DESIGN AND SIMULATION OF FULLY-DEPLETED
SILICON-ON-INSULATOR BASED ISFET USING A TCAD TOOL

BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI

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BY

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BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE PILANI (RAJASTHAN)

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Title of the Project: *Design and Simulation of Fully-Depleted Silicon-on-Insulator Based ISFET using TCAD Tool.*

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Abstract: *We propose a new approach to describe in commercial TCAD (SILVACO), the chemical reactions that occur at dielectric/ electrolyte interface and make the ion sensitive FET (ISFET) sensitive to pH. The earlier attempts to model the electrolyte and chemical reactions at the interface are done on Sentaurus TCAD tool. We try to demonstrate the method proposed earlier by performing, 2-D simulations in TCAD (SILVACO) environment, a full 2-D analysis of ISFET operation, and a comparison between threshold voltage and drain current differential sensitivities in the linear and saturation regimes. The method paves the way to accurate and efficient ISFET modeling with standard TCAD tools.*

Signature of Student   Signature of Instructor In-Charge

Date   Date

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Chapter 1 – Introduction

The possibility of chip technology to develop silicon based sensors has been exploited by biomedical engineers for a long time now. One of the first attempts was to establish such sensors at the tip of a catheter. Such technology would provide clinicians with cheap sensors, which become cheaper and cheaper every year, even with improved characteristics. Reproduction of such sensors would be easier as it is the very basis of silicon technology. As expected, the very first research attempts to develop silicon based sensors in biomedical engineering were focused at ion sensors. The ISFET sensor is one of the most well-known examples.

What is ISFET?

ISFET stands for Ion Sensitive Field Effect Transistor. It is nothing but a MOSFET with the gate connection separated from the chip in the form of a reference electrode inserted in an aqueous solution which is in contact with the gate oxide.
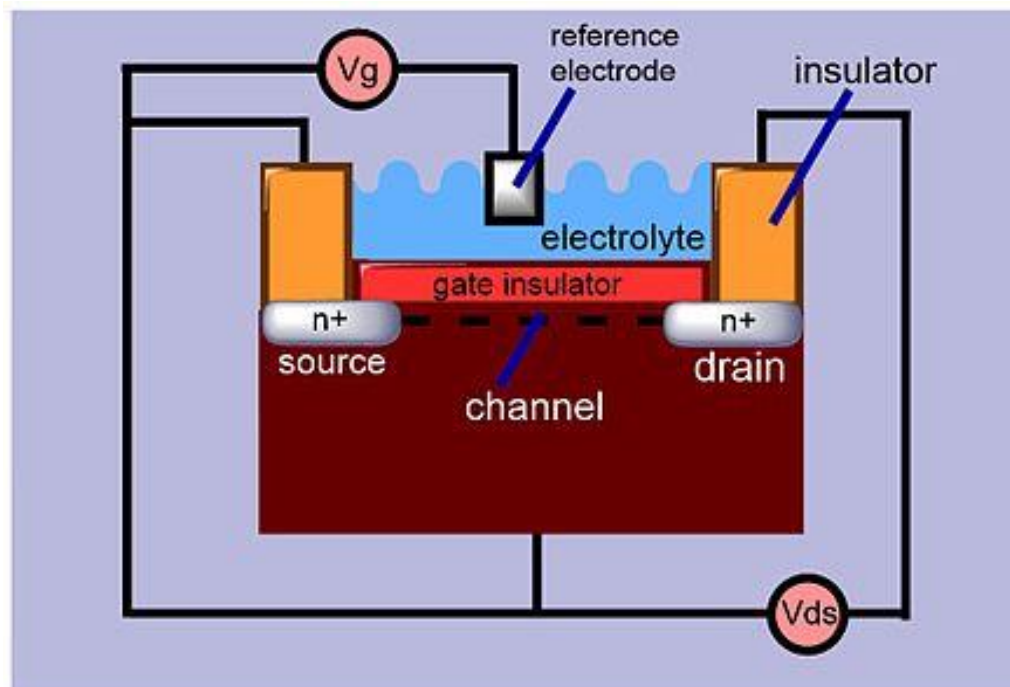

Fig. 1.1 Model of ISFET

History

The introduction of silicon as a substrate for microelectrodes, specifically meant for electrophysiological measurements (action potentials), started in the late sixties at the Stanford University. Applying an etching technique for the silicon needles and evaporation of gold for the electrode leads resulted in 5 mm long and 0.2 mm wide electrodes, insulated with silicon dioxide, except for the tip. The needle ended in a silicon part of some square millimeters, which was meant to contain fully integrated buffer amplifiers in a later version. Reading this, P Bergveld (regarded as the inventor of ISFET), thought that integrating a complete amplifier was not "wise", as only the impedance transforming part of the amplifier was necessary. This

function at the time was performed by a JFET. He further proposed that a MOSFET without gate metallization should be applied, leaving the bare oxide as the actual contact between the electronic system and the biological environment. Since this device could measure ion concentrations along with electric potentials, it was primarily known as ISFET.

