Quantum corrected full-band Cellular Monte Carlo simulation of AlGaN/GaN HEMTs†

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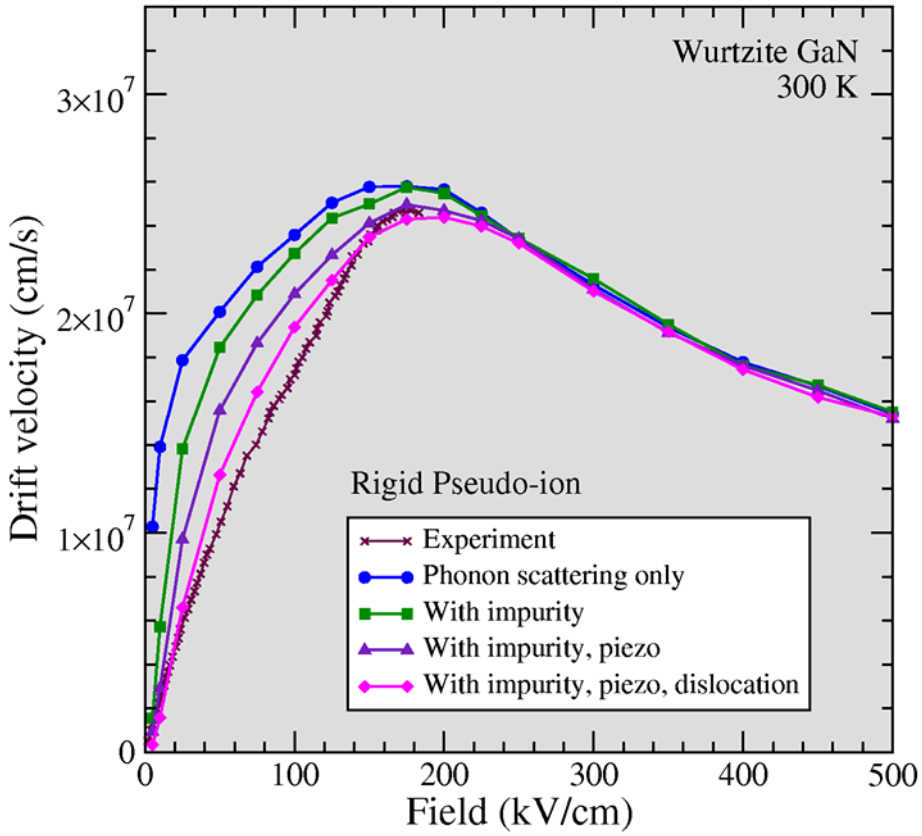
Motivation and Approach

- AlGaN/GaN HEMT is the attractive candidate for high-temperature, high-power and high-frequency device.
  - wide band gap, high saturation velocity
  - high electron density by spontaneous and piezoelectric polarization effect
- Here the full-band Cellular Monte Carlo (CMC) approach is applied to HEMT modeling.
- The effect of the quantum corrections is examined based on the effective potential method.

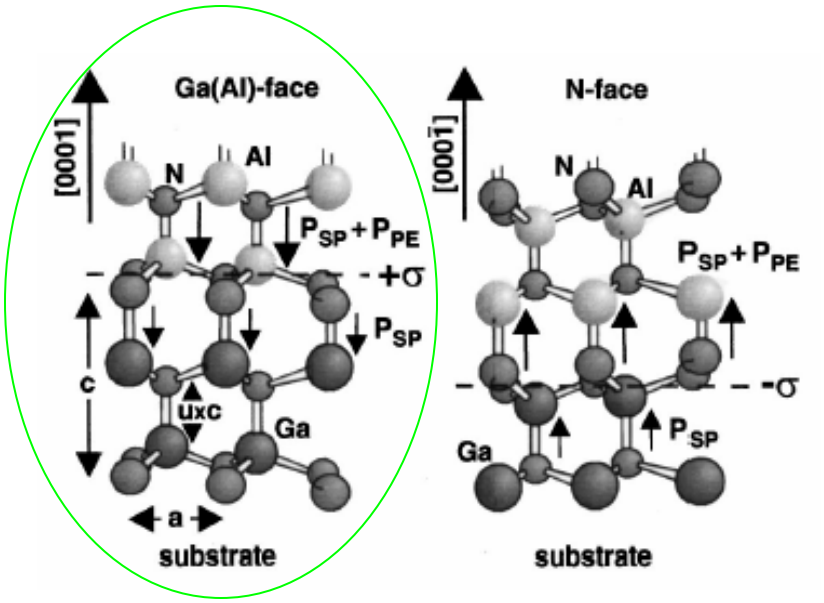
Full-band transport model

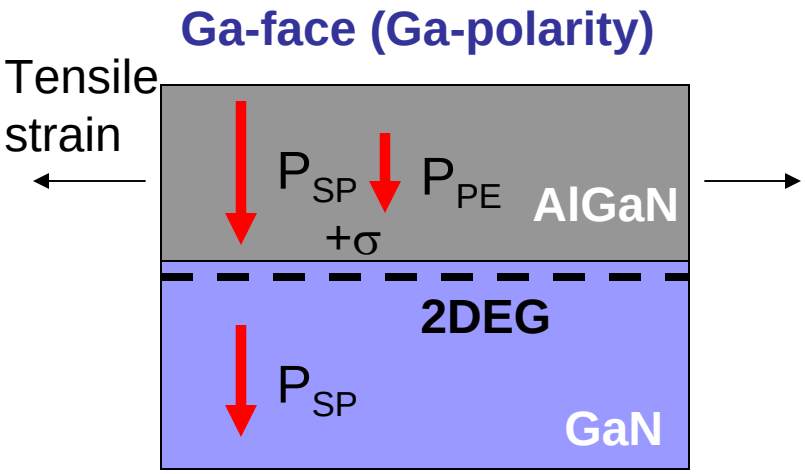
Transport is based on the full electronic and lattice dynamical properties of Wurtzite GaN:

