Silicon-on-insulator devices with metal contacts for pH sensing based on out-of-equilibrium body potential

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THÈSE

Pour obtenir le grade de

DOCTEUR DE L'UNIVERSITÉ GRENOBLE ALPES

Spécialité : NANO ELECTRONIQUE ET NANO TECHNOLOGIES

Arrêté ministériel : 25 mai 2016

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préparée au sein du Laboratoire Institut de Microélectronique, Electromagnétisme et Photonique - Laboratoire d'hyperfréquences et de caractérisation dans l'École Doctorale Electronique, Electrotechnique, Automatique, Traitement du Signal (EEATS)

Dispositifs de silicium-sur-isolant avec contacts métalliques pour détection de pH basée sur le potentiel hors-équilibre

Silicon-on-insulator devices with metal contacts for pH sensing based on out-of-equilibrium body potential

Thèse soutenue publiquement le 8 février 2022, devant le jury composé de :

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Acknowledgments

After three years, this unique journey of pursuing a PhD has come to an end. This journey would be meaningless without the people who were a part of it; to whom, I would like to express my sincere gratitude.

First and foremost, I would like to extend my sincere thanks to the members of the jury Francis Calmon, Jérôme Launay, Adrian Ionescu, Francisco Gamiz, Stéphane Monfray and Anne Kaminski for reading and evaluating my thesis, for providing with constructive comments and for the very interesting and fruitful questions during the defence.

Additionally, I would like to express my deepest gratitude to my PhD advisor, Irina Ionica. Thank you for giving me this amazing opportunity to work in the excellent environment of IMEP-LaHC and trusting me as your student. I appreciate all the time you have invested in me for our scientific discussions, philosophy Fridays, “magic-hand” training and professional mentoring. All this effort made me reach the PhD milestone and helped me to become a researcher.

I am extremely grateful to Maryline Bawedin, Gerard Ghibaudo, Cecile Delacour and Davide Bucci. Their scientific expertise and their valuable advice and comments really helped me to progress on my thesis and approach the problems for various perspectives. It was a great pleasure to work with all of you. Also, many thanks to Frédéric Allibert from SOITEC for providing the SOI wafers used in this work.

Especially helpful during the last three years were Xavier Mescot, Aude Bouchard and Martine Griaud who spent many hours training me and adjusting the equipment for my unconventional experiments and processes. Your contribution was essential to the quality of the experiments in this work, I sincerely thank you for this.

Of course the PhD students of the lab (or doctors by now) and friends: Giuseppe, Vipin, Petros, Aggeliki, Balraj, Olfa, Namanu, Kyungwha, Hyungjin, Andres, Francesco for all the laughs, interesting conversations and great memories. Special thanks to Licinius Benea with whom, besides the above, I also had very long constructive scientific discussions. To all of my friends in Grenoble, I am glad I have met intelligent and open-minded people like you.

To my friends who are next to me from the early university days and especially those with whom we share a similar scientific passion (even if we have chosen different fields): Thank you for always standing by my side.

I am also grateful to my parents and sister for supporting me through this journey. Finally, I would like to express my endless gratitude to Despoina Polaktsidou for all the sacrifices she made to support me and be next to me the last three years, her patience and her profound belief in my abilities that kept me focused on my goals.

Thank you all!
Abstract

This thesis focuses on the development of a (bio)-chemical sensor based on an innovative detection paradigm, the out-of-equilibrium body potential in a silicon-on-insulator (SOI) device. The phenomenon belongs to the family of floating body effects, which are generally considered as parasitic in fully depleted SOI metal oxide semiconductor field effect transistors (MOSFET), but it was exploited for memory applications. The starting point of the thesis was the pseudo-MOSFET configuration with pressure controlled probes, where the bulk serves as gate and the two probes are source and drain. In this structure, typically used for electrical characterisation of SOI wafers, the transport at the interface between the Si film and the buried oxide is influenced by the charges placed on the top, similar to the working principle of an ISFET (ion sensing FET). DNA sensing in dry conditions, based on the out-of-equilibrium body potential was proven previously utilising this structure. In this context, the thesis focuses on three key elements concerning the technological developments needed to obtain a simple SOI sensor with metal contacts based on out-of-equilibrium body potential: (1) implementing dynamic measurements with triangular signals applied to the back-gate, (2) replacing the pressure controlled probes of the pseudo-MOSFET with deposited metal contacts and (3) proving the use of out-of-equilibrium body potential for “in-liquid” sensing. In parallel with the technological developments, significant progress was made on the understanding of the out-of-equilibrium body potential through TCAD simulations and modeling. A new TCAD simulation architecture, able to recreate the out-of-equilibrium body potential for pseudo-MOSFET, showed that its origin relates to the potential barrier created under the contacts. For SOI devices with deposited metal pads this behaviour is simply due to the Schottky junction between the metal and the low doped silicon film. This was elegantly reproduced by solving numerically the Poisson and continuity equations. Based on the above results, the device was modeled by an equivalent circuit made of a Schottky diode in series with a MOS capacitor, where the inversion charge imposed by the back-gate in the capacitor must be provided by the junction. The proof-of-concept of sensing with body potential in our device was done for in-liquid pH detection. Further TCAD simulations revealed optimization paths and possible sensitivity enhancement through the out-of-equilibrium body potential reading with respect to the conductance shifts.
Résumé