Advantages

One of the main advantage of using Silicon Devices is that the size of these devices decreases every year, in accordance with *Moore's Law*. This allows an ISFET to make it possible to make sensors of nanoscale. For example, such sensors can make it possible to develop intelligent catheters, providing fast and accurate measurements. Moreover, since more transistors can now be packed in the same

space, it provides more computing power within the same size limit. This makes it possible to integrate a microprocessor alongside ISFET which can make the sensor smart, enable autocleaning of the sensor and dispense different serums depending on the value sensed. Such applications make ISFET an important part of the development of Smart Sensors.

Silicon on Insulator (SOI) Technology

Silicon on insulator (SOI) technology refers to the use of a layered silicon–insulator–silicon substrate in place of conventional silicon substrates in semiconductor manufacturing, especially microelectronics, to reduce parasitic device capacitance, thereby improving performance. SOI-based devices differ from conventional silicon-built devices in that the silicon junction is above an electrical insulator, typically silicon dioxide.

Chapter 2 – ISFET

2.1 Background Theory

ISFET is an electrochemical device that is based on the concept of the metal-oxide-semiconductor field-effect transistor (MOSFET). Unlike MOSFET, metal gate of MOSFET is replaced by a pH sensing film. In ISFET, the ion sensing film is in contact with the electrolytic solution while the gate region is insulated in MOSFET.
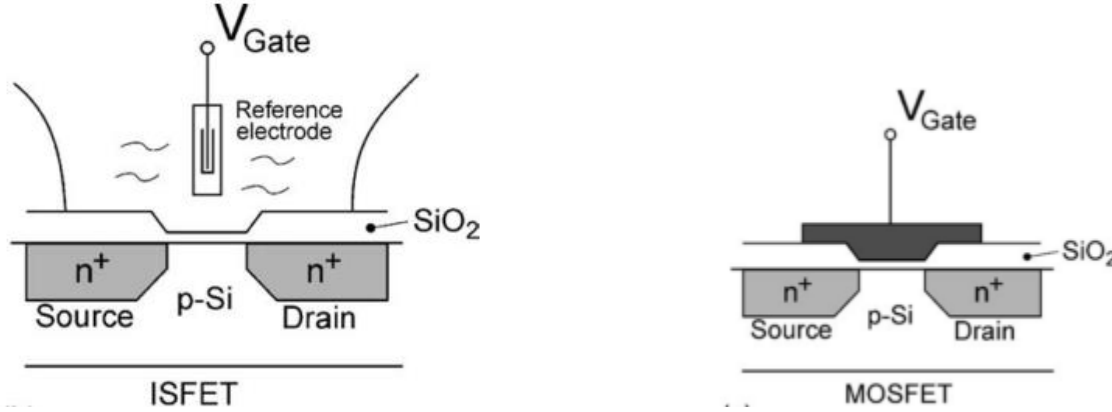
The general expression for drain current of a MOSFET, and thus of an ISFET in non-saturated mode is

$$I_D = \mu C_{ox} \frac{W}{L} \left[(V_{gs} - V_t) V_{ds} - \frac{1}{2} V_{ds}^2 \right]$$

where C_{ox} is the oxide capacitance per unit area, W and L the width and the length of the channel, respectively, and μ is the electron mobility in the channel. With everything else withheld constant, I_D is a function of V_{gs}. Thus, V_{gs} is the only input variable. In case of ISFET, it was initially debated whether the observed ion sensitivity should be described as an additional input variable in terms of a modification of V_{gs} or a modification of V_t. As the metal connection of the reference electrode is defined as a remote gate, we must define any interfacial potential in the input circuit in terms of V_t. For a MOSFET, this relation is

$$V_t = \frac{\phi_M - \phi_{Si}}{q} - \frac{Q_{ox} + Q_{SS} + Q_B}{C_{ox}} + 2\phi_f$$

In case of ISFET, the same fabrication process is used, resulting in the same constant physical part of the threshold voltage. However, in addition to this, two more contributions manifest themselves: the constant potential of the reference electrode, E_{ref}, and the interfacial potential $\psi + \chi^{sol}$ at the solution/oxide interface of which ψ is the chemical input parameter, shown to be a function of the solution pH and χ^{sol} is the surface dipole potential of the solvent and thus having a constant value. Hence the expression for the ISFET threshold voltage becomes

$$V_t = E_{ref} - \Psi + \chi^{sol} - \frac{\phi_{Si}}{q} - \frac{Q_{ox} + Q_{SS} + Q_B}{C_{ox}} + 2\phi_f$$

From above two equations, it may be concluded that an ISFET is electronically identical to a MOSFET and can thus still be seen as an electronic device, with one additional feature: the possibility to chemically modify the threshold voltage via the interfacial potential at the electrolyte/oxide interface.