- Full-band structure
- Full Phonon dispersion
- Anisotropic deformation potential scattering (Rigid pseudo-ion Model)
- Anisotropic polar optical phonon scattering (LO- and TO-like mode phonons)
- Crystal dislocation scattering
- Ionized impurity scattering
- Piezoelectric scattering

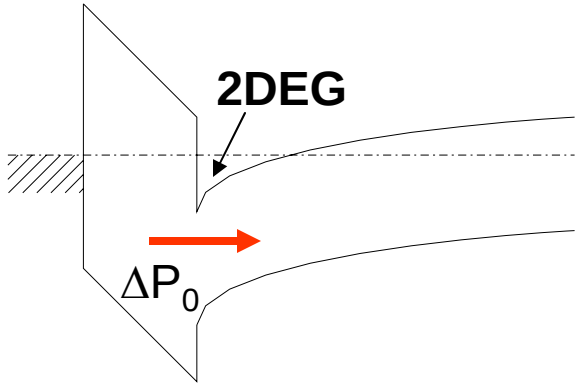


AlGaN/GaN hetero structure





P_{SP} : Spontaneous polarization
P_{PE} : Piezoelectric polarization (strain)

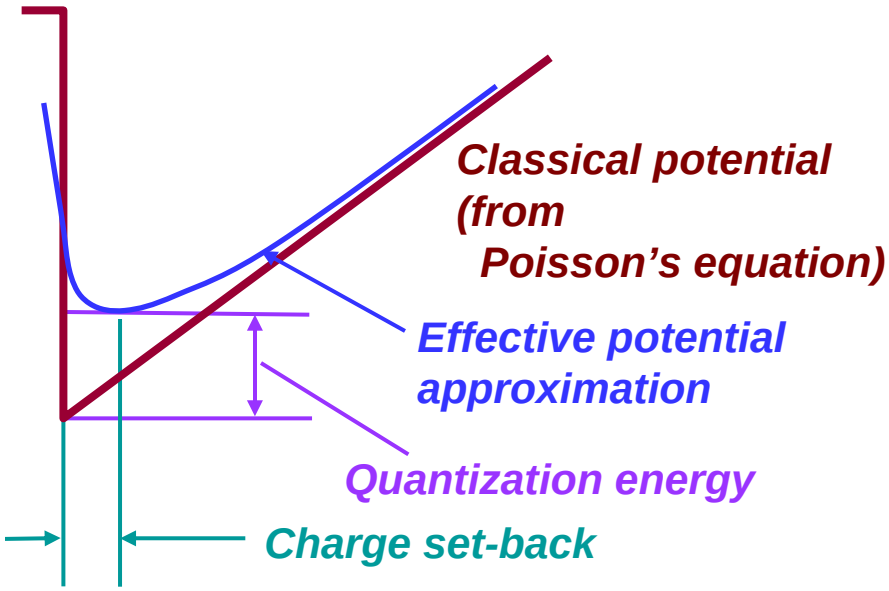


Fixed polarization charge is induced at the AlGaN/GaN interface

$$\sigma = P(GaN) - P(AlGaN)$$
$$= P_{SP}(GaN) - \{P_{SP}(AlGaN) + P_{PE}(AlGaN)\}$$

Ambacher *et al.*, *J. Appl. Phys.* **87**, 334 (2000)

Effective potential approach



$$V_{eff}(x) = \frac{1}{\sqrt{2\pi}a_0}\int_{-\infty}^{+\infty} V(x+\xi)\exp\left(-\frac{\xi^2}{2a_0{}^2}\right)d\xi$$

D.K. Ferry, Superlattices and Microstructures 28, 419 (2000)

Smoothed Effective Potential

Effective potential takes into account the natural non-zero size of an electron wave packet in the quantized system.

This effective potential is related to the self-consistent Hartree potential obtained from Poisson's equation.

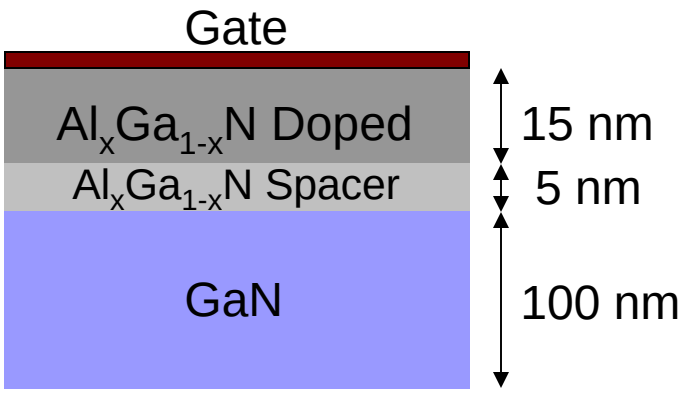
a_0 : Gaussian smoothing parameter

depends on

- Temperature
- Concentration
- Confining potential
- Other interactions

Schrödinger-Poisson calculation

Calculated AlGaN/GaN structure



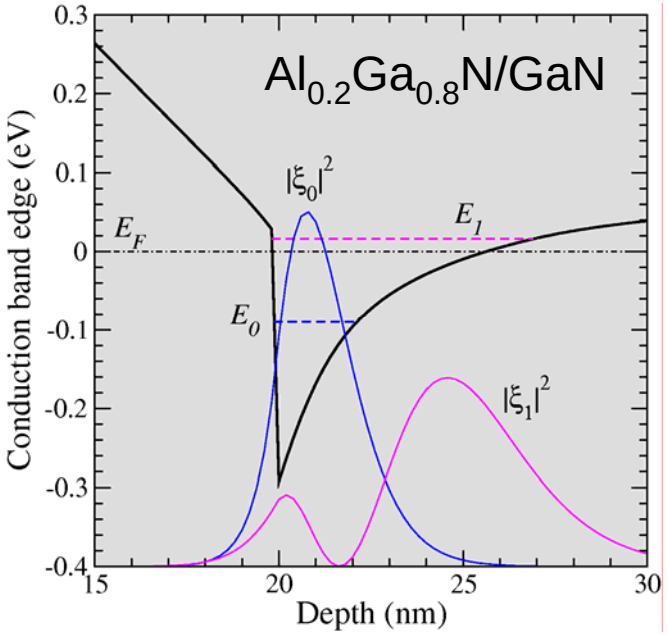
Modulation doping : 10^{18} cm^{-3}
Unintentional doping : 10^{17} cm^{-3}
(for AlGaN and GaN)
Al content x : 0.2 ~ 0.4

