MOS-AK Compact Modeling Workshop
at ESSCIRC-ESSDERC 2020 Virtual Educational Event

Nanowire Junctionless ISFETs

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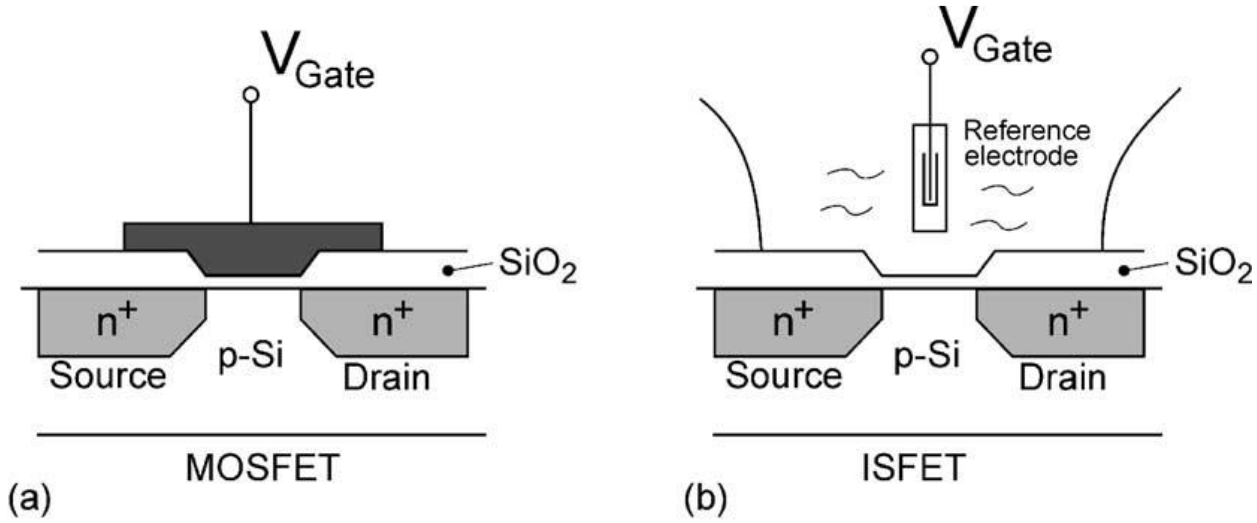
Outlines

- Concept and Art of the State of ISFETs
- Nanowire ISFETs as bio-sensors
- Operation Principle of ISFET sensors
  - The basics of electrolyte-oxide interface interactions
- Modeling of junctionless (JL) ISFET
  - Double-gate (DG) ISFET
  - Nanowire (NW) ISFET
- Validation of the DG and NW JL ISFET model
- Conclusion

Concept of Ion-Sensitive FETs (ISFETs).

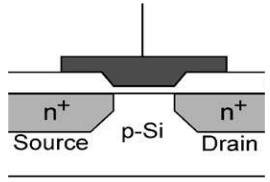


✓ The oxide is the actual contact between the electronic system and the bio-chemical environment.

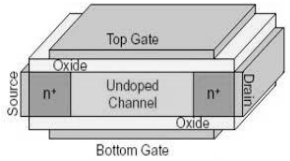
P. Bergveld / Sensors and Actuators B 88 (2003) 1–20

- The ISFET is a MOSFET with the gate replaced by an electrolyte with a reference electrode in it. The electrolyte is in contact with the gate oxide.
- This device measures ion concentrations (e.g. H^+ions) along with electrical potentials and was first called an ISFET in 1970 by Bergveld.

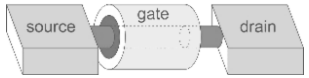
Art of the State



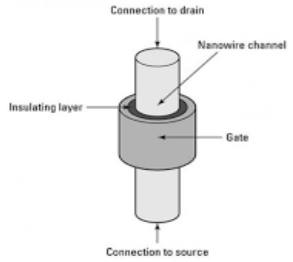
Conventional FET



DG FET

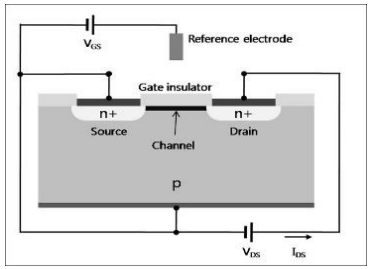


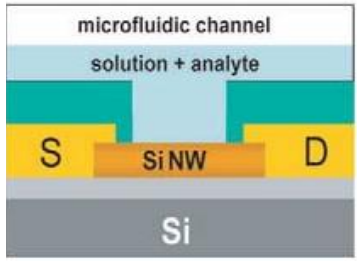
GAA FET



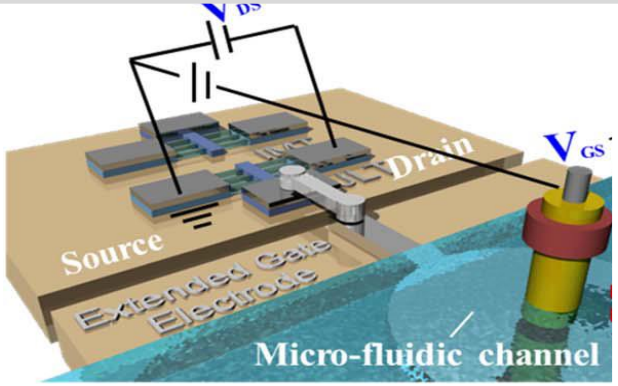
Junctionless NW FET

- **better channel control**
- **reduced short channel effects**
- **no junctions**





F. Patolsky, M. Lieber, Mterials Today, (2005).



Jpn. J. Appl. Phys. 58, 027001 (2019)

- **High sensitivity, selectivity**
- **low detection limit**
- **miniaturization**

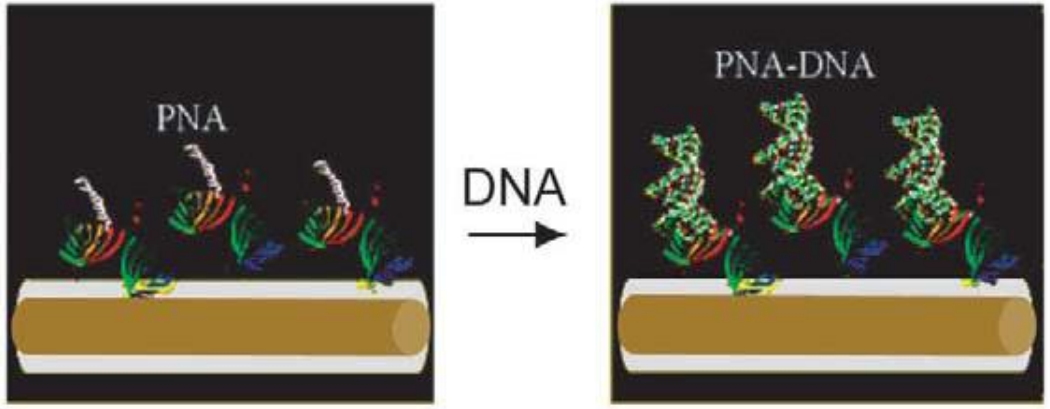
➢ The progress in FET technologies is promoting the progress of ISFETs.