L’objectif de cette thèse est le développement d'un capteur (bio)-chimique basé sur une méthode de détection innovante, le potentiel hors-équilibre dans un dispositif fabriqué sur silicium-sur-isolant (silicon-on-insulator, SOI). Le phénomène fait partie de la famille des effets de «body» flottant, qui sont généralement considérés comme parasites dans les transistors à effet de champ métal oxyde semi-conducteur (MOSFET) sur SOI complètement déserté. Toutefois, il a été exploité pour des applications «mémoire». Le point de départ de la thèse est la configuration pseudo-MOSFET, où le substrat sert de grille arrière et deux pointes métalliques de pression contrôlée sont posées sur le film et sont utilisées comme source et drain. Dans cette structure, typiquement utilisée pour la caractérisation électrique des plaques SOI, le canal formé à l'interface entre le film Si et l'oxyde enterré est affecté par les charges déposées sur la surface, comme dans un ISFET (ion sensing FET). La détection d’ADN dans des conditions sèches, basée sur le potentiel hors-équilibre mesuré dans cette structure, avait déjà été prouvée. Dans ce contexte, la thèse a apporté trois développements technologiques majeurs pour obtenir un capteur en SOI avec contacts métalliques déposés, en utilisant le potentiel hors-équilibre : (1) implémentation des mesures dynamiques avec des signaux triangulaires appliqués sur la grille arrière, (2) remplacement des pointes à pression contrôlée du pseudo-MOSFET par des contacts métalliques déposés et (3) validation de la preuve de concept de détection basée sur le potentiel hors d'équilibre, dans un milieu liquide. En parallèle aux développements technologiques, des progrès significatifs ont été réalisés dans la compréhension de l’origine du potentiel hors-équilibre, grâce à des simulations TCAD et aux modélisations. Une nouvelle architecture de simulation TCAD, capable de recréer la réponse en potentiel hors-équilibre avec la configuration pseudo-MOSFET, a montré que son origine est liée à la barrière de potentiel créée sous les pointes. Pour les dispositifs SOI avec des contacts métalliques déposés, ce comportement est simplement dû à la jonction Schottky entre le métal et le film de silicium faiblement dopé. Cet effet est reproduit en résolvant numériquement les équations de Poisson et de continuité. En s’appuyant sur les résultats ci-dessus, le dispositif a été modélisé par un circuit équivalent constitué d’une diode Schottky en série avec une capacité MOS, où la charge d'inversion imposée par la grille arrière dans la capacité doit être fournie par la jonction. La preuve de concept de la détection par potentiel hors-équilibre a été apportée pour la mesure du pH en solution. Des simulations TCAD complémentaires ont révélé des chemins d'optimisation et une amélioration possible de la sensibilité grâce à la lecture du potentiel hors d'équilibre par rapport à la variation de conductance classiquement utilisée dans les ISFETs.
# Table of contents

Chapter 1: General introduction and context ................................................................. 1  
1.1 Why semiconductors? ................................................................................................. 2  
1.2 Biosensors .................................................................................................................. 3  
1.3 Out-of-equilibrium body potential in SOI: A new detection paradigm ................. 13  
1.4 Objective of the thesis ............................................................................................ 15  
Chapter 2: Transient measurements in the pseudo-MOSFET configuration .......... 23  
2.1 SOI characterization with the pseudo-MOSFET ................................................... 24  
2.2 Implementation of transient voltage ramps in the pseudo-MOSFET ................. 32  
2.3 Conclusions ............................................................................................................. 42  
Chapter 3: Transient TCAD simulations with a novel pseudo-MOSFET structure .... 49  
3.1 Introduction ............................................................................................................... 50  
3.2 Simulation strategy in this thesis ............................................................................. 51  
3.3 Simulations with a novel structure ......................................................................... 54  
3.4 Comparison with experimental results ................................................................... 58  
3.5 Body potential dependence on the contact properties ......................................... 60  
3.6 Impact of channel-related parameters on the dynamic response ....................... 67  
3.7 Effect of electrical parameters effect on the $V_B$ response ................................. 69  
3.8 Conclusions ............................................................................................................. 73  
Chapter 4: SOI devices with deposited metal contacts ............................................. 79  
4.1 Introduction ............................................................................................................... 80  
4.2 Issues with metal contacts on SOI ......................................................................... 80  
4.3 Fabrication process for SOI with metal contacts ................................................... 84  
4.4 Geometry optimization of the device ................................................................... 94  
4.5 Is the body potential a pressure related effect? ..................................................... 104  
4.6 Conclusions ............................................................................................................. 105  
Chapter 5: Origin and modeling of the out-of-equilibrium body potential .......... 111  
5.1 State of the art ......................................................................................................... 112  
5.2 Numerical simulations ......................................................................................... 120  
5.3 Equivalent circuit model ....................................................................................... 132  
5.4 Circuit model and device parameters .................................................................. 135  
5.5 Conclusion ............................................................................................................. 139  
Chapter 6: A novel pH sensor based on out-of-equilibrium body potential reading .... 145  
6.1 Introduction ............................................................................................................. 146  
6.2 Sensing ability of SOI substrates (pseudo-MOSFET): state of the art ............... 147
# Table of contents

6.3 Surface functionalization for our pH sensors .................................................. 152  
6.4 Metal contact SOI devices as pH sensors: current response .......................... 155  
6.5 Metal contact SOI devices for pH sensors: $V_B$ response ............................. 162  
6.6 Optimisation of the sensor through 2D TCAD simulations .......................... 167  
6.7 Conclusion ................................................................................................. 180  

Chapter 7: General conclusion and perspectives .................................................. 189  
7.1 General conclusion ..................................................................................... 190  
7.2 Perspectives .............................................................................................. 194  

Appendices ....................................................................................................... 197  
Appendix A: Data treatment of the transient $V_B$ measurements ....................... 198  
Appendix B: Characterization of the contact through $I_D$-$V_D$ simulations .......... 200  
Appendix C: Does the resist used affect the $V_B$ response? ............................... 203  
Appendix D: $V_B$ TCAD simulations with Schottky contacts ............................... 206  
Appendix E: Details on the W Lambert function ................................................. 208  
Appendix F: DOS calculation for pH simulation ............................................... 209  

Résumé en français ............................................................................................ 212
Chapter 1: General introduction and context

Table of contents of the chapter

1.1 Why semiconductors? ............................................................................................................. 2
1.2 Biosensors ............................................................................................................................... 3
  1.2.1 Types of transducers ........................................................................................................ 3
  1.2.2 The operation principle of ISFETs ..................................................................................... 4
  1.2.3 Figures of merit .................................................................................................................... 6
  1.2.4 Some ISFET architectures .................................................................................................. 8
  1.2.5 Schottky barrier sensing ................................................................................................... 9
  1.2.6 Back gate sensing .............................................................................................................. 10
  1.2.7 Alternative materials ....................................................................................................... 12
1.3 Out-of-equilibrium body potential in SOI: A new detection paradigm......................... 13
1.4 Objective of the thesis............................................................................................................ 15
1.1 Why semiconductors?

Moore’s law has predicted the increase in the number of semiconductor components per wafer since 1965 [1]. This technological growth had a huge socio-economic impact that made the semiconductor devices widely available. Since the cost was driven down with the device size, integrated electronics became vastly accessible. This effect created a virtuous cycle in the semiconductor industry that lead to immense development and growth. In 2005, a second trend arised, named “More-than-Moore” (MtM) [2], focused on adding functionalities to circuits rather than the continuous miniaturization of the device size, named “More-Moore” (MM). The MtM branch is based on the ability of the semiconductor devices to interact with the environment (actuators and transducers) and then transfer the information as electrical signal to the processing unit, opening new options for applications [2]. Additionally, both MM and MtM branches complement each other on the development of the “Internet-of-things”, which refers to complete systems which combine sensors and edge computing, that monitor the environment and then transfer the information via the network [3]. This was very cleverly phrased in [2] as: “More-Moore focuses on the development of the brain and More-than-Moore on the interaction capabilities of a compact system”.