Schrödinger-Poisson (S-P) calculation

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m(z)}\frac{d}{dz}\right)\varphi+\{eV(z)+\Delta E(z)\}\varphi=E\varphi$$

$$\frac{d}{dz}D(z)=\frac{d}{dz}\left\{-\varepsilon(z)\frac{d}{dz}V(z)+P(z)\right\}$$

$$=e\left\{-n(z)+N_D^+\right\}$$



F. Sacconi *et al.*, *IEEE Trans. Electron Devices* **48**, 450 (2001)

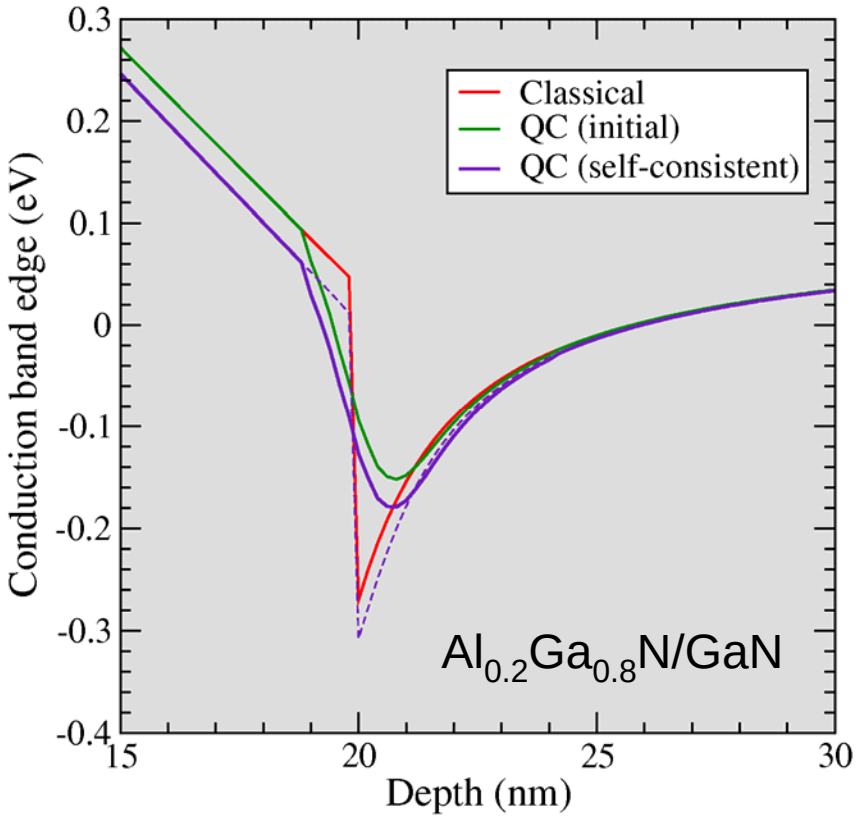
Effective potential calculation

Quantum correction (QC)
with effective potential

Self-consistent calculation :

- Solve Poisson equation with classical electron distribution
- Quantum correction with the effective potential method
- Calculate the electron density with the new potential (Fermi-Dirac statistics)
- Solve the Poisson equation