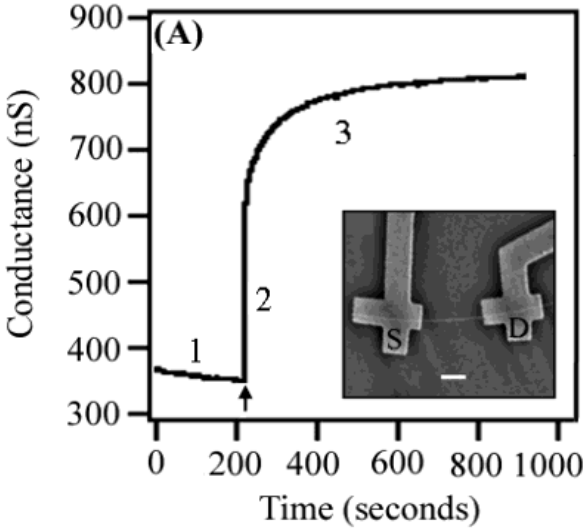
Nanowire ISFET sensors

Why Nanowires (NW) are preferred?

- The high surface to volume ratio of NWs is an advantage over bulk FETs.
  - Ultra-sensitive detection of biological and chemical species
- NW diameters are about the size of the molecules to be detected.
  - Increases the ability to miniaturize the transduction principle
- Decreasing the size of the nanowire decreases capacitance
  - Enables shorter time responses.

Examples of Nanowire bio-sensors





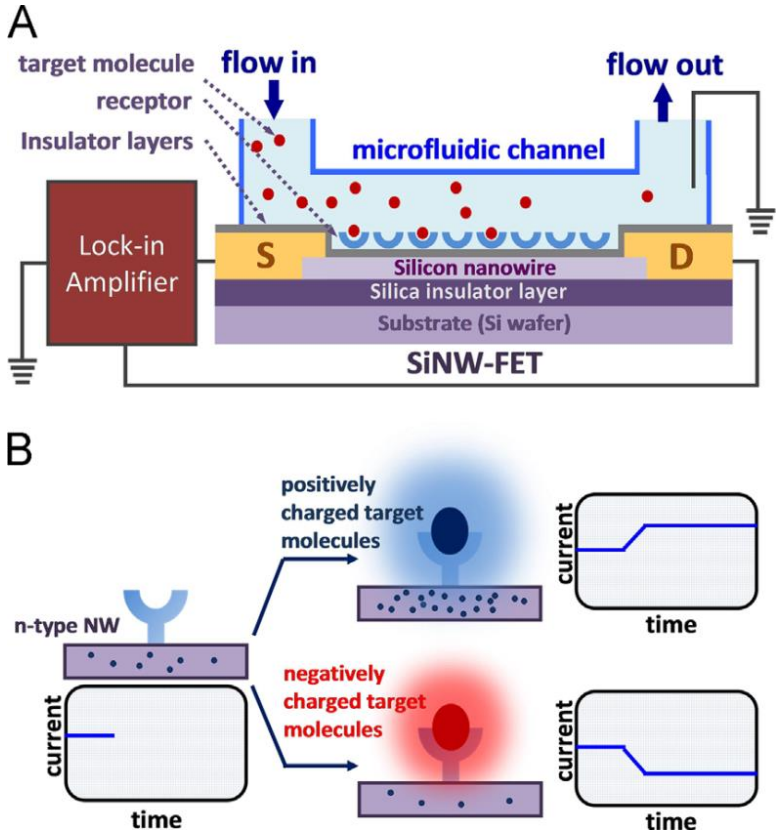
The conductance response from a Si NW device functionalized with PNA receptor.

Si NW sensors functionalized with peptide nucleic acid (PNA) receptors to bind to DNA.

- Electrical detection of DNA molecules with NW sensor* published in 2004.
  - The binding of a charged biomolecule results in conductance change in NW.

* Jong-in Hahm and Charles M. Lieber, Nano Lett., Vol. 4, No. 1, 2004

Examples of Nanowire bio-sensors

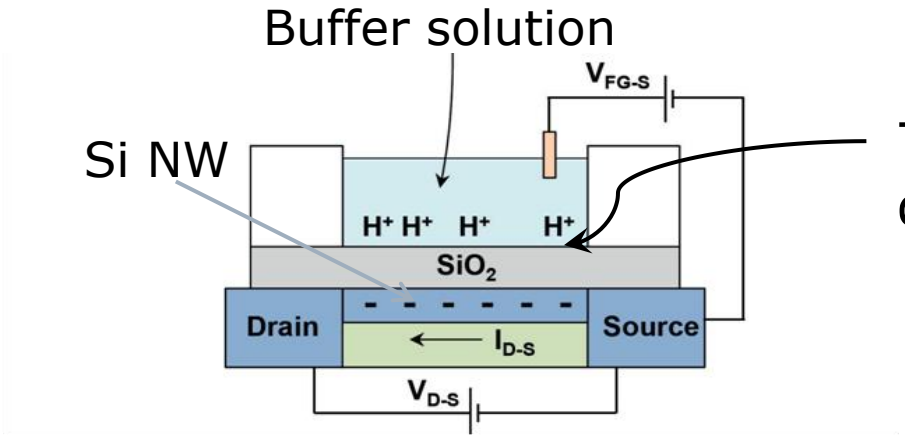


- NW FETs for biomolecules recognition.
  - Grafting 'receptor' on the NW surface: selective binding to molecules.
  - Once the target molecule (antigen) binds to the receptor, a charge transfert occurs: change in the drain current.

Mo-Yuan Shen et. al., Biosensors and Bioelectronics, 60,101–111 , (2014) .

Operation Principle of ISFET sensors

Principle of ISFET sensors



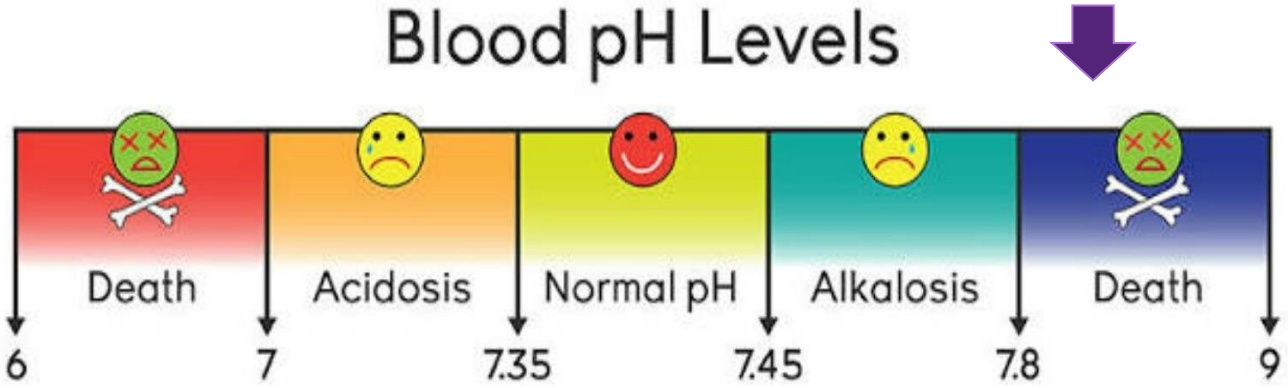
The potential at the SiO_2- solution interface depends on [protons] in the solution.

- The operation principle remains the same as for 'regular' FETs:

But

- The gate electrode is 'removed'.
- The buffer solution acts *almost* as a gate

Why to measure pH ?



To remember: $pH = -log_{10}[H^+]$

Pure water contains equal quantity of (H^+) and $(OH-)$ ions, each equal to 1×10^{-7} M/Liter. Thus for pure water pH=7.