In this context, compact and portable systems for monitoring have a promising future with exciting new applications in many fields such as environment, health, automotive etc. For these systems the semiconductor-based sensors are appealing due to their compatibility with the CMOS technology. This implies simple fabrication and integration to already existing systems and compatibility with the “Internet-of-Things”. Additionally, semiconductor components can be manufactured in millions per wafer, which is cost effective and compatible with mass production. They also require low maintenance, they are stable over time and the can even be implanted, in certain cases [4].

In terms of applications, many challenges today concern medical, environmental and even agricultural monitoring. In all these fields, bio sensors play a key role and the research interest [5] is fully justified. In this thesis, a novel detection paradigm is used in devices similar to the ion sensitive field effect transistors (ISFETs), presented in the next section. Hence a brief review of the ISFET is presented next.
1.2 Biosensors

According to Thevenot et al. [6], a biosensor is a complete system that is capable of displaying an analytical value that describes the species under detection. This system is synthesised by five independent elements (illustrated in the schematic of Figure 1.1): the analyte, the bio-chemical receptor, the transducer, the integrated system and the output display. More specifically, the analyte contains the substance to be detected. It is the starting point of the system since, the sensor development and calibration must be adapted to those specific species (O₂, glucose, H⁺, etc…). The analyte will impose the choice of the biochemical receptor which is defines the selectivity of the sensor by binding the specific molecules of the analyte to the transducer. This transducer, which can be a semiconductor-based device, creates an electrical signal as a response to the presence and properties of the analyte. The signal then travels through the integrated circuits for amplification and processing before being displayed on the output. In the schematic, the output is represented as a screen, but it could be any visual or acoustic signal or vibration.

![Figure 1.1: Schematic representation of a biosensor components [6].](image)

Since the topic of this thesis is the development of a new transducing method, the attention is drawn on the discussion of the transducers.

1.2.1 Types of transducers

Various types of sensors are reported and they can be grouped according to the physical principle on which the transduction is done. The major categories used for bio-chemical detection are the optical, piezoelectric and electrochemical sensors. Each of these categories is divided into sub-categories. For example, in the family of the optical sensors, methods are based on labelling the species under detection. More precisely, the analysis of the evanescent wave is a label based technique. Others, like surface plasmon resonance [7], are so-called “label-free” since they do not require modification of the molecules under detection. While the
optical sensors produce accurate readings, the system is heavy, it uses expensive and fragile lenses and lasers which restricts them mainly to laboratory analysis.

For the piezoelectric sensors, the operation principle is based on the creation of a bias in presence of mechanical deformation [8]. Consequently, they can be adapted for detection of any particle given that it has a mass. They are CMOS-compatible since they can be developed with materials widely used in microelectronics industry, but the integration in a complete system might be challenging.

In the final category, we find the electrochemical sensors. Their operation is based on the modulation of an electrical signal in presence of chemical species (usually charged molecules). Depending on the monitored physical parameter they are characterised as amperometric, potentiometric and conductometric [9]. ISFETs were considered part of the potentiometric sensors until recently, but they were finally recognised as an independent category of electrochemical sensors [6]. The major advantages of the ISFETs are their CMOS-compatibility, integration and scalability which can lead to mass-production of low-cost, low-power and portable devices. This thesis is dedicated to the development of an ISFET sensor, so we will focus on a more detailed description of ISFETs operation.

1.2.2 The operation principle of ISFETs

The ISFET was a game-changer in the field of semiconductors since its discovery in 1970 [10], because it transformed the classic metal-oxide semiconductor transistor (MOSFET) into a sensor. In a classical MOSFET, the gate workfunction or any charge in the proximity of the channel (e.g. in the oxide) tunes the threshold voltage of the device. In the ISFETs, the gate is substituted by a liquid solution as depicted in the schematic of Figure 1.2. The charge in the solution directly affects the device threshold voltage ($V_T$), similar to the gate workfunction. This means that the device operation will be modified by the properties of the solution. Consider an n-MOS device as in Figure 1.2, with a p$^+$ doped channel material. If a positive charge is induced in the gate material, it favours the inversion of the channel and $V_T$ of the MOSFET decreases. Similarly, for an ISFET the charge in the solution increases or decreases the $V_T$ according to the type and quantity.
Figure 1.2: Schematic of a MOSFET and an ISFET. The solid gate of the MOSFET is replaced by a liquid solution.

To illustrate this more precisely, we present the operation principle of an ISFET fabricated on silicon-on-insulator (SOI) (similar to the devices studied in this thesis). Figure 1.3 is a schematic showing an ISFET on SOI with 3 different solutions as top-gate and a qualitative shift of the drain current ($I_D$) versus gate voltage ($V_G$) characteristic in a semi-logarithmic scale. Under the back-gate operation, when the gate voltage increases, the current follows an exponential increase until $V_G = V_T$, after which a conductive channel is formed at the interface between the silicon and the buried oxide (BOX). If the “liquid-gate” is negatively charged, the conductivity of the channel will decrease for a given $V_G$. This results in a parallel shift of the characteristic towards higher $V_G$, since higher gate bias is required to achieve a certain current value. The opposite is true for a positively charged liquid-gate. The shift of the characteristic can be quantified either as a change in the drain current ($\Delta I$) for a given $V_G$ value or as a $\Delta V_G$ for a fixed $I_D$. Often the threshold voltage shift ($\Delta V_T$) is used. The current or voltage variations are proportional to the quantity of charge in the solution and the type of charge can be recognised by the direction of the shift. This makes the ISFET capable of quantitatively measuring the amount of charges in the solution.
For actual applications, the sensors must comply the qualification standards required specifically for the category of the product, country regulations, etc. The parameters used for qualification are generally given by the figures of merit of the sensor, as we will see in the next section.

1.2.3 Figures of merit

There is a plethora of criteria for the selection of the correct transducer for a system, and the final choice depends on the application. For example, robustness is key for a sensor that operates continuously or low power and low weight are necessary for a portable device. In any case, various criteria must be considered during development stages. An in-depth list of them is presented in [11] and summarised in [12]. Here, the most important of these figures-of-merit are presented briefly.

Accuracy, precision and trueness

Regardless of the application, the reading output of the sensor should correspond to the real value measured. To define whether or not that applies to a transducer, its accuracy needs to be evaluated. The accuracy is the combination of precision and trueness of the produced outcome [13]. The term “trueness” describes how much the average output of the device differs from the real value measured, while “precision” refers to the variation of the device output.
during the reading of a certain analyte. The latter is related to repeatability and reproducibility [12].

