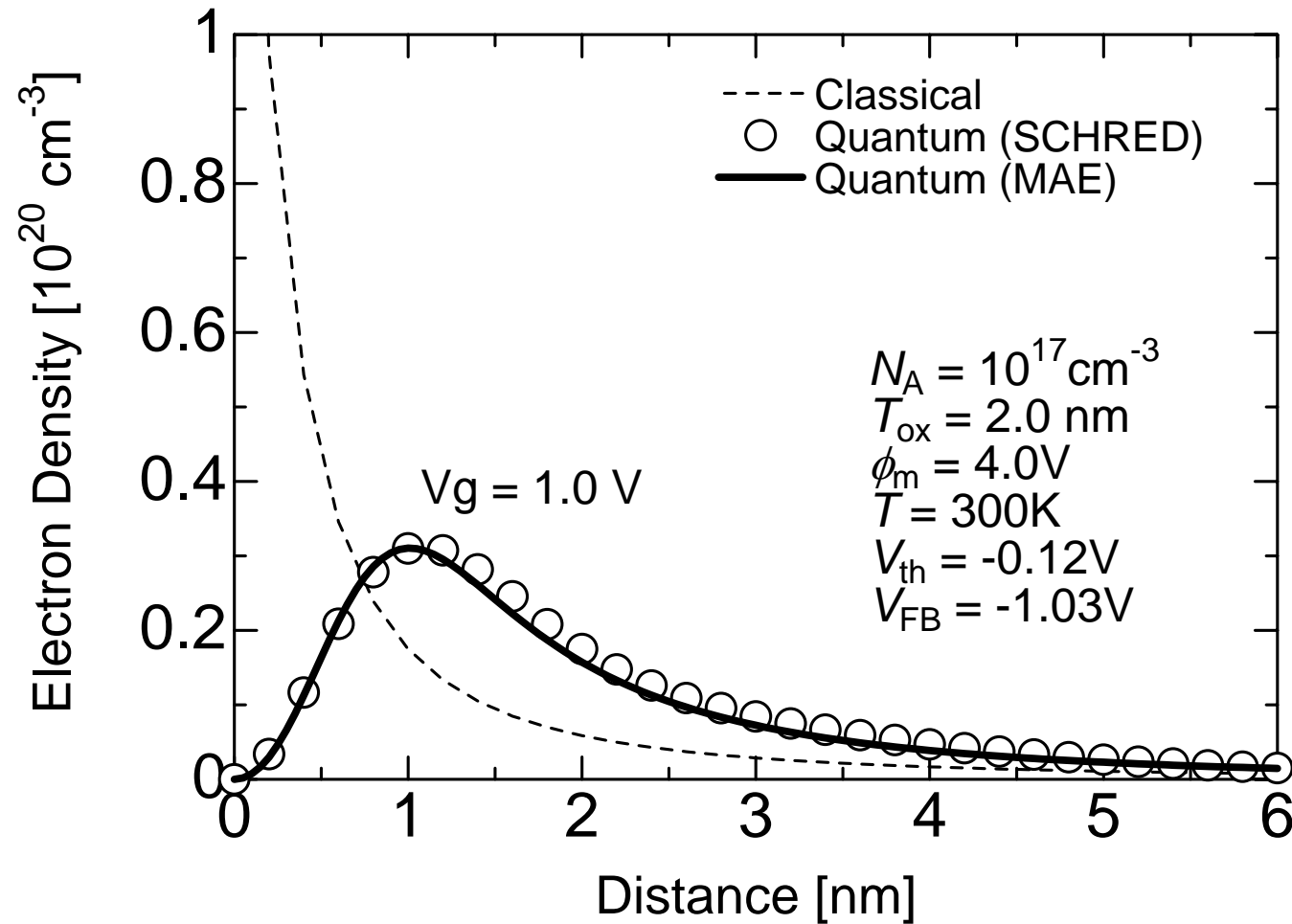
# Comparison 1: Band Bending



**Excellent Accuracy !**

# Comparison 2: Electron