Repeat until convergence

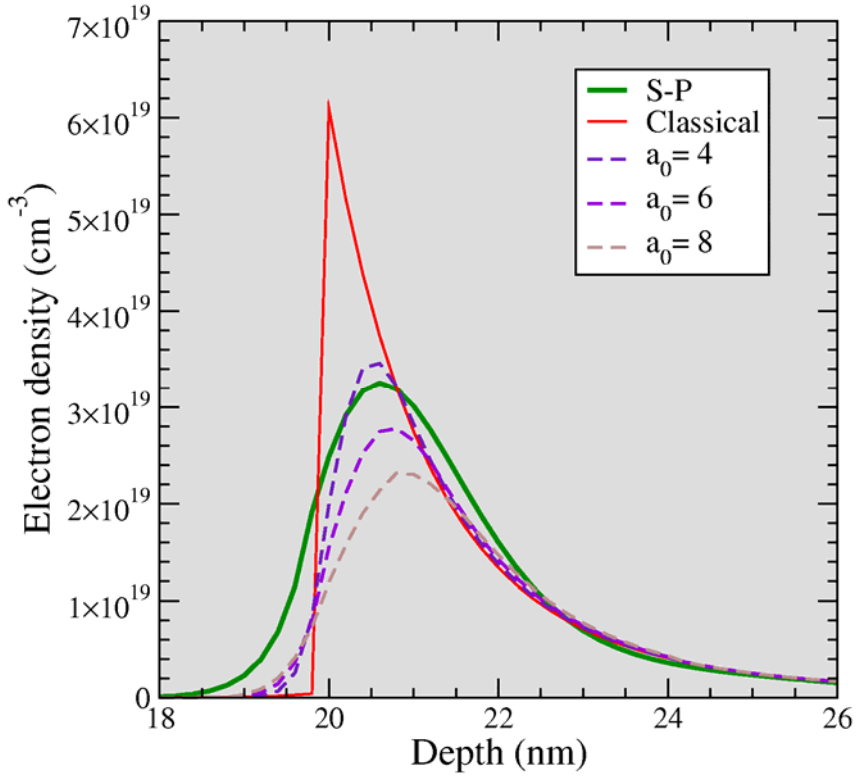


The final effective potential shifts due to the polarization charge

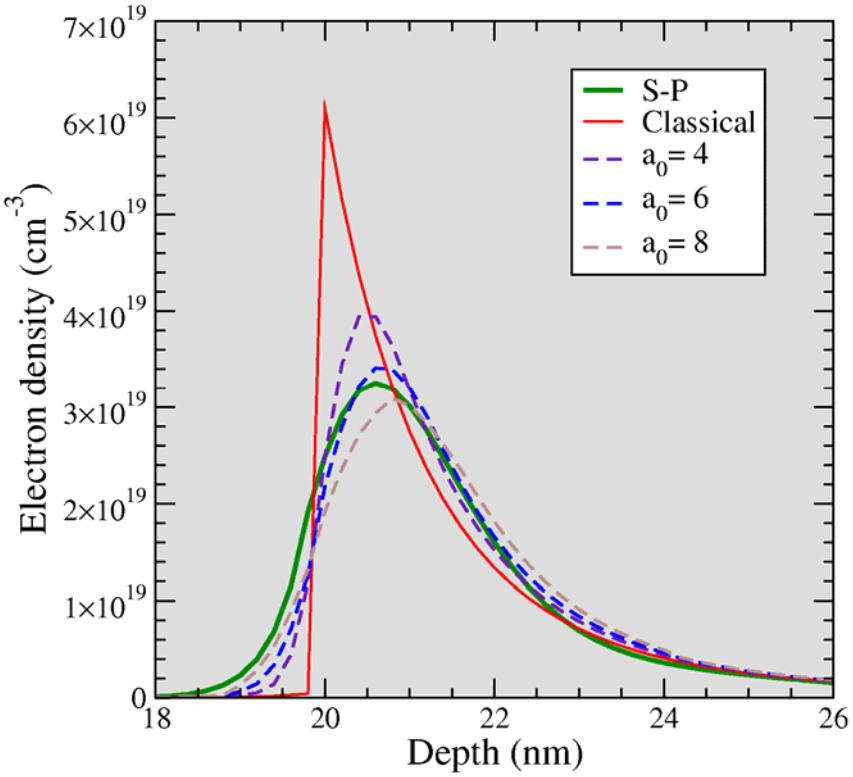
Electron distribution

Electron distribution for S-P, classical and quantum correction ($Al_{0.2}Ga_{0.8}N/GaN$)

Quantum correction (initial)



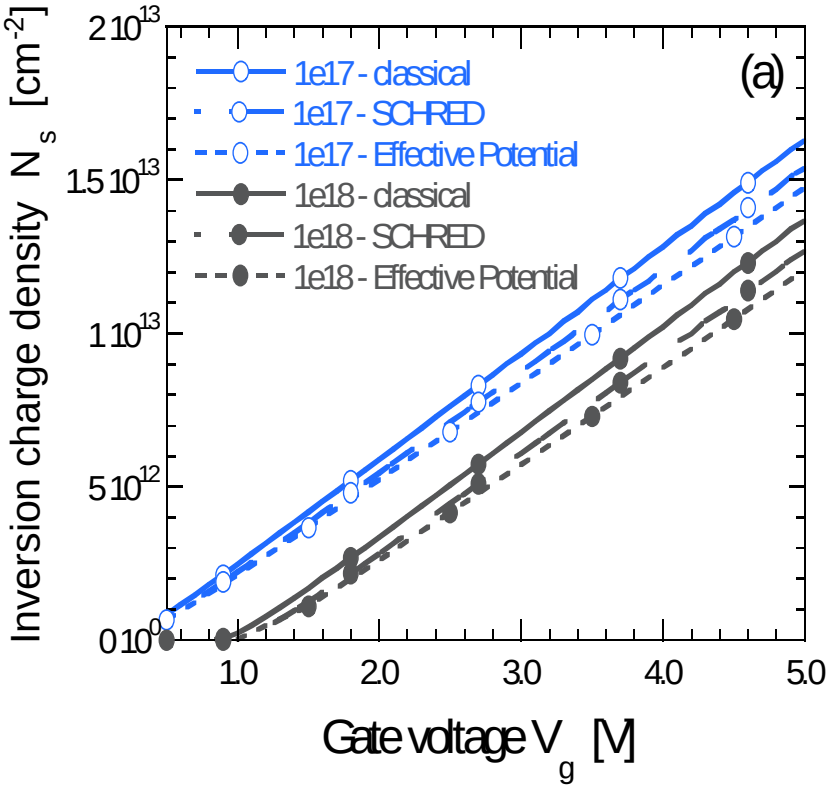
Quantum correction (self-consistent)