**Repeatability, variability and reproducibility**

A sensor is characterised with good repeatability when it produces the same reading output values under consecutive measurements with the same conditions. The repeatability can be quantified as the average deviation from the real value when one device detects the same analyte, under short periods of time, in the same laboratory. The variability of the sensor is assessed when the above protocol is repeated for many samples. If the device under test generate the same output in other laboratories/environments with different measurement equipment, then it has good reproducibility.

**Stability**

The stability refers to the operational stability, but also to reliable use of a device after a long period of storage time. The first one indicates whether the results are affected by external parameters such as temperature, humidity or system aging. The second, gives the ability of the device to read a value with similar accuracy after long time periods. Additionally, the sensor should also reach the operational stability in a reasonable amount of time, this property is given by the response time.

**Sensitivity and limit of detection**

One of the most discussed figures-of-merit during the research stage of a sensor is the sensitivity. The sensitivity describes the signal change for a finite variation of the number of the species under detection. For sensors, the sensitivity is estimated through the calibration curve, which also illustrates the relationship between output values and the detected parameter. The simplest case would be a linear calibration curve in which the sensitivity is constant along the operation range. However, non-linear calibration curves can also occur depending on the measurements conditions [14] and in this cases the closeness to linearity could also be used as an additional figure of merit. Moreover, there is a point under which the sensor is not able to produce a signal related to the measured analyte and corresponds to the limit-of-detection. This can be for example, the minimum detectable concertation of the analyte.

**Other figures of merit**

It is already stated that sensors are designed for a specific analyte. This ability is described by the selectivity of the sensor and depends on the biochemical receptor (see Figure 1.1). Also,
the noise in the system is a major factor for an accurate result. In some cases, instead of defining a limit of detection, researchers chose to use the signal to noise ratio to determine a minimum detectable concentration [15]. Finally, properties like toxicity, reusability and bio-compatibility could be considered.

Most of the above mentioned factors are directly connected to the material quality, detection method, fabrication process refinement or the system design. However, the sensitivity strongly depends on the device architecture and this motivated their description in the next subsection.

1.2.4 Some ISFET architectures

To understand the need for new architectures, one should understand first the limitations in semiconductors imposed by physics (and chemistry) for ISFETs. In 1995, the sensitivity of a liquid-gate ISFET was modelled by van Hal et al. [16] The idea was to construct a physics-based model that describes the effect of the solution on the device operation. Starting from the equation of AOH⁻ and H⁺ species (AOH⇌AO⁻+H⁺ and AOH₂⁺⇌AOH+H⁺, where A an ion) for a solution in equilibrium, one can quantify the charge imposed by the liquid on the sensing interface. By estimating the disassociation constants of the ions and combine them with the Nernst equation is possible to obtain the amount of charge on the surface of the sensing layer of the ISFET (for example SiO₂). The surface potential of the semiconductor will be modified by the charge placed on the top surface according to the equation [16]:

$$\Delta \psi_s = -2.3 \cdot \frac{kT}{q} \cdot a \cdot \Delta pH$$  \hspace{1cm} (1.1)

where $$\psi_s$$ is the surface potential at the Si/oxide interface, $$k$$ is Boltzmann’s constant and $$\Delta pH$$ is the variation of the pH value. The parameter $$a$$ is a capacitive coefficient which has the form:

$$a = \frac{1}{\left( \frac{2.3 \cdot kT \cdot C_{\text{diff}}}{q^2 \cdot \beta_{\text{int}}} \right) + 1}$$  \hspace{1cm} (1.2)

where $$C_{\text{diff}}$$ is the Stern layer differential capacitance and $$\beta_{\text{int}}$$ is the intrinsic capacity of the buffer. In the best case scenario, parameter $$a$$ could be equal to one. This means that the maximum slope of equation (1.1) is 59mV/pH. This value, in the world of the biosensors is called the Nernst limit and give the best sensitivity possible by ISFETs. In practical applications, SiO₂ is not always the ideal material to be in contact with the analyte. A solution
to this arrives with the addition of an extra sensing layer [17], eventually extending the top gate.

Figure 1.4 illustrates two modified ISFET structures. In Figure 1.4a an extended gate FET (EGFET) [18] is presented. Instead of the SiO$_2$ dielectric layer in the ISFET, in the EGFET the gate is connected to a larger sensing layer adding a capacitance in series to the gate. For this structure, and additional term multiplied on the right hand side of equation (1.1) which corresponds to the capacitive ratio between the sensing capacitance and the oxide capacitance $C_{\text{sensing}}/(C_{\text{sensing}}+C_{\text{ox}})$. While the device accurately detected the solution under test, the reported performance was 45mV/pH [18]. The reduction in sensitivity is a consequence of the capacitive term which is inferior to the unit. Similarly, the ion sensitive front-gate FET with the control gate [19] (Figure 1.4b) is still limited in terms of sensitivity due to the added capacitances but it has the additional advantage of the control over the device operation through the control gate ($V_{CG}$).

![Figure 1.4: Schematic of an extended gate FET [18] in (a) and ion sensitive front-gate FET in (b) [19].](image)

However, if the increase of the sensitivity is the first priority, then sensing through the top gate might not be the optimum solution and other options are presented in the next two subsections.

### 1.2.5 Schottky barrier sensing

Instead of the linear dependence of the threshold voltage with the pH, observed with ISFETs and modeled in equation (1.1), one could chose to modify the conductivity exponentially utilising a Schottky diode for sensing. For the purpose of this demonstration, we just consider a semiconductor device with an ohmic contact at the source terminal and a Schottky contact on the drain side, as in Figure 1.5a. The current through the Schottky junction
depends exponentially on the difference between the workfunction values of the semiconductor and of the metal, called Schottky barrier. Thus, a small variation in the Schottky barrier (Figure 1.5b) induces a substantial variation in the conduction current through the device. This variation can be provoked by the presence of charges close to the depletion region due to the Schottky contact at the drain. For n-type ZnO wire with Pt contacts, an enhancement of 3 orders of magnitude was reported over the ohmic contact equivalent [21].

![Schottky barrier diagram](image)

*Figure 1.5: a) Schematic of a semiconductor device adapted for sensing and based on the Schottky barrier modification [21]. b) Schottky barrier modulation of the structure in the presence of charges [22].*

However, this method has also its drawbacks. First, the device is not conductive for low applied voltage on the drain and no charge under detection, which might lead to integration difficulties. Additionally, the charge-sensitive region is limited around Schottky diode.