Density Profile

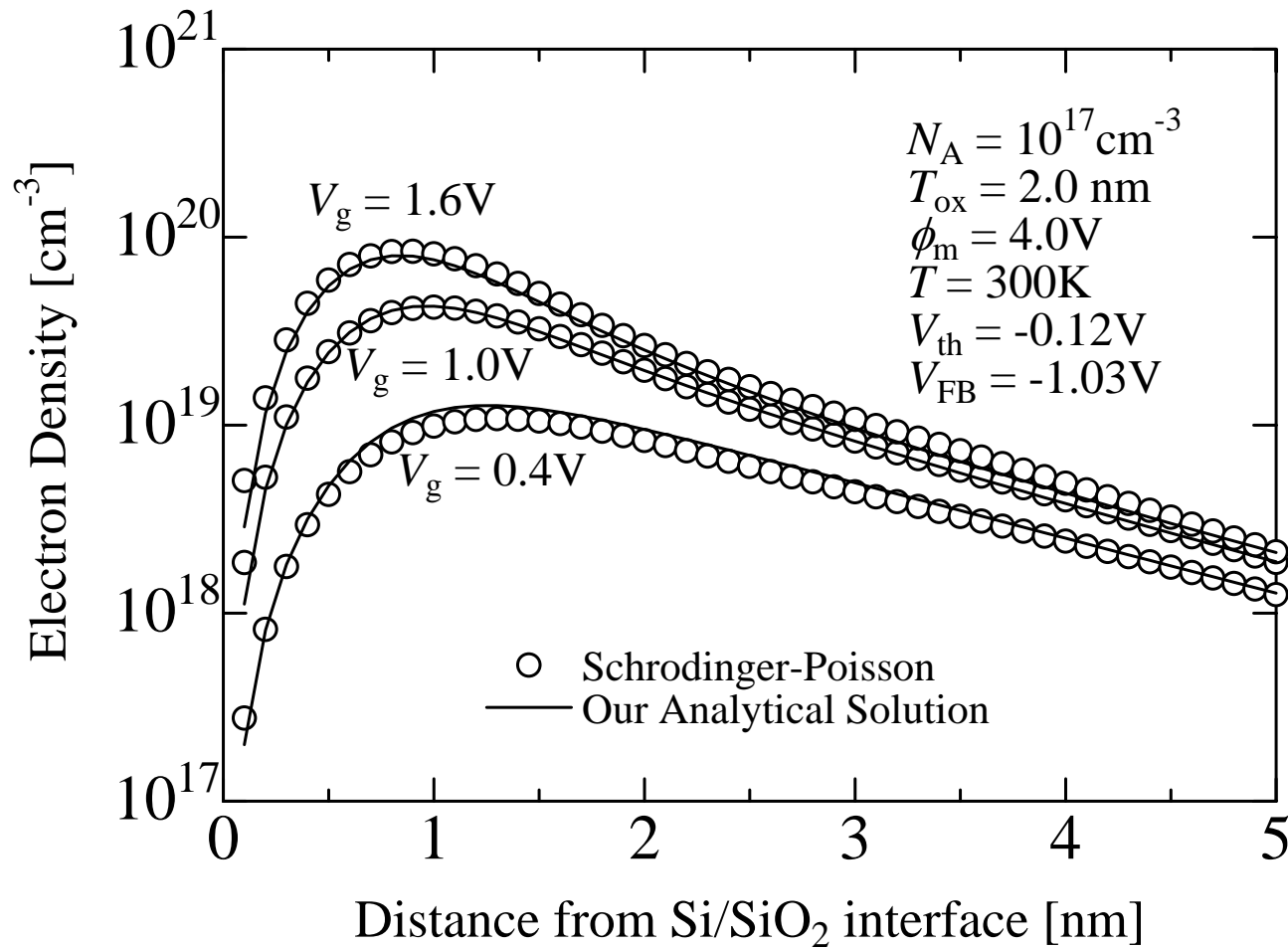
$$n(x)$$



**Brilliant Accuracy !**

# Comparison 3: Electron Density Profile, Log Scale

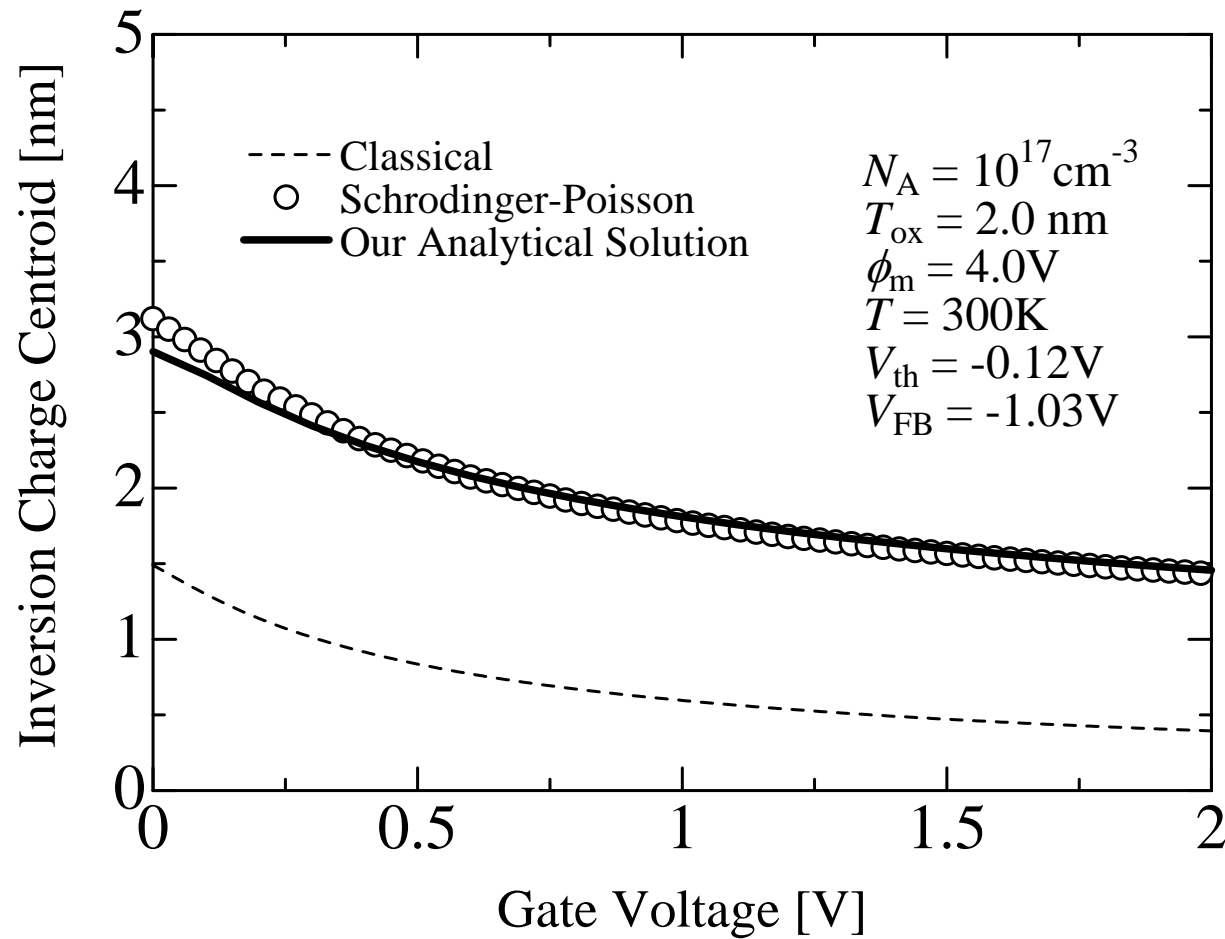
$$n(x)$$



**Fantastic Accuracy !