MOS-AK Compact Modeling Workshop
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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).

➢ This device measures ion concentrations (e.g. H\(^+\) ions) along with electrical potentials and was first called an ISFET in 1970 by Bergveld.

➢ 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.

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

- Conventional FET
- DG FET
- GAA FET
- Junctionless NW FET

- Better channel control
- Reduced short channel effects
- No junctions

- High sensitivity, selectivity
- Low detection limit
- Miniaturization


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

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.

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.


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Operation 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?

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: \[ \equiv \text{SiOH} + H^+ \rightleftharpoons \equiv \text{SiOH}_2^+ \quad \text{Positive surface charge} \]

High pH: \[ \equiv \text{SiOH} - \text{H}^- \rightleftharpoons \equiv \text{SiO}^- \quad \text{Negative surface charge} \]

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:

$$Q_{s\text{-}ox} = q N_s \left( \frac{a_{H_S^+}^2 - K_a K_b}{K_a K_b + K_b a_{H_S^+} + a_{H_S^+}^2} \right)$$

with

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

Surface concentration of H$^+$ ions

$\Phi_{ox}$: is the potential drop inside the electrolyte

$\frac{a_{H_B^+}}{a_{H_S^+}}$: 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.

$$K_a = [\text{A-0}^-] \ [\text{H}^+] / [\text{A-OH}] \quad K_b = [\text{A-OH}] \ [\text{H}^+] / [\text{A-H}_2\text{O}^+]$$

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: \( K_aK_b \ll 1 \)  
\( Q_{s_{-}o} \ll qN_s \)  
true for inorganic oxides

\[ \ln(10) \left( pH_{zpc} - pH \right) = \frac{\phi_{ox}}{U_T} + \text{arcsinh} \left( \frac{Q_{s_{-}ox}}{qN_s \delta} \right) \]

(Bousse et al., 1983)

where:
\[ pH_{zpc} = \sqrt{K_aK_b} \]  
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 Helmholtz 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  \( C_{\text{Stern}} = \frac{\varepsilon_2 \varepsilon_0}{d} \)

Diffusion layer is attributed a varying capacitance
Gouy Chapman-Stern model

\[ \frac{d^2 \psi}{dx^2} = \frac{q}{\varepsilon} n_0 \left( \frac{\psi}{e^U - e^{-U}} \right) \]

Poisson equation in the diffuse layer, considering Boltzmann distribution of ions

\( n_0 \) is concentration of ions in the bulk

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

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

\[ Q_{\text{diff_el}} = 2\varepsilon_1 \varepsilon_0 \frac{U_T}{l_D} \sinh \left( \frac{\varphi_{el}}{2 U_T} \right) \]

where \( l_D = (\varepsilon_1 \varepsilon_0 U_T/2qn_o)^{1/2} \) is the Debye screening length in diffuse layer and \( (\Psi_{el}) \) is the potential at OHP.

*A. Bard, L.Faulkner / Electrochemical methods : fundamentals and applications /
Modeling of Junctionless NW ISFET
Why Junctionless (JL) NW FET?

**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.
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].

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?**


For the ISFET the gating potential is the potential at the oxide/electrolyte interface $\Phi_G$.

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

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

Modeling DG JL-ISFET: Potentials

\( \Phi_{\text{ox}} \) is defined with respect to the neutral electrolyte and is a function of pH in the bulk.

From semiconductor side: 
\[
\Phi_G = -\frac{Q_{sc}}{V_{Cox}} + \psi_S
\]

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

\( v = 2 \) for DG and \( v = 1 \) for NW

\( Q_{sc} \) and \( \psi_S \) are semiconductor charge density and surface potential respectively, both are functions of semicond. central potential: \( \psi_0 \) [2].

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

Source Fermi level is the reference
Modeling DG JL-ISFET: Charges

Charge neutrality requires: \( Q_{s,ox} = -Q_{\text{diff}_el} - Q_{cs} / \nu \)  
\( \nu = 2 \) for DG and  
\( \nu = 1 \) for NW

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

\[
Q_{\text{diff}_el} = C_{\text{eff}} \Phi_{ox},
\]

where

\[
C_{\text{eff}} = C_{d,sc} C_{\text{Stern}} / (C_{\text{Stern}} + C_{d,sc})
\]

\[
C_{d,sc} = \frac{\varepsilon_1 \varepsilon_0}{l_D}
\]

\[
\ln(10) (pH_{zpc} - pH) = \frac{\Phi_{ox}}{U_T} + \text{arcsinh} \left( \frac{Q_{s,ox}}{q N_s \delta} \right)
\]

\[
Q_{sc} = 2 \text{sign}(\psi_o - \psi_s) \left\{ 2 q \varepsilon_{si} n_i U_T \left[ \exp \left( \frac{\psi_s - V}{U_T} \right) - \exp \left( \frac{\psi_0 - V}{U_T} \right) - \frac{N_D}{n_i} \left( \frac{\psi_s - \psi_0}{U_T} \right) \right] \right\}^{1/2}
\]

/ 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 \( \psi_0 \) of the semiconductor will be defined. Whereas for a given central potential \( \psi_0 \) we got a unique correspondence of pH, which simply can be calculated with the expression below:

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

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

Thus we can simulate \( I_d(\mathrm{pH}) \) characteristics.

Vice versa, for a given pH we can calculate \( \psi_0 \), 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:

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

where \( \eta = \frac{2\pi q n_0}{\varepsilon_1 \varepsilon_o} \).

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

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

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

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]

The Nanowire JL-ISFET: Mapping between the NW and DG topologies

- 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**

<table>
<thead>
<tr>
<th>Physical parameters</th>
<th>DG JL ISFET</th>
<th>NW JL ISFET</th>
</tr>
</thead>
<tbody>
<tr>
<td>NW radius</td>
<td>-</td>
<td>( R )</td>
</tr>
<tr>
<td>Semiconductor thickness</td>
<td>( T_{sc} )</td>
<td>( T_{sc}^* = 2 \times R )</td>
</tr>
<tr>
<td>Semiconductor width</td>
<td>( W )</td>
<td>( W^* = \pi \times R )</td>
</tr>
<tr>
<td>Doping concentration</td>
<td>( N_D )</td>
<td>( N_D^* = N_D/2 )</td>
</tr>
<tr>
<td>Intrinsic carrier concentration</td>
<td>( n_i )</td>
<td>( n_i^* = n/2 )</td>
</tr>
<tr>
<td>Oxide thickness</td>
<td>( t_{ox} )</td>
<td>( t_{ox}^* = R \ln(1 + t_{ox}/R) )</td>
</tr>
<tr>
<td>Stern layer thickness</td>
<td>( d )</td>
<td>( d^* = (R + t_{ox}) \ln[1 + d/(R + t_{ox})] )</td>
</tr>
<tr>
<td>Diffuse layer thickness</td>
<td>( l_D )</td>
<td>( l^<em>_D = l_D ((R^</em> + 3l_D)/R^<em>)^{1/2} ), where ( R^</em> = R + t_{ox} + d )</td>
</tr>
</tbody>
</table>

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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: $K_a = 10^{-6}$, $K_b = 100$, $n_0 = 4 \cdot 10^{20} \text{cm}^{-3}$, $d=0.5 \text{ nm}$, $\varepsilon_2 = 11$, $\varepsilon_1 = 75.5$, $\varepsilon_{ox} = 3.9$, $T=300K$.

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

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

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 [*].


Linear regime ($V_g = 1\,\text{V}$) and in nearly saturation regime ($V_g = 0\,\text{V}$), $V_{DS} = 0.1\,\text{V}$. 

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:

Thank you