### 1.2.6 Back gate sensing

ISFETs could potentially be fabricated on SOI substrates in a double-gate configuration which amplifies the sensitivity of the device. In 2010, an ISFET capable of surpassing the physical limitation of 59mV/pH was reported for the first time [23]. The idea was based on the interface coupling which is an intrinsic property of the double-gate transistors with thin films. The interface coupling was modelled by Lim and Fossum in 1983 [24]. According to their findings, the threshold voltage ($V_T$) of the channel formed close to the primary gate could be tuned through the voltage applied to the secondary gate. For the front-gate operation the front-gate threshold voltage ($V_{TF}$) is modulated by the back-gate bias $V_{BG}$; the equivalent is true for the back-gate threshold $V_{TB}$ and $V_{FG}$. A schematic of a double-gate along with the $V_T$ dependence on the secondary gate is presented in Figure 1.6, for front and back-gate operation respectively for an n-MOS with p' doped Si film. When the channel of e' is formed at the top interface if a positive voltage applied on the back-gate ($V_{BG}$), $V_{TF}$ is reduced until the point in which the back interface goes inverts and the threshold voltage modulation stops. The
equivalent is true for negative $V_{BG}$. When the back interface is depleted, the $V_{TF}$ is linear with $V_{BG}$ and the slope is called coupling coefficient and reads [25]:

$$
\alpha_{FG} = \frac{dV_{TF}}{dV_{BG}} = \frac{C_{Si} \cdot C_{BOX}}{C_{ox}(C_{BOX} + C_{Si} + C_{it,B})}
$$

(1.3)

where $C_{ox}$, $C_{BOX}$, $C_{Si}$ and $C_{it,B}$ are the front-oxide, BOX and Si film capacitances respectively. $C_{it,B}$ capacitance associated to the Si/BOX interface state densities and in a first approximation it can be neglected for high quality wafers. Evidently, the slope can be tuned via the thicknesses of the Si and BOX layers. An equivalent equation can be written for the back-gate operation. This implies that a change on the electrostatic condition of the top gate can change the conductivity of the back-channel by a factor $\alpha_{BG}$, which depends on the ratio of the capacitances.

![Schematic of a thin film double-gate MOSFET on SOI](image)

In reality, the correlation between the signal amplification through coupling was made in [26]. The equivalent circuit of an ISFET with a front-liquid gate and a back-gate is depicted in Figure 1.7. $C_{lg}$ is the liquid capacitance including $C_{ox}$ and $C_{dl}$ (standing for the top-oxide and double-layer capacitances respectively). Also, $C_{c}$ is the contact and $C_{Si}$ the silicon film capacitance respectively. The variation of the back-gate threshold voltage is then [26]:

$$
\Delta V_{T_{-BG}} = -2.3 \frac{kT}{q} \cdot \alpha \cdot C_{ox} \cdot C_{BOX} \cdot \Delta pH
$$

(1.4)

$\alpha$ has the same meaning as in equation (1.1). Observe how, the back-gate threshold voltage shift can be improved thanks to $C_{ox}/C_{BOX}$ ratio. This ratio is a result of interface coupling and leads to devices with increased sensitivity. Exploiting this intrinsic property of the double-gate structure with $t_{BOX}>t_{ox}$, Go et al. [23] achieved a sensitivity of 240mV/pH. A more precise model should also include the capacitance of the Si film [27].
Although the above “engineering-trick” effectively improved the sensitivity through the back-gate operation, the size of the device still holds and important role for the limit of detection of the FET sensors. If the application demands the detection of a small amount of charges then, a nanowire FET might be a better choice since, the high surface-to-volume ratio establishes the nanowires very effective in this case [28]. Note also that, besides the surface-to-volume ratio, the geometry of the architecture is of equal importance since it reduces the screening of the charge under detection [29]. The above properties of the nanowire FETs lead to limit-of-detection of about ~30aM for antibody–antigen interaction of about ~1pM for DNA and even got to single virus detection [30].

Aside from architectures and geometries, devices with more exotic materials could also be explored to improve the performance [31] as presented in the next sub-section.

### 1.2.7 Alternative materials

Obviously, the starting point was the classic bulk Si substrates on which the ISFETs was developed. Those kind of structures are robust due to the extensive knowledge on Si devices and technology generally. However, they present limitations as mentioned in subsection 1.2.4, or additional functionalisation steps are required [28]. To find new improvement paths 2D materials have been proposed. For example MoS$_2$ has a tunable band gap [32], high electron mobility and potentially low toxicity [33]. Moreover, graphene seems to be the most promising material for biosensors development since it is cheap, flexible, has a high electron mobility and in certain cases could be directly compatible with the species under detection [34]. However, graphene has been characterised as toxic in some cases [35]. Moving down in size, we arrive to nanowire carbon nanotubes. Such devices exploit the high surface-to-volume ratio achieving a limit-of-detection in the range of aM [36]. Although carbon nano-tube structures are cost
effective, they might be hard to align and create highly resistive junctions when the orientation of the wires is random (nanonets) [37]. Finally, even a single molecule switch was reported in [38] where the conductance of the structures changes as the molecular structure is modified in the presence of specific species to be detected.

1.3 Out-of-equilibrium body potential in SOI: A new detection paradigm

This brief review of biochemical transducers highlights the endless options in terms of materials and structures that were explored within the world of (bio)-chemical sensors. However, the majority of the studies focus mainly on the proof-of-concept with current measurements. This thesis aims to the development of a new reading method utilising a transient phenomenon in thin film SOI MOSFETs: the out-of-equilibrium body potential that we explain in this section.

Indeed, the novelty of this work relays on a particular floating body effect specific to fully depleted (FD) MOSFETs [39]–[44]. Even if, in the majority of cases, these effects are not desirable, the out-of-equilibrium body potential has been successfully exploited for DRAM applications [42] and detection [45]. The phenomenon stems from the lack of carriers in the silicon film during the fast scan of the gate which induces the out-of-equilibrium potential variation. A schematic representation of this transient effect is depicted in Figure 1.8 for a double gate FD-SOI MOSFET. When \( V_{BG} \) is swept from inversion to accumulation, because the source and drain are \( N^+ \) contacts, there is no source to provide holes rapidly, the Si body is driven into an out-of-equilibrium state and its potential \( (V_B) \), follows the variation of the signal applied on the operating gate. Meanwhile holes start to be produced with \( V_G \) (e.g. due to band-to-band tunnelling) and the film is finally driven into accumulation. The potential returns abruptly to the equilibrium value and the device is now at a steady state. The equivalent phenomenon manifests itself also in SOI wafers measured with the pseudo-MOSFET configuration [45].
Chapter 1: General introduction and context

Figure 1.8: Schematic representation of a double-gate FD-SOI MOSFET during the transition from inversion to accumulation through a front-gate scan [42].