**

# Comparison 4: Charge Centroid

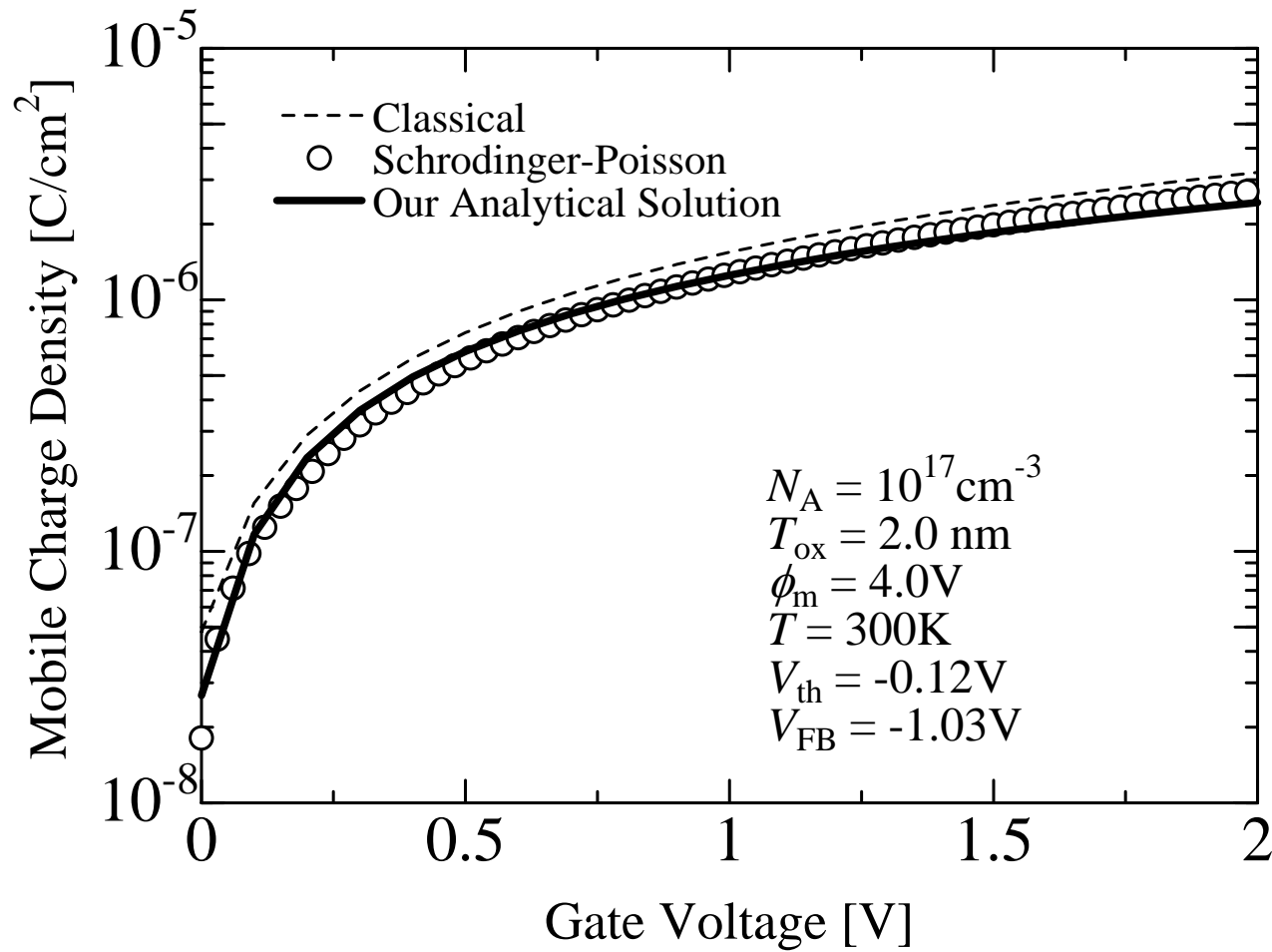
$$\bar{x} = \frac{\int x n(x) dx}{\int n(x) dx}$$