2.2 Working Principle

The differentiating factor between MOSFET and ISFET is that the latter employs a pH sensing gate material. This also explains the fact that most of explanation till now has focused on the electrolyte/oxide interface phenomena.

As mentioned before, the first ISFET gate material tested was silicon dioxide, of which it is known that it needs a certain amount of hydration of the surface to become pH sensitive. From similar experiments with Silicon Nitride, it was concluded that we need to consider pure surface phenomena at the insulator/electrolyte interfaces. The site binding model has been considered as a reliable concept to describe the electrical-double layers at the colloidal oxide-water interfaces. In this model, the oxide surfaces are assumed to be amphoteric, meaning that the surface hydroxyl groups can be neutral, protonized (thus positively charged) or deprotonized (thus negatively charged) depending on the pH of the bulk solution.
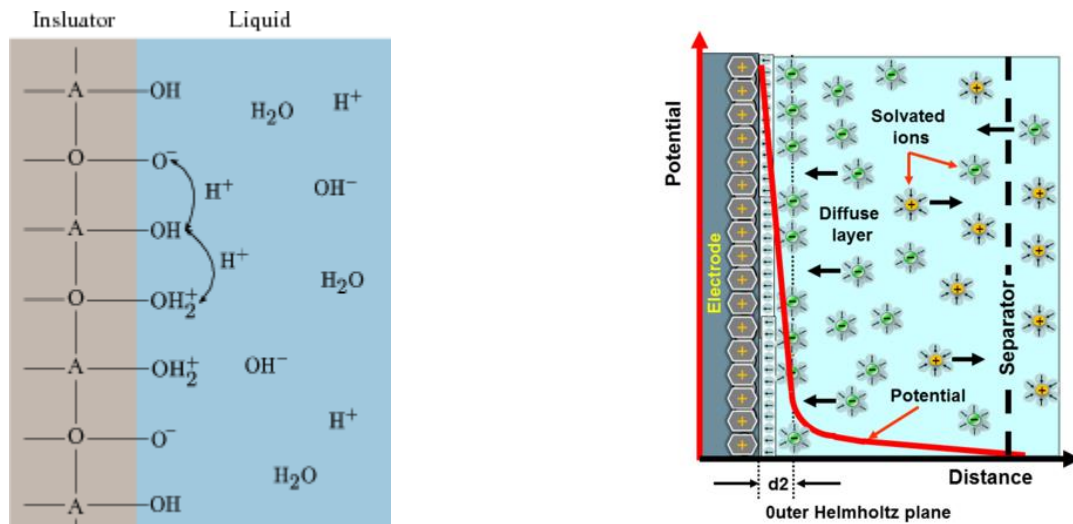
This model was proven to be applicable for ISFET surfaces of SiO_2 and Al_2O_3 by Bousse, a Ph.D. student of P Bergveld in 1980.

There are many ways of utilizing ISFETs. In case the ISFET is treated as a MOSFET and connected to a curve tracer with the reference electrode connected to the V_{gs} port, I_d/V_{gs} curves can be recorded as is done with MOSFETs. However, with the reference electrode connected to the source ($V_{gs} = 0$) similar curves can be achieved by changing the pH of the solution. The latter effect is due to the relation

$\psi = f(pH)$. With the help of above described site-binding model, Bousse derived this relation

$$\psi = 2.3 \frac{kT}{q} \frac{\beta}{\beta + 1} \left(pH_{pzc} - pH \right)$$

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where pH$_{pzc}$ is the value of pH for which the oxide surface is electrically neutral and β is a parameter used to determine final sensitivity (α).

From further analysis, the above mentioned equation led to the following result

$$\Delta\psi = -2.3\alpha\frac{RT}{F}\Delta pH_{bulk}$$

with

$$\alpha = \frac{1}{(2.3kT/q^2)(C_s/\beta_s) + 1}$$

where β$_s$ symbolizes the surface buffer capacity and C$_s$ is the differential double-layer capacitance, of which the value is mainly determined by the ion concentration of the bulk solution via the corresponding Debye length.

This equation illustrates that only in the case α approaches 1, the maximum Nernstian sensitivity of 58.2 mV per decade (at 20 °C) can be obtained, whereas for oxides having α < 1, a sub Nernstian response can be expected.