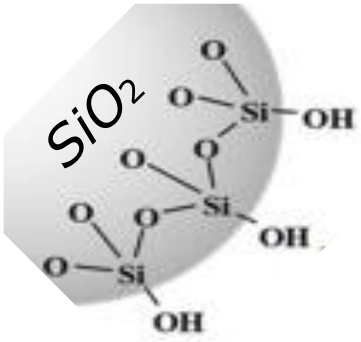
Fluids in human body (saliva, blood, spinal fluid) all have pH of about 7.4.

- **pH** is an important indicator for the composition changes of aqueous solution.

e.g. 'H' release takes place during DNA replication and pH sensing can be applied for tracking of DNA replication.

E. Accastelli, EPFL Thesis n.. 6468 (2015)

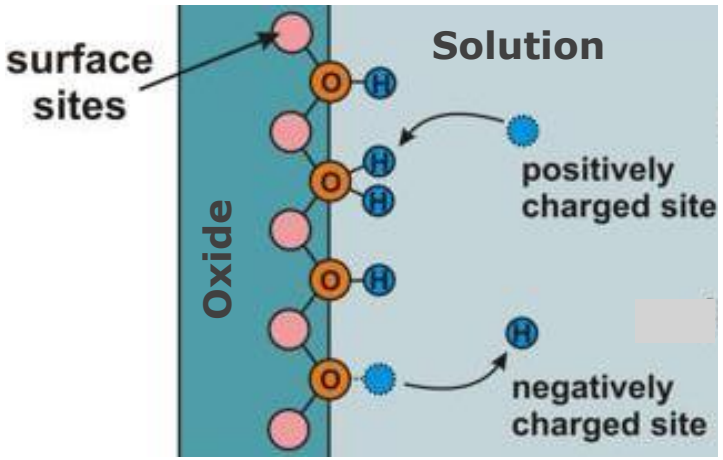
The basics of electrolyte-oxide interface interactions



The surface of oxide reacts with moisture in the air and hydroxyl groups are rapidly formed.

The sites on oxide surface are amphoteric, they act as proton donors or acceptors, depending on activity of surrounding solution.

An **acidic** solution is a proton **source**, a **basic** is a proton **sink**. (*An acid act as an acid if there is a suitable base to accept the proton, v.v.*.)



Low pH: $\equiv SiOH + H^+ \rightleftharpoons \equiv SiOH_2^+$ *Positive surface charge*

High pH: $\equiv SiOH - H^- \rightleftharpoons \equiv Si0^-$ *Negative surface charge*

$\equiv SiOH + 0H^- \rightleftharpoons \equiv Si0^- + H2O$

- A positive or negative charge on the oxide surface is governed by the pH of the surrounding aqueous solution.

The Site Binding Model: Charge Density on the Oxide Surface

The site-binding model describes the charging of an oxide as the result of an equilibrium between the A-OH surface sites and the H^+ ions in the bulk of the solution. According to the site-binding model* the charge on oxide surface is:

$$Q_{s_ox} = qN_s\left(\frac{a_{H_S^+}{}^2 - K_aK_b}{K_aK_b + K_b a_{H_S^+} + a_{H_S^+}{}^2}\right)$$

with

$$a_{H_S^+} = a_{H_B^+}\exp\left(-\frac{\Phi_{ox}}{U_T}\right),$$

$a_{H_S^+}$: Surface concentration of H^+ ions

Φ_{ox}: is the potential drop inside the electrolyte

$a_{H_B^+}$ is the concentration in H+ ions in the bulk

N_s is the number of sites per unit area

K_a, K_b *are* dimensionless intrinsic dissociation constants.

$K_a = [A\text{-}O^-]\ [H^+] / [A\text{-}OH]$ $\qquad$ $K_b = [A\text{-}OH]\ [H^+] / [A\text{-}H_2O^+]$

* Hal et al. Adv. Colloid Interface Sci. 68 (1996) 31-62

The Site Binding Model

$$Q_{s_ox} = qN_s\left(\frac{a_{H_S^+}{}^2 - K_aK_b}{K_aK_b + K_b a_{H_S^+} + a_{H_S^+}{}^2}\right)$$

Assuming: $K_aK_b \ll 1$ / true for inorganic oxides

$Q_{s_o} \ll qN_s$ / true for aqueous solutions

$$ln(10)\left(pH_{zpc} - pH\right) = \frac{\Phi_{ox}}{U_T} + arcsinh\left(\frac{Q_{s_ox}}{qN_s\delta}\right)$$

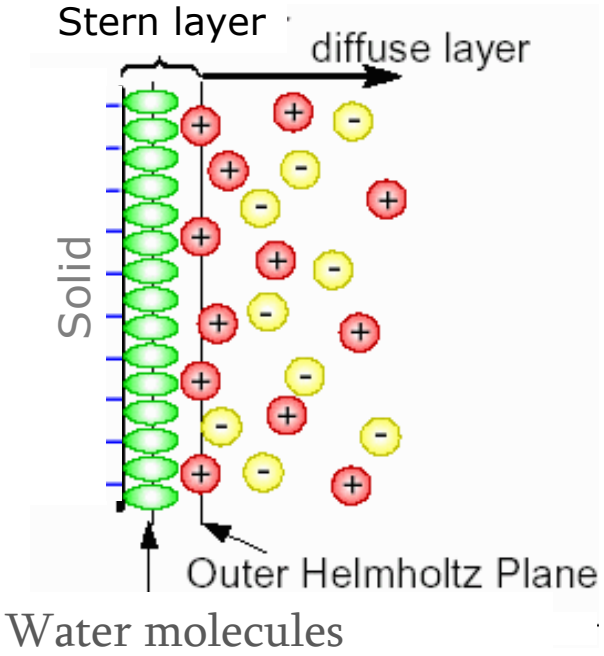
(Bousse et al., 1983)

where:

$\mathrm{pH}_{zcp} = \sqrt{K_aK_b}$ is the pH in the bulk, when oxide surface is neutral and $\delta = 2\sqrt{K_a/K_b}$

Thus for each surface-electrolyte system, characterized by a pH_{zcp}, there is a unique correspondence between the pH in the neutral electrolyte and the charge density at the oxide-electrolyte interface.

The diffusion layer



- Ions having the same sign as the charge on the oxide surface will be repelled, creating a diffusion layer in the electrolyte.
- Ions of opposite sign will be attracted and create the so-called double layer

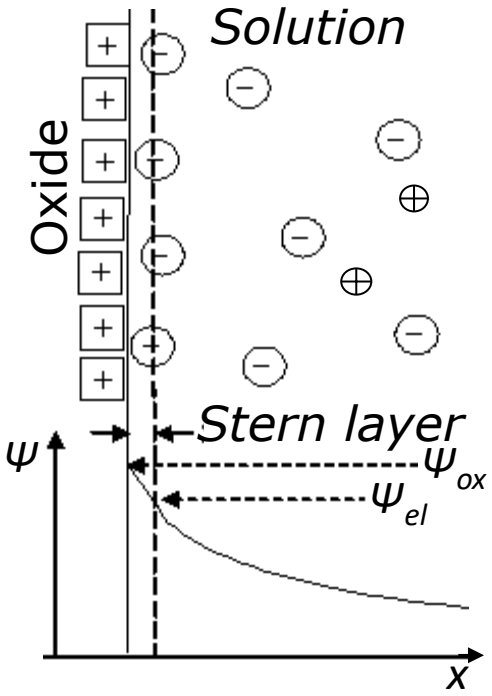
The outer Helmoltz plane OHP is defined as the plane of the center of the hydrated ions closest to the solid.