In the pseudo-MOSFET, two metallic probes are placed directly on the SOI and they act like source and drain [46]. The gate voltage \( V_G \) is applied directly to the substrate, as shown in Figure 1.9a. Depending on the \( V_G \) value, a channel is formed at the Si/BOX interface and creates an upside down MOSFET structure. In this configuration, a third probe is placed on the film, between the source and drain, to monitor the body potential during the \( V_G \) scan. As illustrated in Figure 1.9b, the body potential \( V_B \) occurs when the film is depleted. This is an asset for detection applications, since in this region the device seems to be more sensitive to charges [14]. The detection ability with \( V_B - V_G \) shifts in SOI with thin films was also demonstrated in [45] as depicted in Figure 1.9c. In this experiment, the top SiO\(_2\) surface was modified with APTES (aminopropyltriethoxysilane), which is positively charged, followed by the binding of negatively charged gold nano-particles. Observe, the body potential shifts in two different directions depending on the charge type, proving the legibility of the technique as a detection method.

Figure 1.9: Schematic of the pseudo-MOSFET configuration adapted for body potential measurements (a). Drain current, gate current and body potential versus gate voltage (b). Body potential shift when charges are placed on the top SiO\(_2\) surface (c) [45].

The proof of concept for biochemical detection was performed already during the previous thesis in our group, for the detection DNA molecules with this method in the pseudo-MOSFET.
configuration [47]. Having this as a starting point, this thesis aims to the development of a practical device for sensing based on the out-of-equilibrium body potential reading, which is explained in the next section.

### 1.4 Objective of the thesis

The development of a more practical sensor necessitates two independent development paths: (1) the technological development of the device and (2) the theoretical understanding necessary for device integration for the next development stages.

Evidently, the device and method are at the early stages of development. Although the development of a commercial product requires additional steps to the above two, this thesis focuses on the transition from an experimental configuration, which depends on a particular probe station, towards an independent device operating based on the out-of-equilibrium body potential. The technological objectives of this thesis are illustrated in Figure 1.10.

![Figure 1.10: A schematic of the starting point [47] of the thesis along with the definition of main technological the objectives.](image)

The defined objectives where achieved in five individual steps, each of which corresponds to one of the core chapters of this thesis.

In chapter 2, the dynamic character of the out-of-equilibrium body potential is explored. This requires the replacement of the quasi-static experimental conditions by transients ones. The new experimental set-up is benchmarked and validated with the previously established quasi-static measurements.

In chapter 3, TCAD simulations are performed to provide with an insight concerning the physics behind the transient out-of-equilibrium response. The chapter addresses simulations
concerning the type of contacts for the $V_B$ response and investigates the dependence of the transient effects on the geometrical/technological parameters.

In chapter 4, the development of SOI devices with deposited metal contacts is discussed. Questions concerning the material selection for the contacts, the fabrication processes followed and the design of the contact layout are answered.

In chapter 5, we extend the understanding of the out-of-equilibrium body potential through numerical simulations based on fundamental physical equations. The origin of the phenomenon is identified, modeled and benchmarked with experimental data.

In chapter 6, the new SOI devices with deposited metal contacts are evaluated as sensors. Solutions with various pH values were detected and the $I_D$ and $V_B$ responses from the devices were compared. Further optimisation paths were revealed through TCAD simulations.

In chapter 7, the general conclusions are presented and thoughts for further development of the project are shared.
References


Chapter 1: General introduction and context


Chapter 2: Transient measurements in the pseudo-MOSFET configuration

Table of contents of the chapter

2.1. SOI characterization with the pseudo-MOSFET ............................................. 24
   2.1.1. Static electrical characterization with the pseudo-MOSFET: \( I_D-V_G \) ............ 25
   2.1.2. Contact behaviour of the pseudo-MOSFET with pressure controlled probes . 29
   2.1.3. Transient \( I_D \) measurements in the pseudo-MOSFET ................................ 30
   2.1.4. Out-of-equilibrium body potential ............................................................... 31

2.2. Implementation of transient voltage ramps in the pseudo-MOSFET ............ 32
   2.2.1. Linear ramps applied to the pseudo-MOSFET configuration ......................... 34
   2.2.2. Impact of the scanning speed on the currents ............................................. 36
   2.2.3. Effect of the transient measurement on the body potential .............................. 39

2.3. Conclusions ........................................................................................................ 42
Chapter 2: Transient measurements in the pseudo-MOSFET configuration

The aim of this chapter is to give the starting point of this thesis, the pseudo-MOSFET configuration typically used for SOI wafer characterization (section 2.1), to implement the transient measurements with triangular voltage ramps and to explore the out-of-equilibrium body potential monitoring in a configuration with pressure-controlled probes (section 2.2).

2.1. SOI characterization with the pseudo-MOSFET

Silicon on insulator (SOI) wafers consist of a silicon (Si) film separated from the bulk by an insulator, usually SiO$_2$ as shown in Figure 2.1. The three important regions are: 1) the active Si layer on which the electrical components are fabricated, 2) the buried oxide (BOX) which isolates the top Si from the substrate and, 3) the bulk which serves as mechanical support. SOI wafers were introduced to improve the circuit performance [1]. However, the development of SOI devices requires high quality Si and insulating layers [1]. Smart-CutTM process development [2] played a key role for the improvement of the SOI quality during fabrication. To evaluate if the SOI meets the specifications, the wafer must undergo an electrical characterization for quality control. The pseudo-MOSFET [3], [4] was proposed as a solution to this need at the early stages of the SOI technology, as a fast and inexpensive electrical characterization configuration.