a_0 (Å) : Gaussian smoothing parameter

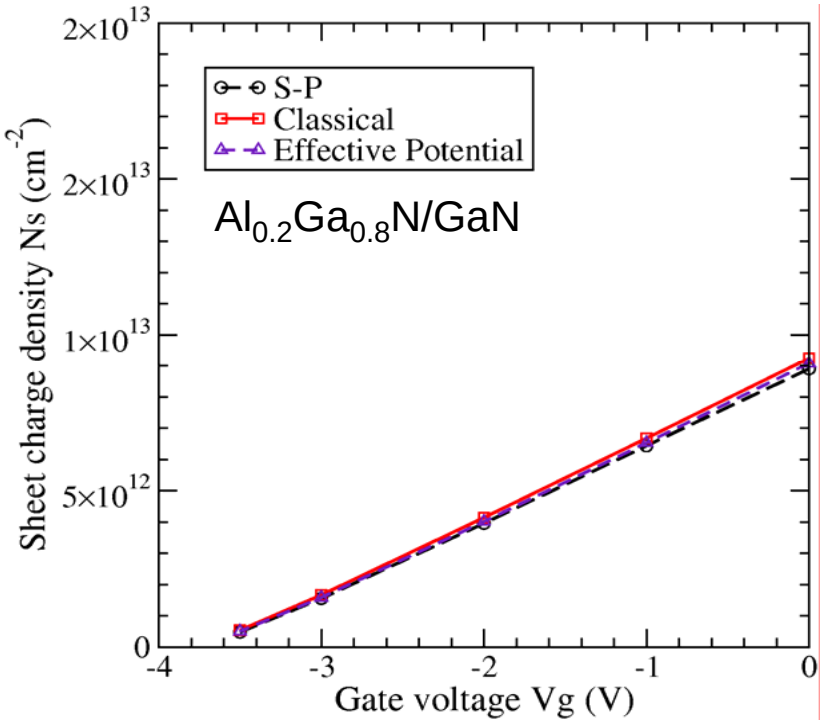
Electron sheet density

N_s for Si MOSFET



MOSFET with 6nm gate oxide.
Substrate doping is 10^{17} and 10^{18} cm^{-3}.

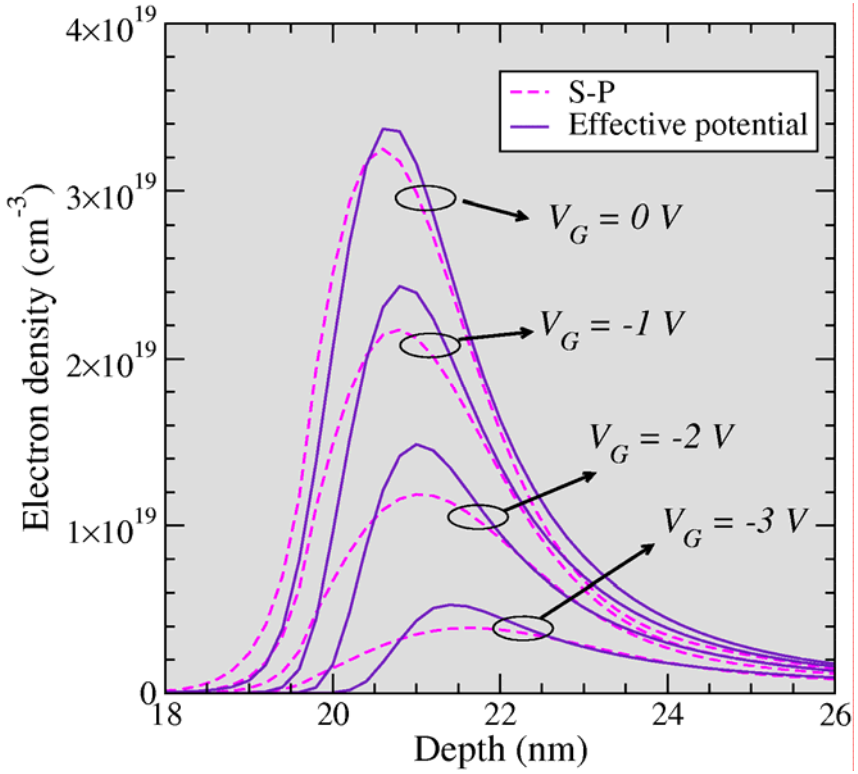
N_s for AlGaN/GaN HEMT



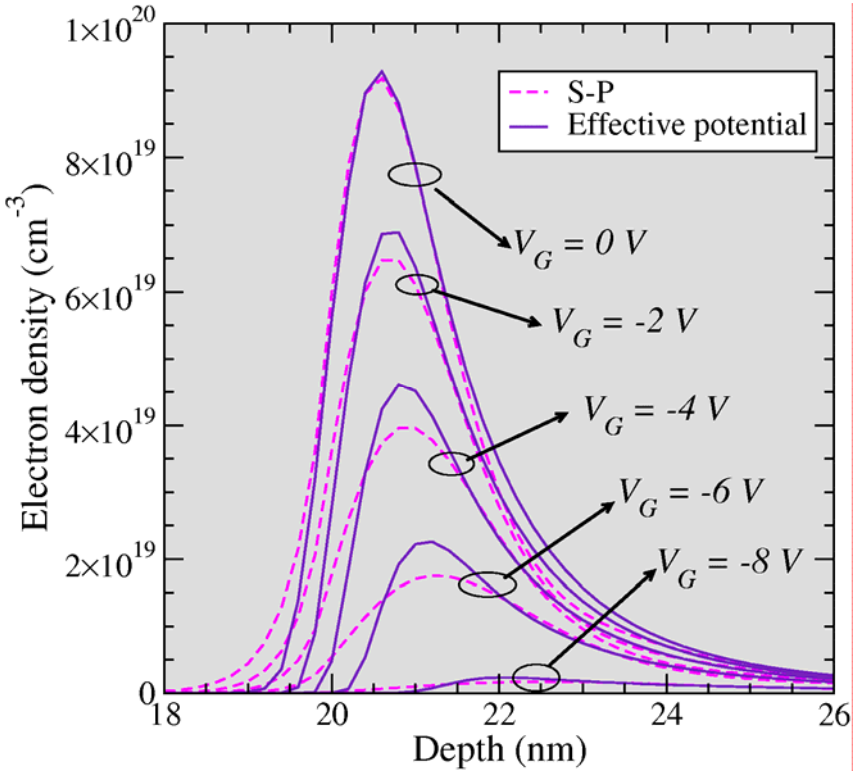
MOSFET data:
I. Knezevic *et al., IEEE Trans. Electron Devices* **49**, 1019 (2002)