The Stern layer is a charge-free layer between the OHP and the insulator.

Stern layer is attributed a constant capacitance $C_{Stern} = \frac{\varepsilon_2 \varepsilon_o}{d}$

Diffusion layer is attributed a varying capacitance

Gouy Chapman-Stern model



$$\frac{d^2\Psi}{dx^2} = \frac{q}{\varepsilon} n_o \left(e^{\frac{\Psi}{U_T}} - e^{-\frac{\Psi}{U_T}} \right)$$ Poisson equation in the diffuse layer, considering Boltzmann distribution of ions

n_o is concentration of ions in the bulk

B.C. $\Psi(\infty)=0$, $E(\infty) = 0$

The integration of Poisson-Boltzmann eq. togethor with Gauss law provides the charge density (Q_{diff_el}) in diffussion layer*:

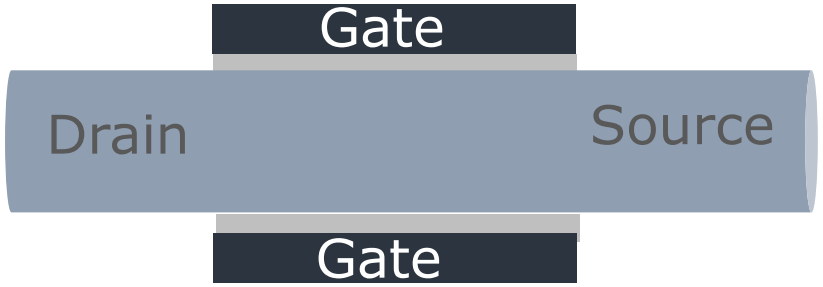
$$Q_{diff_el} = 2\varepsilon_1\varepsilon_o \frac{U_T}{l_D} \sinh\left(\frac{\varphi_{el}}{2\,U_T}\right)$$

where $l_D = (\varepsilon_1\varepsilon_o\, U_T/2qn_o)^{1/2}$ is the Debye screening length in diffuse layer and (Ψ_{el}) is the potential at OHP.

*A. Bard, L.Faulkner / Electrochemical methods : fundamentals and applications /

Modeling of Junctionless NW ISFET

Why Junctionless (JL) NW FET ?



Vertical cut-off JL NW FET

What means junctionless ??

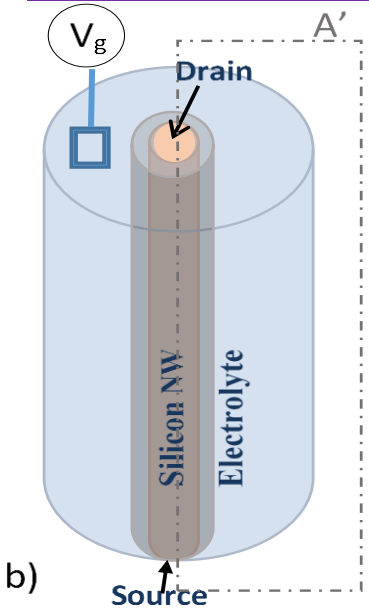
Neither junctions nor doping gradients for source and drain contacts!

Why junctionless FET is preferred??

Fabrication requires less processing steps with respect to standard inversion mode FETs

However the modeling scheme we developed here for NW junctionless (JL) ISFET, is not limited only for junctionless but can be extended also for inversion mode NW ISFETs.

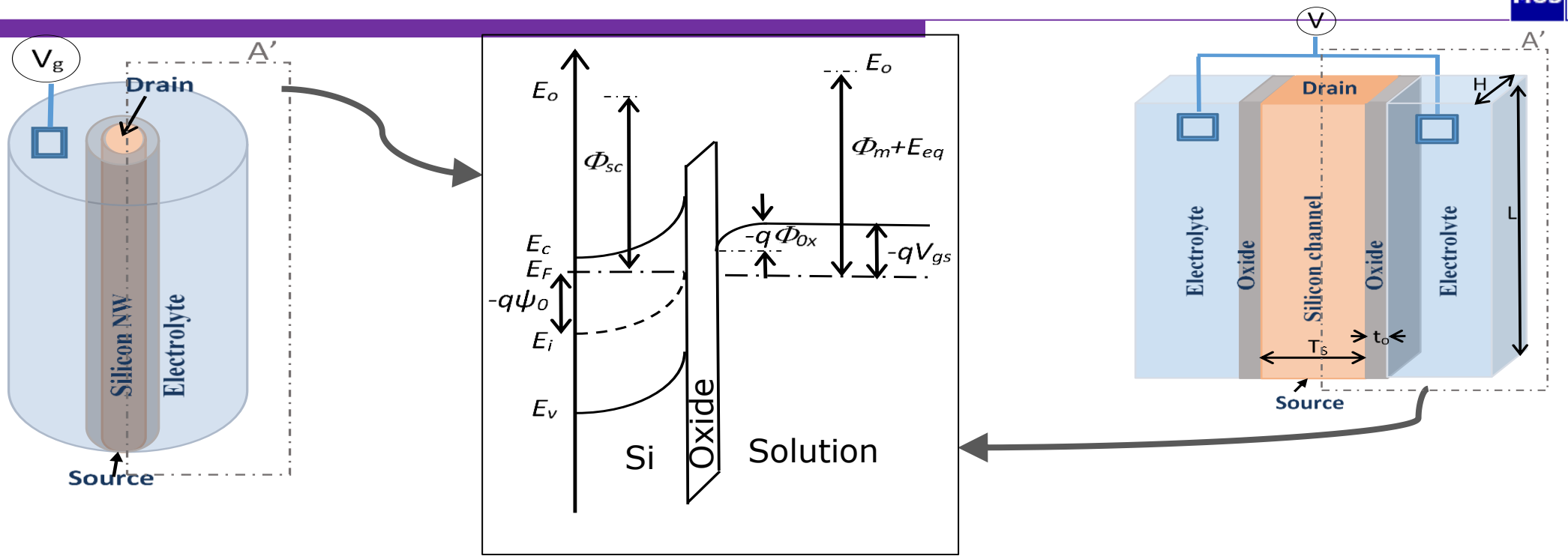
Modeling NW JL-ISFET



- ✓ Likewise a conventional nanowire JL FET but gate electrodes is replaced by the electrolyte.
- ✓ The effective 'gate voltage' will depend on the physico-chemical properties of the electrolyte and surface affinity to protons (i.e. pH).

The model must treat on the same ground the electrostatics of the semiconductor, the electrolyte and the surface chemical reactions.

Nanowire and Double-Gate ISFETs



✓ DG and NW ISFETs have **similar** energy band diagrams in vertical cuts!

✓ Once the model is developed for DG ISFET, it can be extended to NW geometry by applying equivalent parameters method, as it has been done for NW JL FET [1].

1. J. M. Sallese, et al. TED, 60,, p. 4277, 2013

Self-consistent charge based modeling of DG JL ISFET

Modeling DG JL-ISFET

- ISFET Principal: By measuring changes in the drain current (I_d) , the pH value of the solution can be determined.

- Our aim is: to define I_d(pH) characteristics of DG JL ISFET.

What we already have?

The charge-based compact, explicit drain current model of DG JL FET [2] which predicts $I_d(V_{gs})$ characteristics.