2.3 SOI Technology

2.3.1 Introduction

Silicon on insulator (SOI) technology refers to the use of a layered silicon–insulator–silicon substrate in place of conventional silicon substrates in semiconductor manufacturing, especially microelectronics, to reduce parasitic device capacitance, thereby improving performance. SOI-based devices differ from conventional silicon-built devices in that the silicon junction is above an electrical insulator, typically silicon dioxide or sapphire (these types of devices are called silicon on sapphire, or SOS). The choice of insulator depends largely on intended application, with sapphire being used for high-performance radio frequency (RF) and radiation-sensitive applications, and silicon dioxide for diminished short channel effects in microelectronics devices. The insulating layer and topmost silicon layer also vary widely with application.
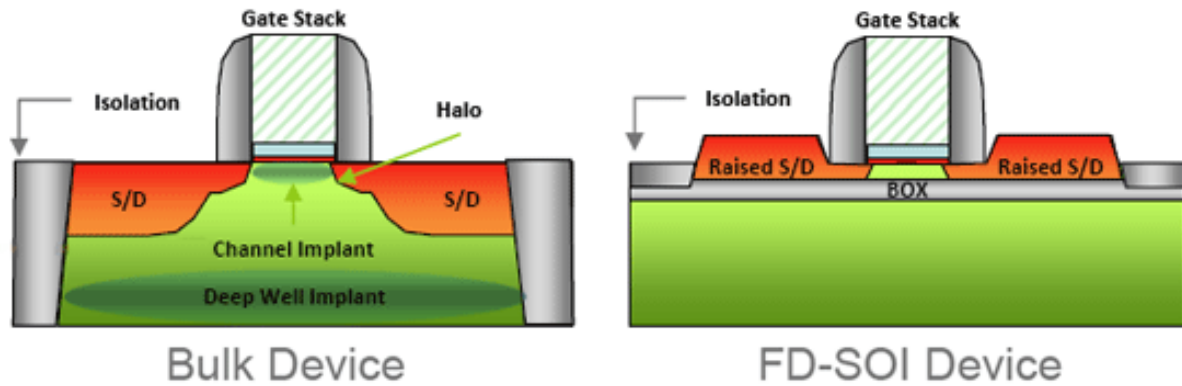
The fully depleted SOI transistor at 20 nm is significantly simpler than even a simplified version of the bulk CMOS transistor.

As demonstrated in the above illustration, contrary to the Silicon substrate over which bulk MOSFET is developed, SOI Device has a Buried Oxide (BOX) implant over which a thin Silicon Layer is deposited over which the MOSFET is developed. This thin Silicon layer is commonly referred as Silicon-on-Insulator (SOI) Layer.

The provision of BOX Layer insulates the upper part of MOSFET from the bottom substrate layer, removing latchup effect and parasitic capacitances. Since the channel region's thickness is reduced drastically, there is no need of extensive doping in the channel region.

There are two types of SOI Devices: PDSOI (partially depleted SOI) and FDSOI (fully depleted SOI) MOSFETs. For an n-type PDSOI MOSFET the sandwiched p-type film between the gate oxide (GOX) and buried oxide (BOX) is large, so the depletion region can't cover the whole p region. So, to some extent PDSOI behaves like bulk MOSFET. Obviously, there are some advantages over the bulk MOSFETs. The film is very thin in FDSOI devices so that the depletion region covers the whole film. In FDSOI the front gate (GOX) supports less depletion charges than the bulk so an increase in inversion charges occurs resulting in higher switching speeds. The limitation of the depletion charge by the BOX induces a suppression of the depletion capacitance and therefore a substantial reduction of the subthreshold swing allowing FD SOI MOSFETs to work at lower gate bias resulting in lower power operation. The subthreshold swing can reach the minimum theoretical value for MOSFET at 300K, which is 60mV/decade. This ideal value was first demonstrated using numerical simulation. Other drawbacks in bulk MOSFETs, like threshold voltage roll off, etc. are reduced in FDSOI since the source and drain electric fields can't interfere due to the BOX.

2.3.2 Advantages over Bulk Devices

The implementation of SOI technology is one of several manufacturing strategies employed to allow the continued miniaturization of microelectronic devices, colloquially referred to as "extending Moore's Law" (or "More Moore", abbreviated "MM").

Reported benefits of SOI technology relative to conventional silicon (bulk CMOS) processing include:

- Lower parasitic capacitance due to isolation from the bulk silicon, which improves power consumption at matched performance.
- Resistance to latchup due to complete isolation of the n-well and p-well structures.
- Matched Performance at lower V_{DD}.
- Reduced temperature dependency due to minimal doping.
- Better yield due to high density, which leads to better wafer utilization.
- Lower leakage currents due to isolation thus higher power efficiency.
- Inherently radiation hardened (resistant to soft errors), thus reducing the need for redundancy.