**Terrific Accuracy !**

# Comparison 5: Mobile Charge Density

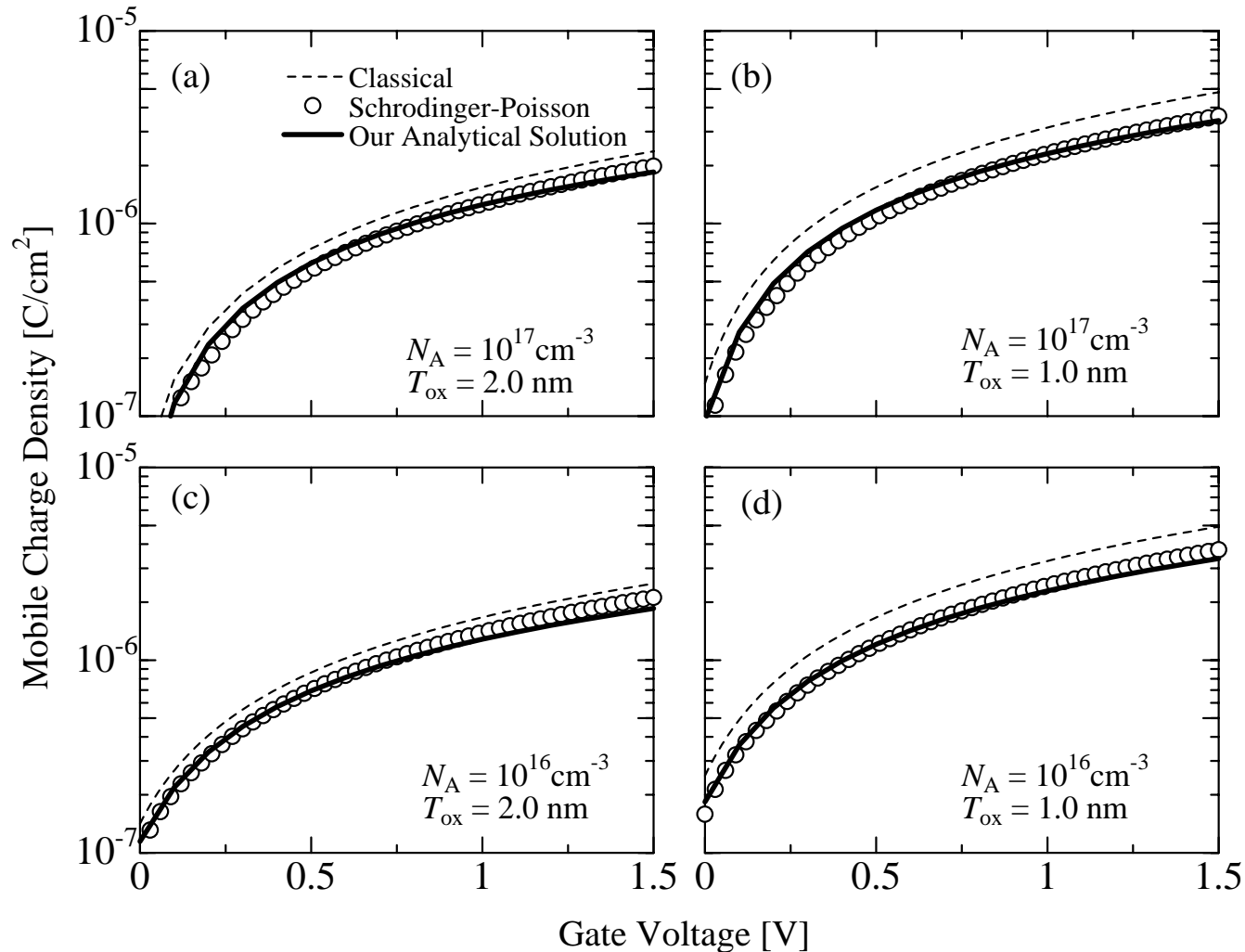
$$Q = \int e n(x) dx$$



Great Accuracy !

# Comparison : Mobile Charge Density, Various Devices

$$Q = \int en(x) dx$$



**Wonderful Accuracy !**

# Conclusion

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- Governing equations in density gradient model were analytically solved.
- Perturbation method was used.
- Analytic solutions have been successfully obtained.
- Potential, electron density, charge centroid, mobile charge density have been compared with exact solution.
- Our formulae have been shown to give excellent accuracy.
- These formulae can be used for more accurate circuit simulation & faster device simulation.

# Acknowledgement

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