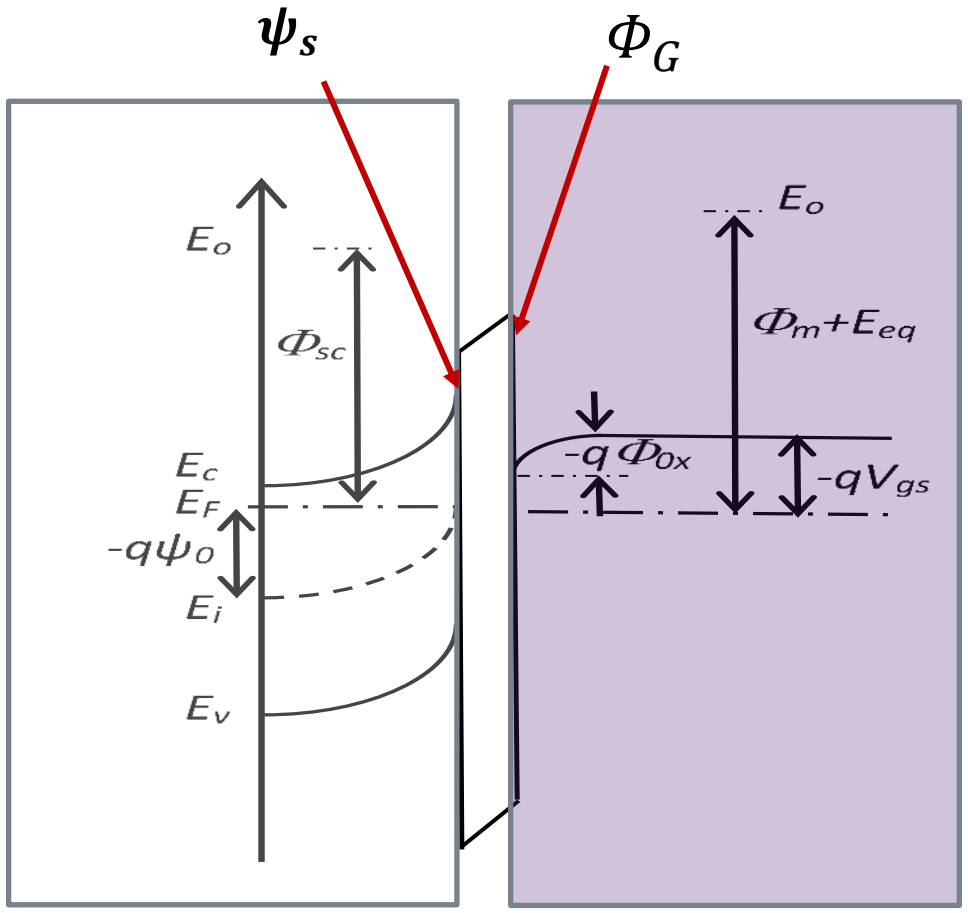
For the ISFET the gating potential is the potential at the oxide/electrolyte interface Φ_G.

$$\Phi_G = V_{gs}{}^{*} + \Phi_{ox}, \qquad \text{where } \Phi_{ox}(pH) \Rightarrow \Phi_G(\text{pH})$$

$$V_{gs}{}^{*} \textit{is the effective gate voltage applied on the reference electrode}$$

2. J. M. Sallese, et al.,*TED*, 58, p. 2628, 2011.

Modeling DG JL-ISFET: Potentials



Source Fermi level is the reference

Φ_{ox} is defined with respect to the neutral electrolyte and is a function of pH in the bulk..

From semiconductor side: $\Phi_G = -\frac{Q_{sc}}{\nu C_{ox}} + \psi_s$

ν=2 for DG and ν =1 for NW

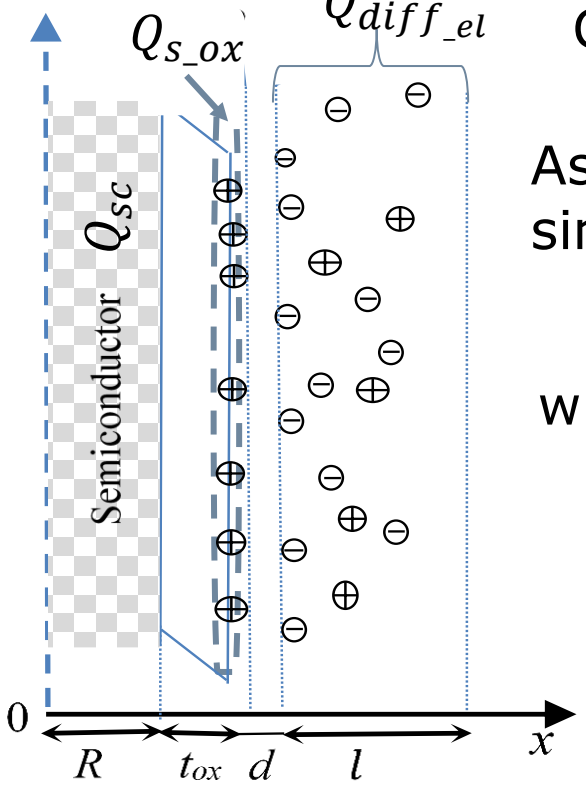
From electrolyte side: $\Phi_G = V_{gs}{}^* + \Phi_{ox}$

$$\Phi_{ox} = -\frac{Q_{sc}}{n\,C_{ox}} + \psi_s - V_{gs}{}^* = f(\psi_0)$$

Q_{sc} and ψ_s are semiconductor charge density and surface potential respectively, both are functions of semicond. central potential: ψ_0 [2].

$$\psi_s = \frac{qT_{Si}{}^2}{8\,\varepsilon_{si}}\left(n_i \exp\left(\frac{\psi_0 - V}{U_T}\right) - N_D\right) + \psi_0$$

Modeling DG JL-ISFET: Charges



Charge neutrality requires: $Q_{s_ox} = -Q_{diff_el} - Q_{cs}/\nu$ *ν=2 for DG and ν =1 for NW*

Assuming small potential drop ($<2U_T$) in diffuse layer & linearizing sinh function (see slide 16):

$$Q_{diff_el} = C_{eff}\Phi_{ox},$$

where $C_{eff} = C_{d_sc}\,C_{Stern}/(C_{Stern} + C_{d_sc})$ $\qquad C_{d_sc} = \frac{\varepsilon_1\varepsilon_o}{l_D}$

$$ln(10)\left(pH_{zpc} - pH\right) = \frac{\Phi_{ox}}{U_T} + arcsinh\left(\frac{Q_{s_ox}}{qN_s\delta}\right)$$ (see slide 14)

$$\ln(10)(\mathrm{pH}_{zpc} - \mathrm{pH}) = \frac{\Phi_{ox}}{U_T} + \mathrm{arcsinh}\left(\frac{C_{eff}\ \Phi_{ox} - Q_{sc}/n}{qN_s\delta}\right)$$

$$Q_{sc} = 2\ \mathrm{sign}(\psi_o - \psi_s)\left\{2\ q\varepsilon_{si}n_iU_T\left[\exp\left(\frac{\psi_s - V}{U_T}\right) - \exp\left(\frac{\psi_0 - V}{U_T}\right) - \frac{N_D}{n_i}\left(\frac{\psi_s - \psi_0}{U_T}\right)\right]\right\}^{1/2}$$ / from DG JLFET model [2]

Modeling DG JL-ISFET: Summarizing

For the measured drain current, by using charge based model the corresponding gating potential and then the central potential (ψ_0) of the semiconductor will be defined. Whereas **for a given central potential ψ_0 we got a unique correspondence of pH**, which simply can be calculated with the expression below:

$$\ln(10)(\mathrm{pH}_{zpc} - \mathrm{pH}) = \frac{\Phi_{ox}(\psi_0)}{U_T} + \operatorname{arcsinh}\left(\frac{C_{eff}\,\Phi_{ox}(\psi_0) - Q_{sc}(\psi_0)/n}{qN_s\delta}\right)$$

There are known expressions for $\Phi_{ox}(\psi_0)$ and $Q_{sc}(\psi_0)$.