Comparison of electron distribution with S-P

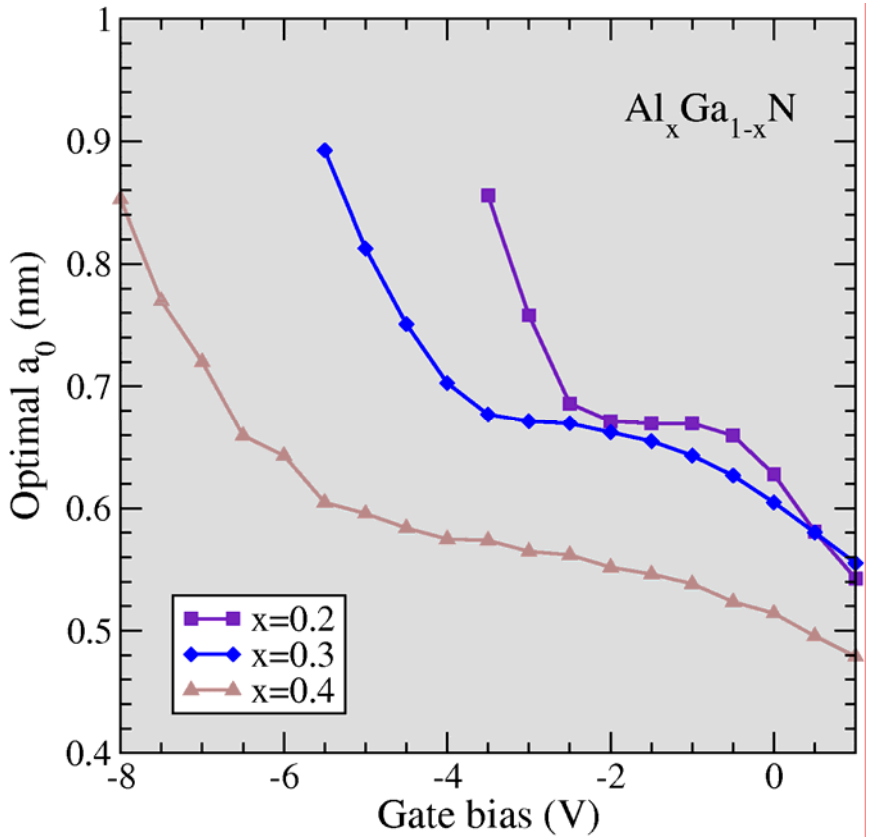
$Al_{0.2}Ga_{0.8}N/GaN$



$Al_{0.4}Ga_{0.6}N/GaN$

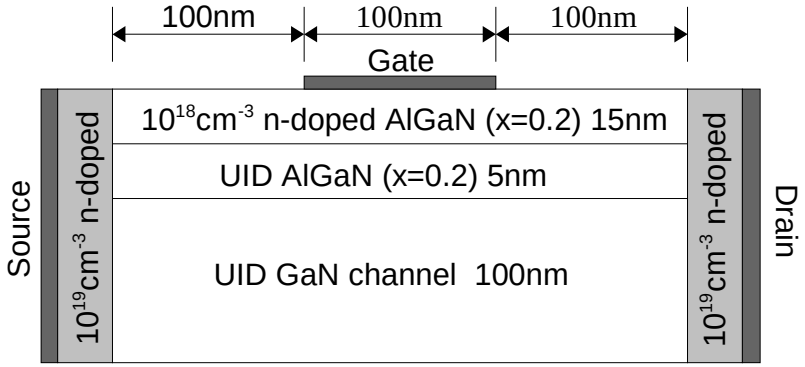


Gaussian smoothing parameter (a_0) fitting



HEMT device simulation

Simulated HEMT device



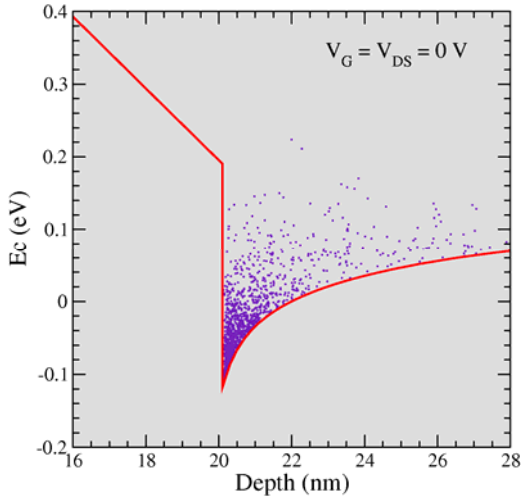
UID density : 10^{17} cm^{-3}

ΔE_c = 0.33 eV

Schottky barrier ϕ_B=1.2eV

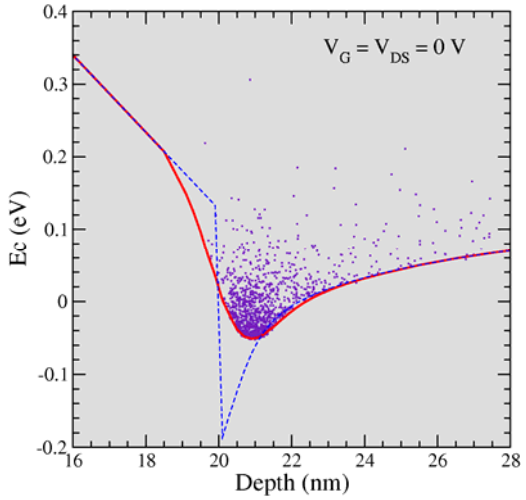
Electron distribution under the gate

Classical



Quantum correction

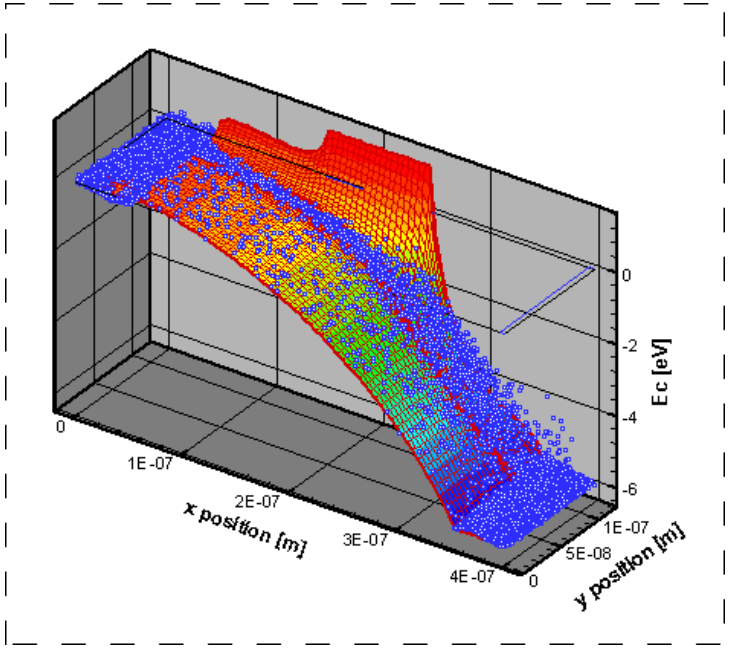
a_0=6.4 Å