From a manufacturing perspective, SOI substrates are compatible with most conventional fabrication processes. In general, an SOI-based process may be implemented without special equipment or significant retooling of an existing factory. Among challenges unique to SOI are novel metrology requirements to account for the buried oxide layer and concerns about differential stress in the topmost silicon layer. The

threshold voltage of the transistor depends on the history of operation and applied voltage to it, thus making modeling harder. The primary barrier to SOI implementation is the drastic increase in substrate cost, which contributes an estimated 10–15% increase to total manufacturing costs.

2.4 Applications of ISFET

ISFETs show potential for development of many game-changing instruments:

Smart Cell Culture Chambers

In such chambers, ISFETs along with other sensors, like temperature sensors (diodes), conductivity sensors (interdigitated electrodes) and oxygen sensors (amperometric), will all be integrated in a silicon wafer at the bottom of the chamber. With a fluid perfusion system for cell culture media the cells can be kept alive or be stimulated by added drugs. It is can be proved that for the pH changes of 0.1 pH/min in a chamber volume of 10 ml, the application of an ISFET as pH sensor is advantageous.

Catheter Tip Sensors

The R&D group of Cordis in Roden, The Netherlands, developed a catheter tip pH sensor, based on an Al_2O_3 ISFET of which the temperature and drift behavior could be predicted by testing MOSFETs made on the same wafers as the ISFETs. These predicted parameters were stored in a PROM, which was an integral part of the connector of the catheter and could be read out by the signal processing unit, resulting in an accuracy of 0.02 pH units over a period of 10 h. It was the first time that it could be shown that blood pH changes periodically with the lung ventilation and that after stopping artificial ventilation during an operation a patient is not always able to take control of his acid–base balance.

Flow-through cells

To combat the problem of biocompatibility, Flow-through cells were developed. These cells are basically a cartridge with four-function ISFET chip (for pH, pNa, pK and pCa) as well as rinsing and calibration facilities, controlled by a microprocessor. The cartridge basically takes in a small "bloodline" and performs all the necessary measurements. Such a cartridge was developed by Sibbald and could perform 200 bedside measurements, using 18 ml/h un-heparinized blood from the patient, resulting in a semi-continuous monitoring of a patient's condition over 24 h.

Sensor/actuator systems

Especially with respect to a pH sensitive ISFET, the integration with a pH actuator is relatively easy: deposit a noble metal electrode around the gate area and generate coulometrically protons or hydroxyl ions by means of a current pulse applied to the actuator electrode with respect to a remotely placed counter electrode. The electrolysis of water will result in a pH change in the direct vicinity of the gate, which will thus be measured by the ISFET with only a small delay, determined by the diffusion of protons from actuator to gate.

ISFETs thus provide a vast range of possibilities. Above examples not only illustrate the benefits of small sizes of ISFET based sensors but also the capability to integrate many such electronic devices like amplifiers on a single chip and thus make the development of nanoscale sensors feasible.

Chapter 3 – Electrolyte Modelling of SOI ISFET

3.1 Electrolyte Model

In Electrolyte Model, we exploit the similarity between the equations for cations and anions in the electrolyte at equilibrium and those for holes and electrons in a semiconductor. A monovalent symmetric (1:1) electrolyte is thus described as an undoped semiconductor with a zero bandgap (hence, n· p = NCNV), a constant permittivity (ϵel $\approx$ 80ϵo), and an effective density of states

$$N_C = N_V = \begin{cases} 10^{-3}.N_{av}(c_0 + cH_B), & for\ pH_B \leq 7 \\ 10^{-3}.N_{av}(c_0 + 10^{-14}/cH_B), & for\ pH_B > 7 \end{cases}$$

Where NC and NV are expressed in cm-3, Nav = 6.02214 · 1023 mol-1 is Avogadro's number, c0 the salt ion molar concentration (M = mol/l) in the bulk of the solution, and cHB = [HB+] = 10-pHB is the hydrogen concentration in the bulk of the solution normalized to 1 M. The bulk electrolyte is defined as the region with constant potential and a zero net charge density as a result of equal total concentrations of positive and negative ions, respectively, represented by p and n; hence, nB = pB = NC = NV.