Thus we can simulate I_d(pH) characteristics.

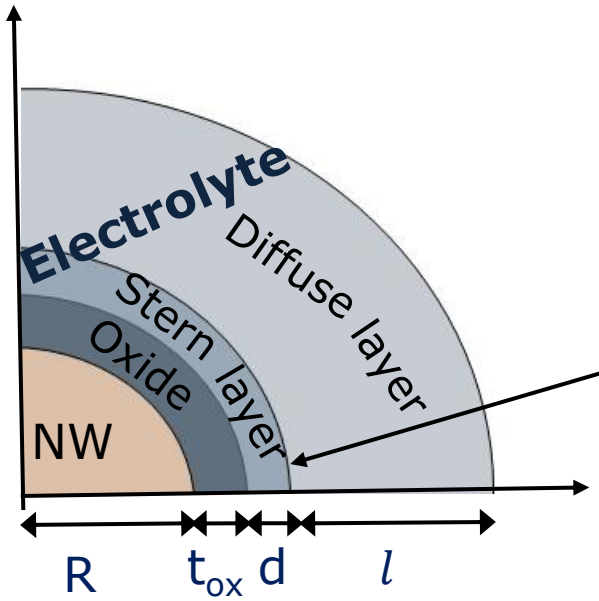
Vice versa, for a given **pH** we can calculate $\boldsymbol{\psi_0}$, and further the corresponding semiconductor charge, potentials and the drain current.

The Nanowire JL-ISFET

In case of nanowire JL ISFET, the electrolyte is also 'cylindrical' and satisfies the Poisson Boltzmann equation in cylindrical coordinates:

$$\frac{d}{dr}\left(\frac{d\,\Phi}{dr}\right)+\frac{1}{r}\frac{d\,\Phi}{dr}=\eta\,sinh\left(\frac{\Phi}{U_T}\right), \quad \text{(P-B)}$$

where $\eta = 2\pi q n_0/\varepsilon_1\varepsilon_o$.



B.C. $\Phi(R^*+l)=0$ and $\left.\frac{d\,\Phi}{dr}\right|_{r=R^*+l}=0$,

where $R^* = R + t_{ox} + d$ OHP is the inner cylinder.

There is a distance l beyond which the electric field is negligible and we write it in terms of the Debye length: $l = n\,l_D$, and n=3.

The Nanowire JL-ISFET

Applying trapezoidal integral rule on the first integral of (P_B) equation, together with B.C. and Gauss law, we calculated the charge in cylindrical diffuse layer:

$$Q_{diff} = \varepsilon_1 \varepsilon_o \frac{U_T}{l_D^*} \sinh\left(\frac{\Phi_{el}}{2U_T}\right)$$

The equation is the same as for planar case !!

BUT

$$\boldsymbol{l_D^* = l_D \sqrt{\frac{R^* + 3l_D}{R^*}}}.$$

is the equivalent Debye length in cylindrical system.

✓ Consequently, the electrolyte in cylindrical geometry can be modelled as a planar one by applying the equivalent Debye length and also the Stern capacitance per unit area derived for the cylindrical geometry.

For the semiconductor part we apply equivalent parameters method developed for NW JL FET [1]

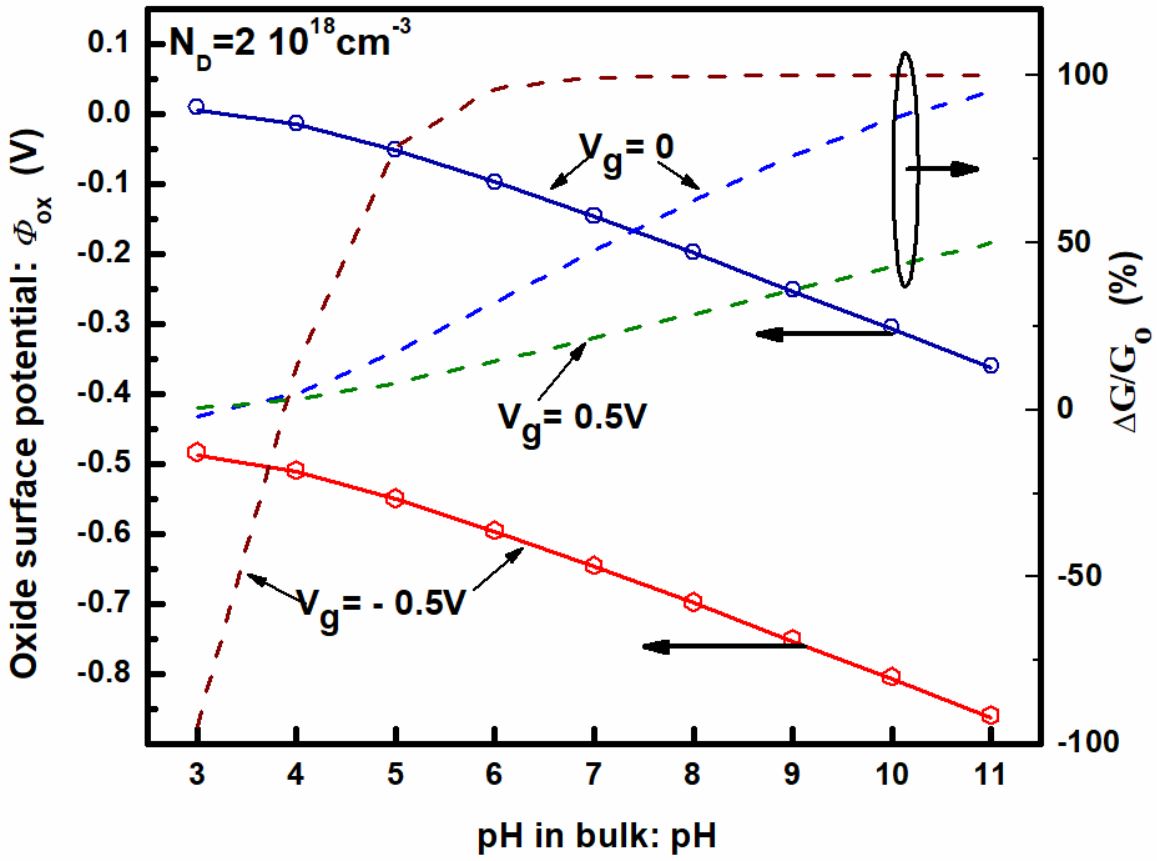
[1] J. M. Sallese, et al. TED, 60, p. 4277, 2013

- NW JL ISFET can be modelled as a DG one with equivalent parameters.