![Figure 2.1: Schematic of an SOI wafer.](image)

In the pseudo-MOSFET, the substrate is utilised as gate and the BOX as gate dielectric of the inverted pseudo-transistor. Additionally, two metallic probes placed directly on top of the Si film of the SOI serve as source and drain. With all these elements, we obtain an inverted MOSFET structure. The configuration requires a special probe station with controlled-pressure probes. The probes penetrate in the Si film, creating an electric contact with the semiconductive material (Figure 2.2a). When a positive bias is applied to the substrate through the chuck (referred hereafter as gate voltage, $V_G$), electrons are attracted to the Si/BOX interface. For the lightly doped p-type ($N_a=10^{15}$ cm$^{-3}$) wafers used in this thesis, when $V_G$ surpasses the threshold voltage ($V_T$), the film inverts and a conductive path of electrons is formed between the two metallic probes. Similarly, a negative $V_G$ inferior to the flat-band voltage $V_{FB}$ ($V_G<V_{FB}$) will
drive the film into the accumulation regime. Between $V_{FB}$ and $V_T$ the Si film is depleted. Contrary to the conventional MOSFETs that require an n-MOS and a p-MOS device for the extraction of hole and electron parameters, the metallic pressure probes permit the injection of both types of carriers with a single pseudo-MOSFET measurement, allowing for a complete electrical characterization of SOI wafers.

![3D schematic of the pseudo-MOSFET configuration](image)

*Figure 2.2: 3D schematic of the pseudo-MOSFET configuration for a Si island of an SOI wafer (a). The applied voltage on the substrate used as gate defines the state of the interface between the top silicon layer and the BOX. The p-type film is in inversion for $V_G>V_T$ (b), in accumulation for $V_G<V_{FB}$ (c) or depleted in between (d).*

2.1.1. Static electrical characterization with the pseudo-MOSFET: $I_D$-$V_G$

In the pseudo-MOSFET, the SOI wafer can undergo various electrical characterization tests, as a classical transistor. Drain current ($I_D$) versus gate voltage ($V_G$) analysis is mostly used and gives access to the calculation of important parameters such as mobility ($\mu$) and $V_T$. For advanced MOSFET structures a widely used method for parameter extraction from $I_D$-$V_G$ curves is the Y-function [5]. To construct the Y-function one needs to plot the drain current ($I_D$) and transconductance ($g_m$) versus gate voltage curves, presented in Figure 2.3. For $V_G<$-2V, the film is in accumulation (Figure 2.2c) with an ON hole current of over 1μA. For -2V<$V_G<$3V, the device is in depletion (Figure 2.2d) and the current drops exponentially to 100p. For $V_G>$3V the film is inverted (Figure 2.2b) with an electron current of over 2μA. In inversion and accumulation regimes and for low drain voltage ($V_D$), the current in the pseudo-MOSFET is modelled similarly to the classic MOSFETs [3], [6]:

$$I_D = f_g \cdot C_{BOX} \cdot \frac{\mu_0}{1+\theta(V_G-V_{T,FB})} \cdot (V_G-V_{T,FB}) \cdot V_D \quad (2.1)$$
where $f_g$ is the geometrical factor [7] (replacing the W/L term of the MOSFETs), $C_{BOX}$ is the buried oxide capacitance, $\mu_0$ is the low field mobility for electrons or holes, $V_T$ is the threshold and $V_{FB}$ the flat-band voltage respectively. $V_D$ is the voltage applied to the drain terminal. The term $\theta$ is the mobility attenuation factor, which includes the effect of the series resistance of the contacts [5] and the phonon scattering mobility limitation [8]. Evidently, equation (2.1) is not linear with $V_G$. Additionally, it contains three unknown parameters, $V_T$, $\mu$ and $\theta$. The $Y$-function [5] solves this problem through a manipulation of equation (2.1). First, the transconductance is calculated as the derivative of $I_D$ with respect to $V_G$:

$$g_m = \frac{dI_D}{dV_G} = f_g \cdot C_{BOX} \cdot \frac{\mu_0}{[1+\theta(V_G-V_T)]^2} \cdot V_D$$  (2.2)

A typical transconductance curve measured in the pseudo-MOSFET configuration is depicted in Figure 2.3b. For $V_G > 0$, $g_m$ shows an increase until the maximum, for $V_G \approx 5V$, and then the value reduces. For negative $V_G$, $g_m$ has a similar shape for negative values. Notice, the smaller $g_m$ values for holes due to their lower mobility with respect to the electrons mobility.

![Figure 2.3: Drain current (a) and transconductance (b) versus gate voltage of an SOI with 88nm silicon film over 145nm thick BOX. $V_D=0.1V$.](image)

A simple division of the drain current by the square root of the transconductance yields the $Y$-function ($Y$) [5], which is linear with $V_G$ and independent from $\theta$:

$$Y = \frac{I_D}{\sqrt{g_m}} = \sqrt{f_g \cdot \mu_0 \cdot C_{BOX} \cdot V_D \cdot (V_G - V_T)}$$  (2.2)

The intercept of the linear part with the x-axis corresponds to $V_T$ and the slope is proportional to the square root of $\mu_0$. The strength of the method is that both quantities are extracted from the same linear fit. An example of the $Y$-function for the pseudo-MOSFET, fitted for electrons and holes, is depicted in Figure 2.4. Since, pseudo-MOSFET has a channel of holes and a channel of electrons, depending on $V_G$, mobility and $V_T$ ($V_{FB}$ for holes current) could be
Chapter 2: Transient measurements in the pseudo-MOSFET configuration

extracted for both carrier types. The extracted values from the curves presented above are
\( \mu_n = 280 \text{cm}^2/(\text{V} \cdot \text{s}) \) and \( V_T = 4.35 \text{V} \) for electrons and \( \mu_p = 90 \text{cm}^2/(\text{V} \cdot \text{s}) \) and \( V_{FB} = -3.16 \text{V} \) for holes.

Considering these extracted parameters the only unknown quantity in equation (2.1) is \( \theta \). Thus, with a substitution of the extracted mobility and threshold voltage in the above equation, the last term can be estimated through the plateau of \( \theta \) for high \( V_G \) (see Figure 2.5). Generally, \( \theta = \theta_0 + \theta_1 \cdot R_{SD} \) were \( \theta_0 \) represents the mobility limitation due to phonon scattering [8]. The second term contains the series resistance \( R_{SD} \). The definition of the \( \theta \) according to [5] is

\[
\theta = \left[ \frac{I_D}{\theta_m(V_G - V_{T,FB})} - 1 \right] / (V_G - V_{T,FB}) \tag{2.3}
\]

However, in the pseudo-MOSFET the main impact on \( \theta \) stems from the series resistance (due to the Schottky contact [9]) and \( \theta_0 \) is neglected, especially for thick BOX. According to [5], the series resistance or the pseudo-MOSFET is calculated as:

\[
R_{SD} = \frac{\theta}{f_{\theta} \mu_0 C_{BOX}} \tag{2.4}
\]

From equation 2.3, the series resistance is extracted as \( R_e \approx 2 \cdot 10^4 \Omega \) for electrons and \( R_h \approx 5 \cdot 10^5 \Omega \) for holes.

