Theoretical study of pH response of electrolyte gate AlGaN/GaN field effect transistors

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Motivation

- Applicability of semiconductor devices as sensors
- Effect of solution gate on I-V characteristics
- Non-toxicity and high mobilities of nitride structures

Goal

Prediction of sensitivity of AlGaN/GaN HEMT as a function of:
- pH value of the electrolyte
- charged adsorbates at the semiconductor/electrolyte interface.

Method of calculation

Electronic structure

- 1D self-consistent Poisson-Boltzmann solution of AlGaN/GaN HEMT structure
- Strain and piezoelectric fields fully included

Current calculation

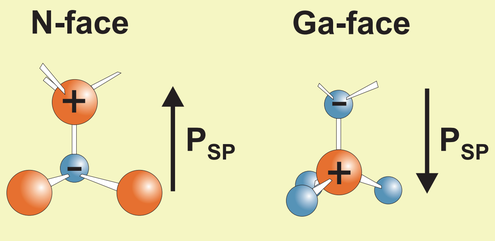
- Fully 2D semiclassical carrier transport within HEMT
- Drift-Diffusion equations with self-consistently determined quasi-Fermi levels

Model of GaN heterostructure

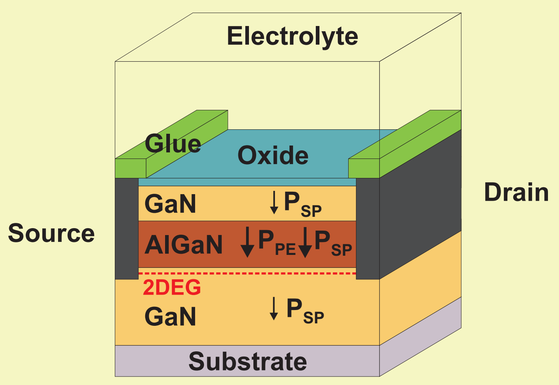
Polarization

Polarity of epitaxially grown GaN

Wurtzite phase is pyroelectric: spontaneous electric polarization along hexagonal axis



Ga-face structure



Interface charge density

Divergence of polarization across interface gives interface charge

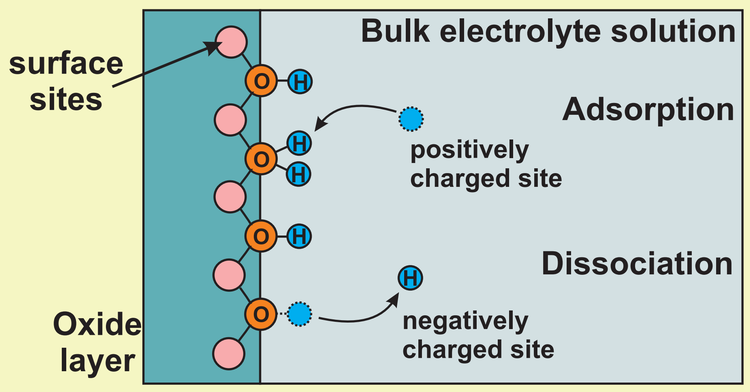
2DEG formation due to polarization fields

Model of Electrolyte

Site-binding model

Amphoteric behavior of surface:
Adsorption or dissociation of hydrogen ions at hydroxyl groups

Reactions characterized by two dissociation constants K



Poisson-Boltzmann model

Describes equilibrium of electro-diffusion processes of ions in solution

Exponential relationship between charge density and potential

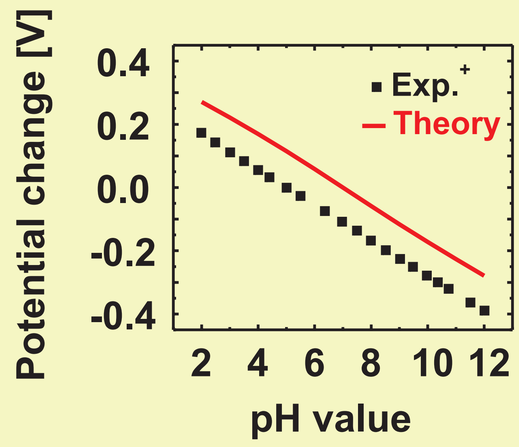
Results

Surface potential sensitivity of 55.9 mV/pH

Determination of material parameters

Calculate variation of surface potential with pH value & compare to experimental data
Surface charge density and dissociation constants determined

Variation of Oxide/Electrolyte potential



Surface charge

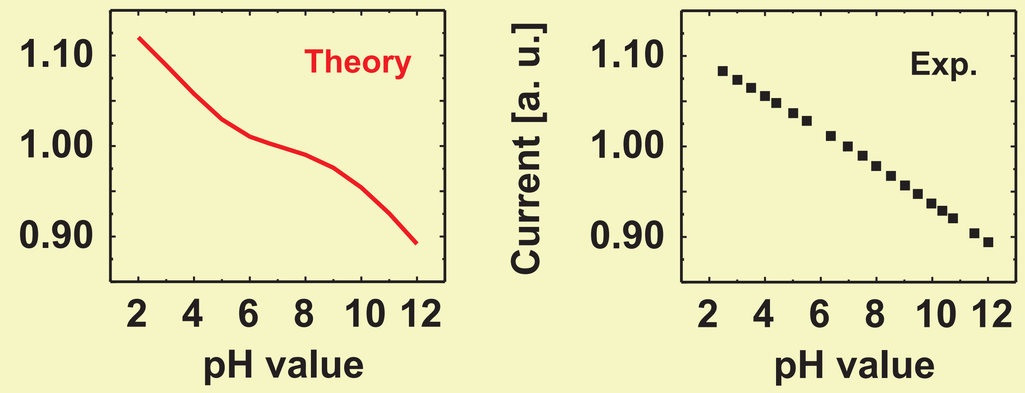
Oxide/electrolyte charge decreases with pH

Point of zero charge for GaO approximately at pH=7

[+] Steinhoff *et al.*, APL **83**, 177 (2003)

Results

Source-drain current as a function of pH



Good agreement with experiment

Ga-face polarity

Calculation of source-drain current with nextnano[3]

Leaky oxide: additional pH-dependent sheet charge at GaN/Oxide interface

nextnano[3] next generation 3D nanodevice simulator quantum

Simulator for 3D semiconductor nano-structures

Predictions

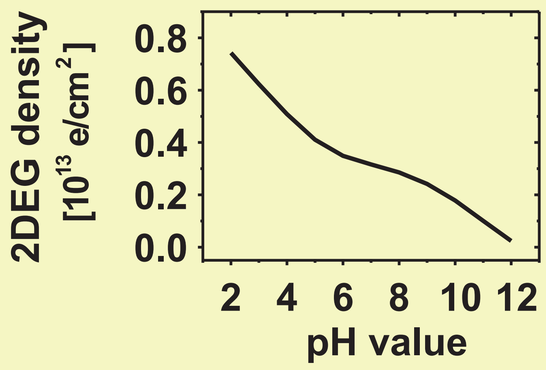
N-face: Significant enhancement in 2DEG variation with pH

N-face polarity

Conducting channel closer to surface charge

Low Al content: closed channel at high pH values possible

BUT: Poorly controlled growth conditions



Conclusion

- Site-binding model and Poisson Boltzmann model successfully explains observed pH sensitivity
- N-face AlGaN/GaN heterostructures promise excellent sensor performance