3.2 Site Binding Model

Chemical reactions at the interface between the ISFET gate dielectric and the electrolyte generate a surface charge density that makes the ISFET sensitive to pH. As a first step toward the development of a general methodology, we implement the default formulation of the well-known site-binding model of the chemical reactions at the amphoteric silanol (SiOH) groups. These reactions generate a surface charge density.

$$\sigma_0(\psi_0) = qN_{sil}\left[\frac{cH_S^2 - K_aK_b}{cH_S^2 + K_bcH_S + K_aK_b}\right]$$

Where, q is the electron charge, N_{sil} is the number of amphoteric silanol surface sites per unit area, $cH_S = 10^{-pH_S}$ is the surface H^+ concentration, and K_a and K_b are the surface dissociation constants. Under equilibrium conditions, as it is most often the case in the electrolyte of an ISFET, and neglecting the steric effects that are relevant only well above physiological salt concentrations ($c_0 \gg 100\ mM$), the surface and bulk concentrations of all monovalent ions are related by the same Boltzmann factor. For H^+ ions, this relation reads,

$$cH_S = cH_B exp\left(-\frac{q\Psi_0}{kT}\right)$$

Where, ψ0 is the potential difference between the interface and the bulk of the solution. Equations (2) and (3) are also valid for dielectrics other than SiO2, where a metal (M) replaces silicon, and amphoteric sites are generated by MOH groups. This category comprises most of the dielectrics used in the semiconductor technology, such as HfO₂, Al₂O₃, and Ta₂O₅. Dielectrics such as Si3N4 and Al2O3 are often preferred because they have better sensitivity, and yield more stable characteristics because of the reduced ion diffusivity.

3.3 Procedure for Modelling the Electrolyte

For a FET device,

$$V_G = V_{FB} + \frac{qN_B x_d}{C_{ox}} + \frac{qN_B x_d^2}{2\varepsilon_s}$$

Where, for different V_G (Reference Gate Voltages), we can get different V_{FB} values using the following formula for x_d

$$x_d = \sqrt{\frac{2\epsilon_{Si} V_{Si}}{qN_B}}$$

As we know the following expression for threshold voltage for a FET

$$V_T = V_{FB} - \frac{Q_B}{C_{ox}} + 2\emptyset_F$$

For an ISFET,

$$V_{FB} = E_{ref} - \Psi_0 + \chi_{sol} - \frac{\Phi_{Si}}{q} - \frac{Q_{ss} + Q_{ox}}{C_{ox}}$$

We can thus get different values of Ψ_0 for different values of V_{FB}. From Site Binding Model, we know that bulk concentration cH_B is given by

$$cH_B = 10^{-pH_B}$$

$$cH_S = cH_B exp\left(-\frac{q\Psi_0}{kT}\right)$$

Calculate N_C and N_V from the Electrolyte Model,

$$n_i = N_C exp\left(-\frac{qE_g}{2kT}\right)$$

$$n_B = \sqrt{N_C N_V}$$

$$p_B = n_B$$

$$n_S = n_B\, exp\left(\frac{q\Psi_0}{kT}\right)$$

$$p_S = p_B\, exp\left(-\frac{q\Psi_0}{kT}\right)$$

As ISFET senses change in pH because of a change in Threshold Voltage, it is essentially working on the principle of change in surface charge due to change in Bias Voltage (change in pH). We can model this property of electrolyte as a semiconductor by introducing interface donor and acceptor traps.

The charge corresponding to a surface trap density of N_S^d donor and N_S^a acceptor traps per unit area is given by

$$\sigma_T = q\left(N_S^d f^d - N_S^a f^a\right)$$

Where f^d and f^a are the occupational probabilities for donor and acceptor traps, respectively. In Silvaco,

$$f^d = \frac{v_n\ SIGN\ n + e_p}{v_n\ SIGN\ n + e_p + v_p\ SIGP\ p + e_n}$$

$$f^a = \frac{v_p\ SIGP\ p + e_n}{v_n\ SIGN\ n + e_p + v_p\ SIGP\ p + e_n}$$

Assuming that donor traps only interact with Valence Band and acceptor traps only interact with Conduction Band,

$$SIGN \approx 0, e_n \approx 0\ for\ f^d$$

$$SIGP \approx 0, e_p \approx 0\ for\ f^a$$

To make this σ_T resemble the behavior of σ_T of Site Binding Model, we make the following substitutions,

$$e_p = K_a K_b n_S$$

$$v_p\ SIGP\ p = K_b c H_B \sqrt{n_s p_s} + c H_B^2 p_s$$

$$e_p = c H_B^2 p_S$$

$$v_n\ SIGN\ n = K_a K_b n_S + K_b c H_B \sqrt{n_s p_s}$$

$$N_S^d = N_S^a = N_{sil}$$

After making these substitutions, we get the values necessary to simulate traps. All the calculations and simulations are shown in the MATLAB and Silvaco Codes in Appendix. Thus, till this step, we have supposedly simulated ISFETs reliably in Silvaco using Site Binding Model.