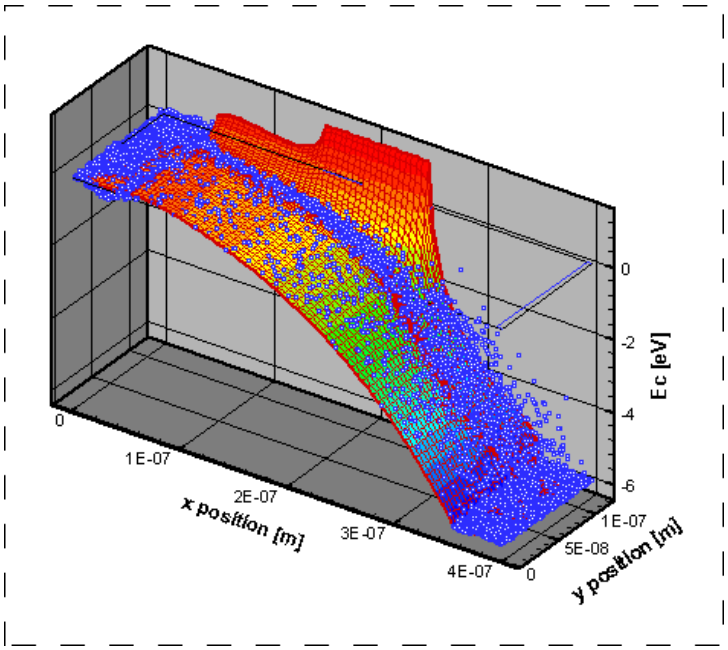


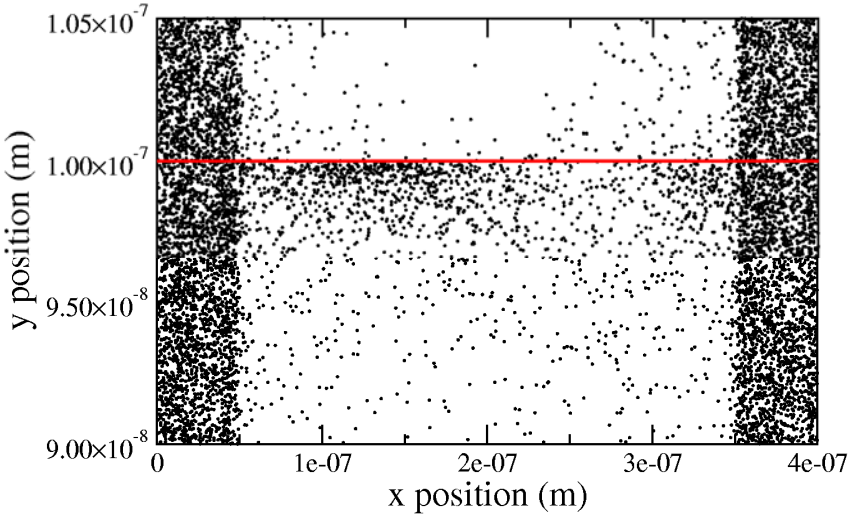
Classical

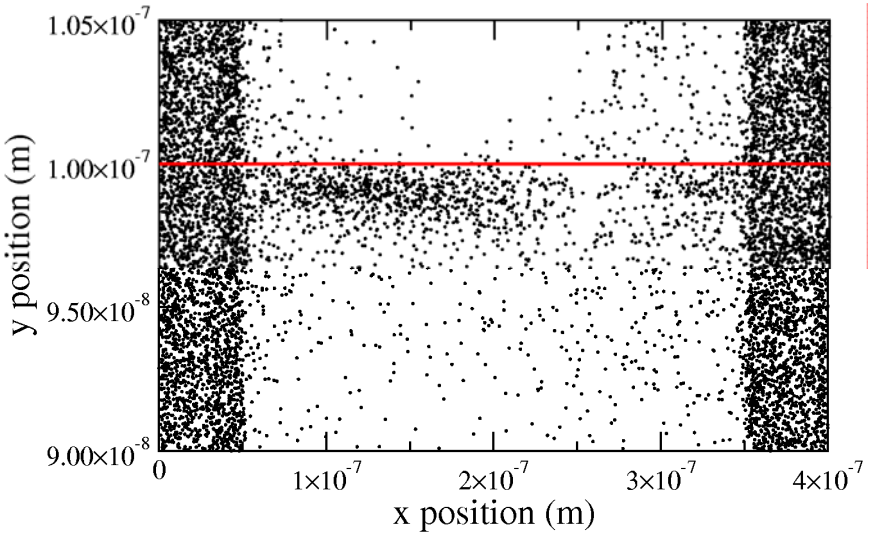
Effective potential

V_G=0V
V_{DS}=6V

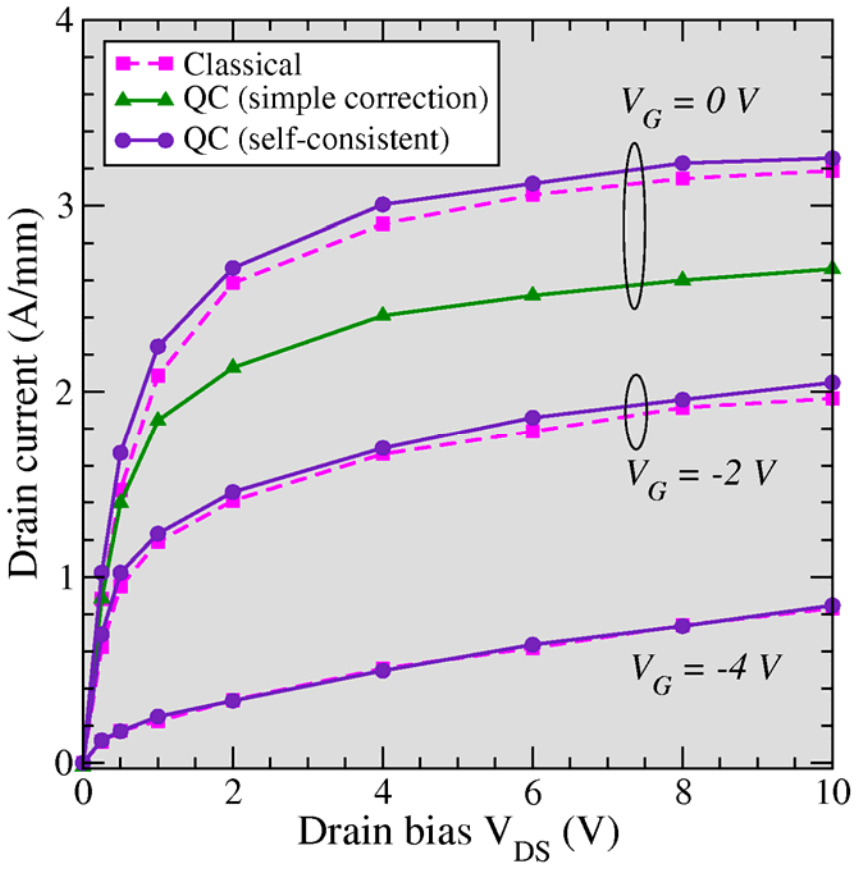


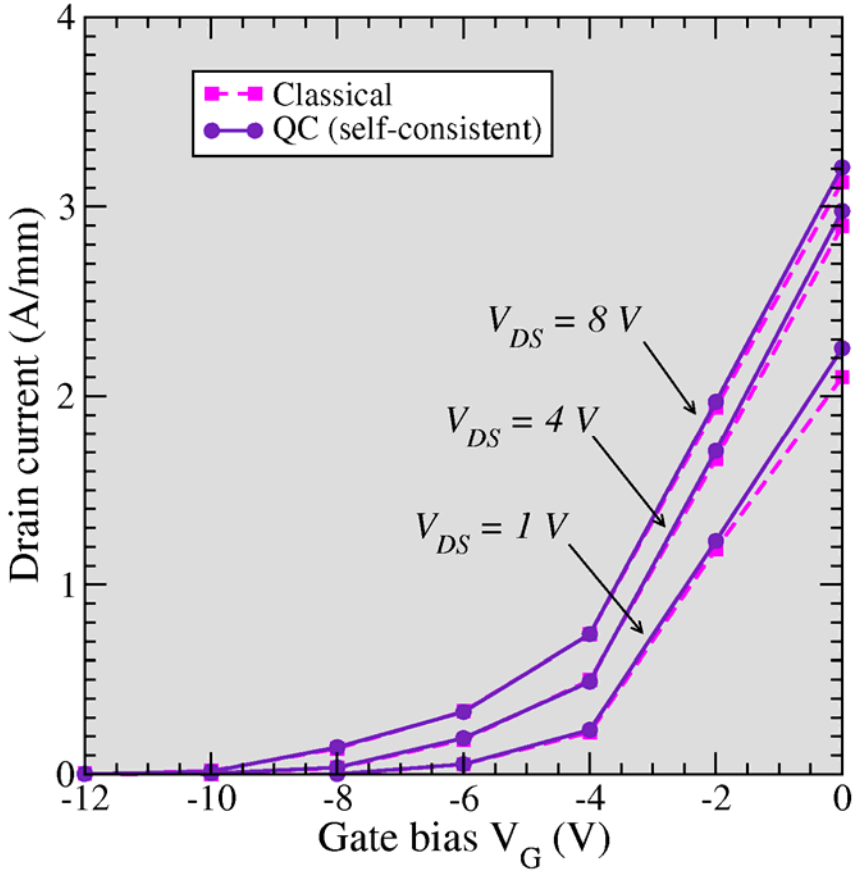






$I_D\_V_{DS}$, $I_D\_V_G$


Classical
QC (simple correction)
QC (self-consistent)
V_G = 0 V
V_G = -2 V
V_G = -4 V
Drain current (A/mm)
Drain bias V_{DS} (V)
0
1
2
3
4
0
2
4
6
8
10


Classical
QC (self-consistent)
V_{DS} = 8 V
V_{DS} = 4 V
V_{DS} = 1 V
Drain current (A/mm)
Gate bias V_G (V)
0
1
2
3
4
-12
-10
-8
-6
-4
-2
0

Conclusion

- The effect of quantum corrections to the classical charge distribution at the AlGaN/GaN interface are examined. The self-consistent effective potential method gives good agreement with S-P solution.
- The best fit Gaussian parameters are obtained for different Al contents and gate biases.
- The effective potential method is coupled with a full-band CMC simulator for a GaN/AlGaN HEMT.
- The charge set-back from the interface is clearly observed. However, the overall current of the device is close to the classical solution due to the dominance of polarization charge.