Equivalent parameters in DG JL ISFET model for reformatting it to NW JL ISFET model

Physical parameters	DG JL ISFET	NW JL ISFET
NW radius	-	R
Semiconductor thickness	T_{sc}	$T_{sc}^{*} = 2\times R$
Semiconductor width	W	$W^{*} = \pi\times R$
Doping concentration	N_D	$N_D^{*} = N_D/2$
Intrensic carrier concentration	n_i	$n_i^{*} = n_i/2$
Oxide thickness	t_{ox}	$t_{ox}^{*} = R\,(ln(1+ t_{ox}/ R)$
Stern layer thickness	d	$d^{*} = (R + t_{ox})ln[1 + d/(R + t_{ox})]$
Diffuse layer thickness	l_D	$l_D^{*} = l_D((R^{*} + 3l_D)/R^{*})^{1/2}$, $where \;\; R^{*} = R + t_{ox} + d$

The DG JL ISFET: Validation of the model



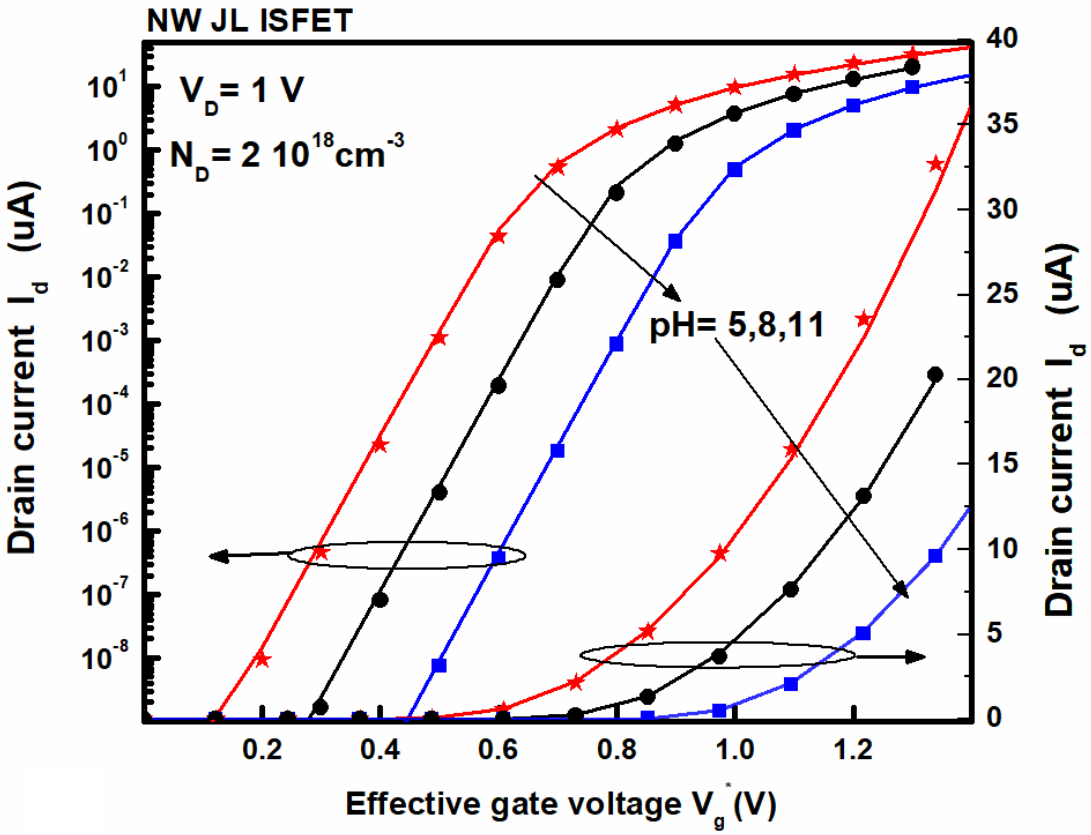
The analytical model has been validated with COMSOL Multiphysics simulations.

Here and further:

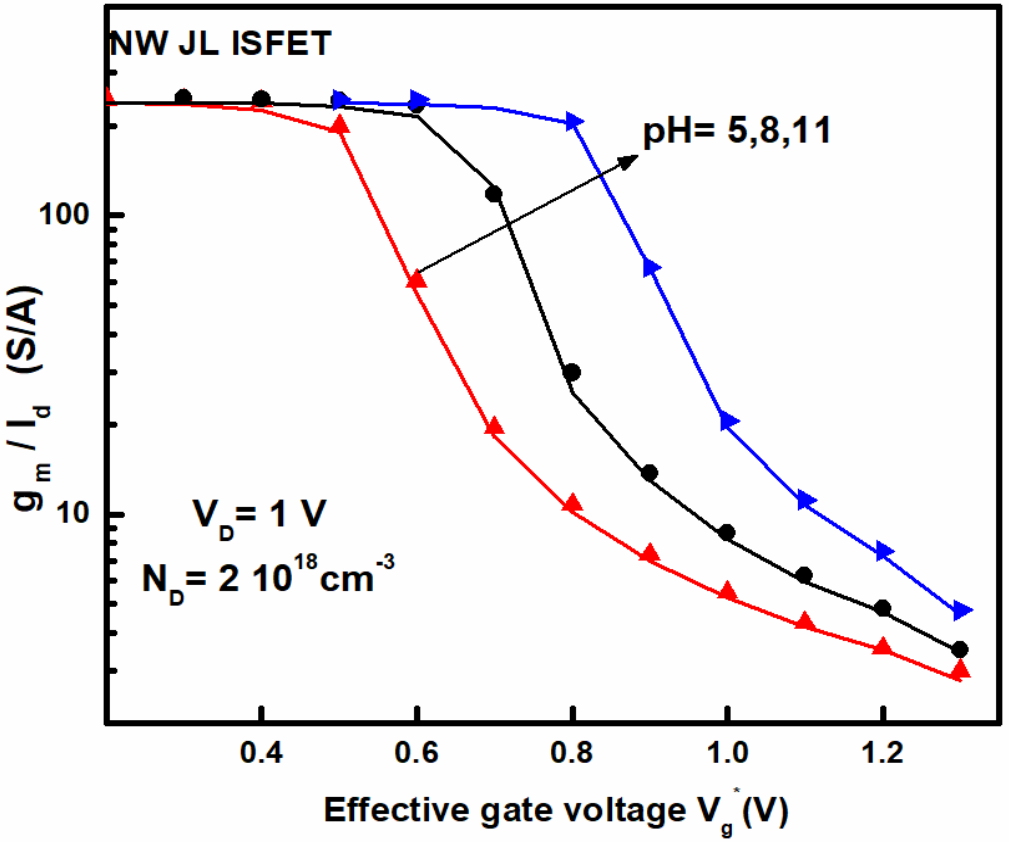
- *Solid and dash lines: analytical model, symbols: COMSOL simulations*
- *The following parameters have been used:* $K_a = 10^{-6}$, $K_b = 100$, $n_o = 4 \cdot 10^{20} cm^{-3}$, *d=0.5 nm,* $\varepsilon_2 = 11$, $\varepsilon_1 = 75.5$, $\varepsilon_{ox} = 3.9$, *T=300K.*

Oxide surface potential and relative change in the conductivity upon pH (V_{DS}=10mV) for different gate voltages.