Chapter 4 - TCAD Simulation of SOI ISFET

4.1 What is a TCAD Tool?

Technology CAD (or Technology Computer Aided Design, or TCAD) is a branch of electronic design automation (EDA) that models semiconductor fabrication and semiconductor device operation. The modeling of the fabrication is termed Process TCAD, while the modeling of the device operation is termed Device TCAD. Included are the modelling of process steps (such as diffusion and ion implantation), and modelling of the behavior of the electrical devices based on fundamental physics, such as the doping profiles of the devices. TCAD may also include the creation of compact models (such as the well-known

SPICE transistor models), which try to capture the electrical behavior of such devices but do not generally derive them from the underlying physics.

Chapter 5 - Future Directions

Up till now we have completed a major portion of the theoretical aspect of the working of the ISFET. We have also learnt to do simulation in the SILVACO TCAD tool. The procedure mentioned in the above section has been implemented, however, simulation results are not in perfect confirmation with the expected results. We have contacted the corresponding authors regarding our queries and are waiting for a response. After performing these simulations for a standard substrate ISFET, we aim to propose some improvements in the current variable dependencies, in order to enhance the device sensitivity. Keeping the above goal in mind, our current ideas are to extend the simulations to FDSOI ISFETs, incorporating permittivity variations in the model and exploring different sensing layers for improved sensitivity.

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Appendix

SILVACO TCAD Program.

```
go athena

#mesh definition
line x loc=0 spacing=0.5
line x loc=0.23 spacing=0.02
line x loc=1.27 spacing=0.02
line x loc=1.5 spacing=0.5

line y loc=0 spacing=0.02
line y loc=0.1 spacing=0.02
line y loc=0.5 spacing=0.2
line y loc=1.0 spacing=0.2

#wafer definition
init silicon orientation=100 c.boron=1.3e15 two.d

#gate oxide
diffuse time=0.18 temp=1050 dryo2
extract name="Tox" thickness oxide mat.occno=1 x.val=0.7

# define active region
etch oxide start x=0 y=0.25
etch cont x=0 y=-0.5
etch cont x=0.25 y=-0.5
etch done x=0.25 y=0.25

etch oxide start x=1.25 y=0.25
etch cont x=1.25 y=-0.5
etch cont x=1.50 y=-0.5
etch done x=1.50 y=0.25

# deposit Silicon for Electrolyte
deposit material=silicon thick=1.0 division=2

# etch Electrolyte
etch silicon start x=0 y=0.0
etch cont x=0 y=-1.1
etch cont x=0.25 y=-1.1
etch done x=0.25 y=0.0

etch silicon start x=1.25 y=0.0
etch cont x=1.25 y=-1.1
etch cont x=1.50 y=-1.1
etch done x=1.50 y=0.0

# deposit platinum for Gate
deposit material=platinum thick=0.2 division=8

etch platinum start x=0.0 y=0.0
etch cont x=0.0 y=-1.3
```

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```
etch cont x=0.1 y=-1.3
etch done x=0.1 y=0.0

etch platinum start x=0.1 y=-0.2
etch cont x=0.10 y=-1.4
etch cont x=0.20 y=-1.4
etch done x=0.20 y=-0.2

etch platinum start x=0.20 y=0.0
etch cont x=0.20 y=-1.4
etch cont x=0.25 y=-1.4
etch done x=0.25 y=0.0

# etch DRAIN

etch platinum start x=1.25 y=0.0
etch cont x=1.25 y=-1.6
etch cont x=1.30 y=-1.6
etch done x=1.30 y=0.0

etch platinum start x=1.30 y=-0.2
etch cont x=1.30 y=-1.6
etch cont x=1.42 y=-1.6
etch done x=1.42 y=-0.2

etch platinum start x=1.40 y=0.0
etch cont x=1.40 y=-1.6
etch cont x=1.50 y=-1.6
etch done x=1.50 y=0.0

ELECTRODE NAME=SOURCE X=0.15 Y=-0.1
ELECTRODE NAME=DRAIN X=1.35 Y=-0.1
ELECTRODE NAME=GATE X=0.8  Y=-0.2
ELECTRODE NAME=SUBSTRATE backside

tonyplot

go atlas

# Defining regions for electrolyte and substrate semiconductors
region num=1 y.max=0 material=silicon
region num=2 y.min=0 material=silicon

material material=silicon permittivity=80 eg300=1.1 nc300=1.2046e18 nv300=1.2046e18
region=1