Nanowire JL ISFET: Validation of the model

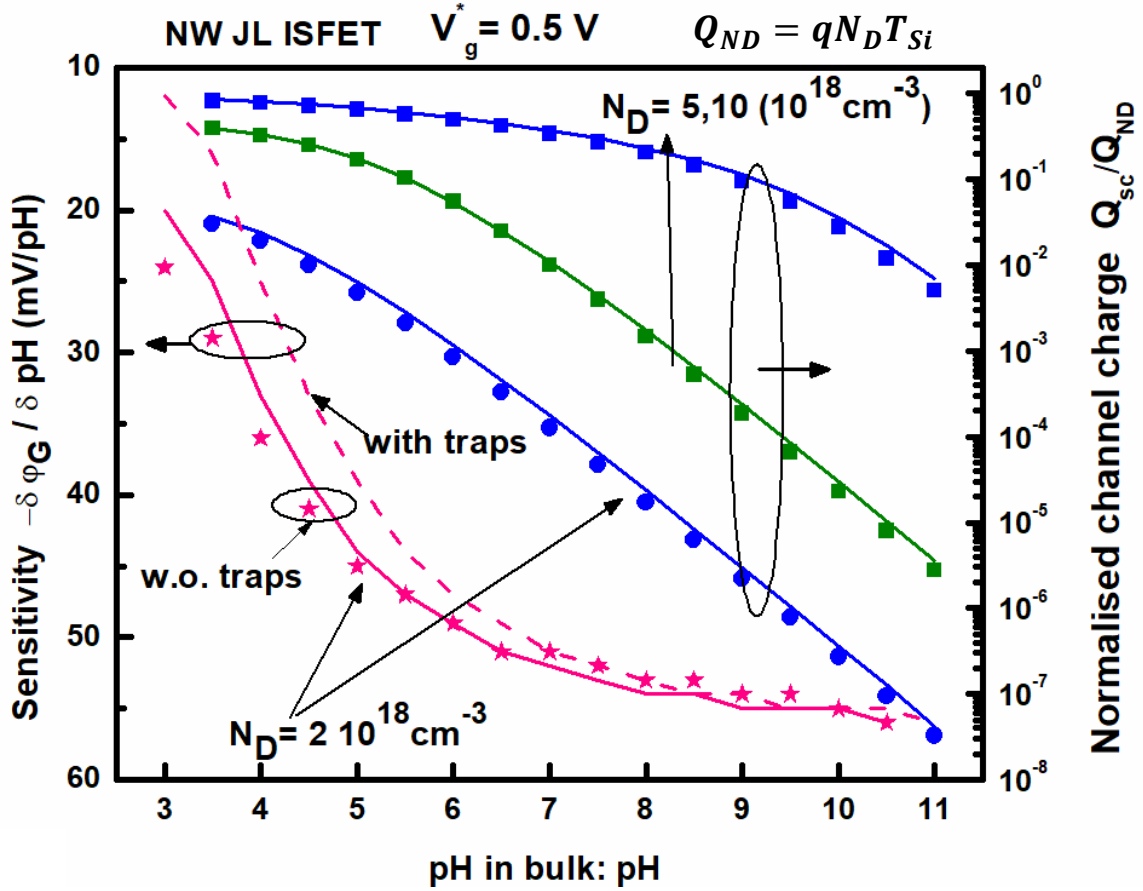


The drain current versus gate voltage for different pH is presented in logscale and linear scale



The transconductance to current ratio

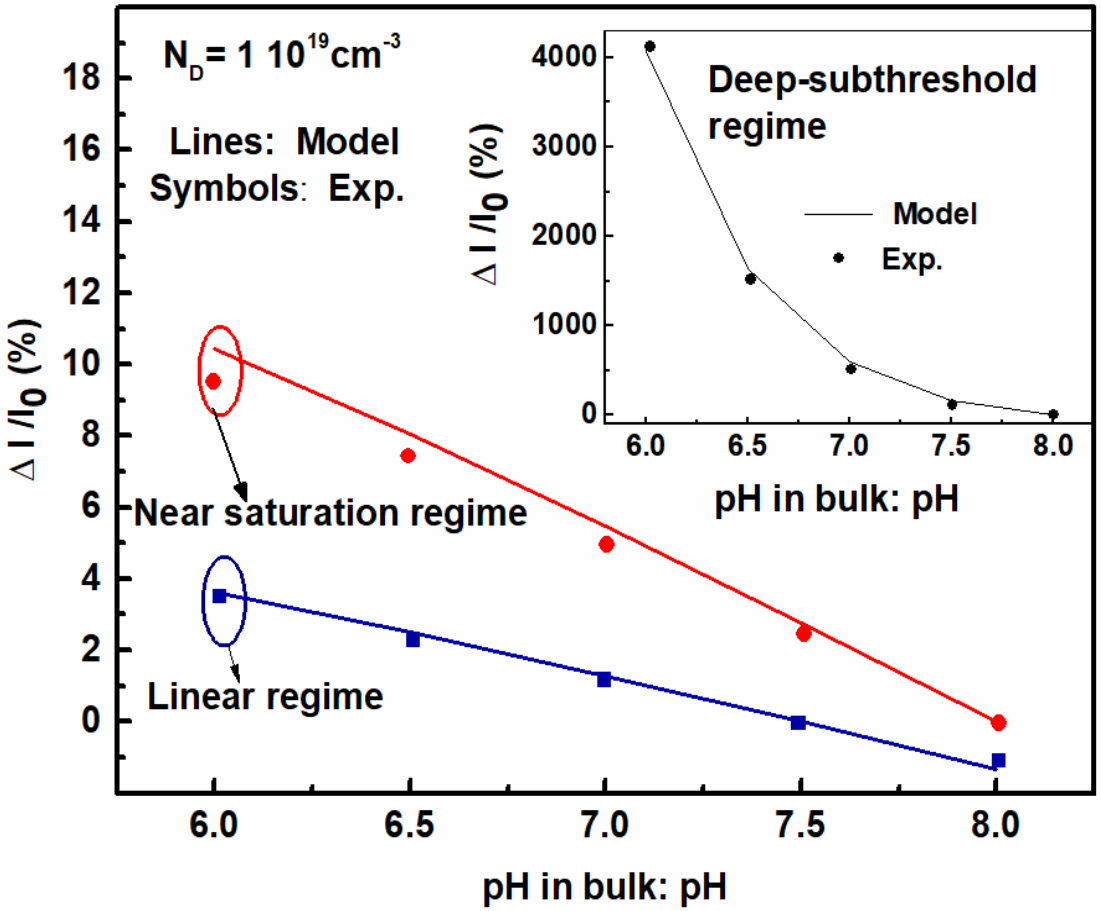
Nanowire JL ISFET: Validation of the model



The dashed line illustrates the sensitivity of JL ISFET considering surface traps with continuous energy distribution. As it was expected, the presence of acceptor type surface traps slightly increases the n type JL ISFET sensitivity

Sensitivity calculated as a derivative of oxide surface potential: left axis, Normalized semiconductor charge at different doping densities: right axis.

NW JL ISFET: Comparison with Experimental Data



- Lines: analytical model, symbols: experimental data from [*].

* C. Chen, et al. "Junctionless gate-all-around nanowire field-effect transistors with an extended gate in biomolecule detection," *Jpn. J. Appl. Phys.*, vol. 58, p. 027001, 2019.

Linear regime (Vg=1V) and in nearly saturation regime (Vg=0V), V_{DS}*=0.1V.*

Conclusion

- An analytical compact model is developed for DG and NW JL ISFETs describing the gating effect of hydrogen ions.
- Relying on cylindrical to planar transformation, NW and surrounding solution are accurately modelled still keeping the compact form.
- The model is valid in all regions of operation.
- The accuracy of the model is proved by validation with comprehensive numerical simulations and experimental data.
- No fitting parameters

For more details refer to:

A. Yesayan, F. Jazaery, J.M. Sallese, 'Analytical Modelling of Double-gate and Nanowire Junctionless ISFETs', IEEE TED, v. 67 (3), pp. 1157-1164, March 2020.

Thank you