# Introducing traps in the electrolyte semiconductor
inttrap e.level=0.5 acceptor density=5e14 sign=0.0021 sigp=0
inttrap e.level=0.3 donor density=5e14 sign=0   sigp=8.6295
models mos srh print
method newton
solve init
solve vdrain=0.5
log outf=e30.log
solve vgate=-10 vstep=2 vstop=10 name=gate
tonyplot e30.log
```

MATLAB Programs

- Constants Used

```
clc; clear;

Eg = 1.1; % Bandgap of Silicon (eV)
Ei = Eg/2; % Energy Level
k = 1.3806*10^-23; % Boltzmann Constant
T = 300; % Temperature
q = 1.6e-19; % Electron Charge (Coulombs)
vn = 2.3e7; % Avg. Velocity of Electron ( Silicon)
vp = 1.65e7; % Average Velocity of Hole ( Silicon)

Ka = 10^-6; % Ka of the Electrolyte
Kb = 10^2; % Kb of the Electrolyte
pH = 3;      % pH of The Solution The Taken
c0 = 1.0e-3; % The Concertation of Salt
cHb = 10^-pH; % Concertation of Hydrogen Ions
Nav = 6.023e23; % Avogadro Constant
Nc = (10^-3)*Nav*(c0+cHb);
Nv = Nc;
ni = Nc*exp(-(Eg/2)/(k*T/q)); % Intrinsic Charge Carriers in Silicon
psi0 = -0.0824; % ASSUMPTION

nb = sqrt(Nc*Nv); % Bulk Concentration of Electrons
pb = nb;  % Bulk Concertation of Holes
ns = nb*exp(q*psi0/(k*T)); % Surface Concentration of Electrons
ps = pb*exp(-q*psi0/(k*T)); % Surface Concentration of Holes
```

- Calculating The Acceptor Trap Values

```
clc; clear;

constants;

% CCA Calculations As Per In Procedure Equation
lhs1 = Ka*Kb*ns;    % Ka, Kb for Electrolyte Interface
Elevel = 0.5; % ASSUMPTION
power1 = exp(q*(Elevel-Ei)/(k*T));  % Calculating The Power Factor
sign = lhs1/(vn*ni*power1); %Calculating The Sign.
sigp = 0;  % Assumption As Compared to The SILVACO Tool Equations

% ECA Calculations
lhs2 = (Kb*cHb*sqrt(ns*ps))+((cHb^2)*ps);
n = lhs2/(vn*sign); % Calculation For The Electrons
p = (ni^2)/n; % Calculation For Holes (Ni of Silicon is Used).
```

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- Calculating The Donor Trap Values

```
clc; clear;

constants; % Getting The Constants

% CVD calculations
p = 2.0408e05; % Calculated From the Acceptor Program
lhs1 = (cHb^2)*ps; % Calculations as per Procedure
sigp = lhs1/(vp*p);
sign=0; % Assumption As Per Equations given by Silvaco

% EVD Calculations
lhs2 = (Ka*Kb*ns)+(Kb*cHb*sqrt(ns*ps));
power2 = lhs2/(vp*sigp*ni); % Power Factor
Elevel = Ei - (k*T*log(power2)/q); % Calculation The Trap Energy Level
```

- Calculating The psi Value

```
clear; clc;

psi = -0.1:0.0001:-0.08; % Variable psi

k = 1.3806*(10^-19); % Boltzmann Constant in cm^2
T = 300; % Temperature
q = 1.6*(10^-19); % Electron Charge
Ka = 10^-6; % Ka of the Electrolyte
Kb = 10^2; % Kb of the Electrolyte
Nsil = 5*(10^14); % Silanol Sites

pH = 3; % pH of The Solution
cHb = (10^-pH)*10^-3;  % Bulk Hydrogen Concertation
nb = 1.2044*(10^18);   % Bulk Electron Concertation
pb = nb;               % Bulk Hole Concertation
power = q*psi./(k*T);  % Power Factor
ns = nb*exp(power);    % Surface Electron Concertation
ps = pb*exp(-power);   % Surface Hole Concertation

% Calculation of the Variables According to the Procedure
a = ((cHb^2).*ps);
b = (Ka*Kb.*ns);
c = (Ka*Kb.*ns);
d = (Kb*cHb*sqrt(ps.*ns));
e = ((cHb^2).*ps);
sigmabyq = Nsil*(a-b)./(c+d+e);

% plotting the Values to Get Approximate Value of psi.
plot(psi,sigmabyq);
grid on;
ylabel('sigma/q');
xlabel('psi');

% Values Calculated From the Graph
% psi=-0.0824 for pH=3 with SiO2-Electrolyte Interface
```

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```matlab
% Final Calculations
psi0 = -0.0824;
power0 = q*psi0/ (k*T);
ns0 = nb*exp(power0);
ps0 = pb*exp(-power0);
```