**Figure 2.4:** Y-function versus gate voltage of an 88nm silicon film over 145nm BOX layer wafer. The curve was calculated with the data from Figure 2.3.
Figure 2.5: $\theta$ versus gate voltage of an 88nm silicon film over 145nm BOX layer wafer.

Additionally, the analysis of the $I_D-V_G$ curves also provide information for the interface states. As for the SOI MOSFETs [10], the sub-threshold swing ($S_{\text{swing}}$) of the current could be exploited for the estimation of interface trap densities ($D_{it}$). The definition of the $S_{\text{swing}}$ is:

$$S_{\text{swing}}^{-1} = \frac{d \log(I_D)}{d V_G}$$  \hspace{1cm} (2.5a)

and in the pseudo-MOSFET the simplest model for the swing gives [5]:

$$S_{\text{swing}} = 2.3 \frac{kT}{q} \left( 1 + \frac{C_{Si}qD_{it}}{C_{BOX}} \right)$$  \hspace{1cm} (2.5)

where $k$ is Boltzmann’s constant, $T$ the temperature, $q$ the elementary charge, $C_{Si}$ the silicon film capacitance and $D_{it}$ the interface traps density. For the curve of Figure 2.3a, the extracted value of interface traps density in inversion is $D_{it,e} = 1.2 \cdot 10^{12} \text{cm}^{-2} \text{eV}^{-1}$.

The above methods were used in this thesis for the electrical characterization of the devices tested in this thesis. However, there is a plethora of other electrical characterization and extraction techniques applied to the pseudo-MOSFET. For example, the estimation of $V_T$ can be done using all the developed methods for MOSFETs [11]. Additionally, a more accurate estimation of the $D_{it}$ value is possible based on capacitance measurements [12], the effective mobility and the inversion charge could be extracted from split C-V measurements [13], or noise characterization was also implemented [14].
2.1.2. Contact behaviour of the pseudo-MOSFET with pressure-controlled probes

The challenge with the pseudo-MOSFET configuration is the nature of the contacts between the metal (tungsten carbide) probes and the low doped Si film. This aspect will also be considered for the deposited metal contacts in chapter 4. Generally, contacts between metals and semiconductor can have a rectifying or non-rectifying behaviour [15], depending on the materials used for the junction. In MOSFETs, the source and drain contacts must have a low resistance and provide the carriers as soon as they are needed in the device channel. Thus, an ohmic contact is always desirable and it is obtained through doping. Although, pseudo-MOSFET has metal/semiconductor junctions as source and drain, the characterization is based on adapted models from MOSFET devices, which always consider ohmic contacts. Schottky contact devices would need model adjustments for accurate parameter extraction [16]. Luckily, pressure-controlled contacts on pseudo-MOSFET show an ohmic behaviour, as reported plenty of times in the literature [9], [17], [18], [4], [19]–[21].

To show the electrical response obtained with the pseudo-MOSFET contacts, the drain current versus drain voltage ($V_D$) characteristics are plotted in Figure 2.6 as an example. The curves were traced for positive gate voltage in Figure 2.6a and for negative $V_G$ in Figure 2.6b. For low $V_D$ and high $V_G$ the curves show a linear dependence on the applied $V_D$. On the contrary, they show a rectifying behaviour for low $V_G$ (when the Si film is depleted). Notice that the models are true for the linear region of the $I_D$-$V_D$ curves. Thus, they are applicable in the pseudo-MOSFET configuration, without any additional adaptation and the parameter extraction remains valid, in the region where the behaviour is ohmic. Note that, the pressure applied on the probes can affect the measurement [18].

![Figure 2.6: Drain current versus drain voltage curves for a) $V_G>0$ and b) $V_G<0$ of an SOI with 88nm thick Si film over 145nm thick BOX measured with the pseudo-MOSFET. The pressure was set to $p=100$g.](image)
In the characterization shown above, the device was into a quasi-static state for each measurement point. As it will be discussed later in this thesis, the contact type plays an extremely important role on the transient body potential \( (V_B) \) and the dynamic response of the configuration. Before reaching this point, some transient results from the literature are presented.

### 2.1.3. Transient \( I_D \) measurements in the pseudo-MOSFET

The first transient measurement in the pseudo-MOSFET configuration was reported four years after its discovery \[22\]. The transient drain current monitored during a negative bias pulse is depicted in Figure 2.7a for various gate voltages. After the \( V_G \) pulse is applied on the gate, the drain current does not return to the equilibrium value directly, unless the wafer is under illumination. As explained in \[22\], the derivative of the current (Figure 2.7b), follows the equation

\[
\frac{dI_D}{dt} = \frac{q \cdot n_i \cdot d_{si}}{\tau_g} \left( \frac{I_D(t) - I_D(\infty)}{R_H + C_{ox} V_G} \right) = \frac{q \cdot n_i \cdot d_{si}}{\tau_g} \cdot RHS(t)
\]  

(2.6)

where, \( q \) is the elementary charge, \( n_i \) the intrinsic carrier concentration, \( d_{si} \) the silicon thickness, \( \tau_g \) the carrier lifetime, \( C_{ox} \) the oxide capacitance and \( K = f_g \cdot q \cdot \mu_0 \cdot V_D \). RHS(t) corresponds to the term inside the brackets in the formula above. The slope of equation (2.5) gives the carrier lifetime in the Si film of the SOI (extracted from the linear fit in the Figure 2.7b). In Figure 2.7a, observe on the right y-axis the small measured potential variation of the top Si interface reported which shows a value close to 50mV. Even if a potential variation was reported in 1996 and other transient studies we published in the pseudo-MOSFET \[23\]–\[26\], they were mainly focused on the current response.

![Figure 2.7](image)

*Figure 2.7: a) Transient \( I_D \) versus time for three \( V_G \) pulses and the potential measured on the top of the SOI. b) Drain current derivative versus RHS(t) \[22\].*
Another type of transient experiments were performed in the last years to explore the out-of-equilibrium body potential response of the pseudo-MOSFET, as we will discuss next.

### 2.1.4. Out-of-equilibrium body potential

This dynamic effect of body potential variation ($V_B$) in the Si film was firstly encountered in SOI transistors. A linear potential variation with respect to the applied $V_G$ was observed in double-gate fully depleted (FD) SOI MOSFETs, under the appropriate bias conditions that lead the device into an out-of-equilibrium state. More specifically, Bawedin et al. [27] showed that a sweep of the front-gate voltage ($V_{G1}$) in a n-MOS double gate FD-SOI device can impose a linear body potential variation. Figure 2.8a illustrates the out-of-equilibrium body potential of the tested device (inset) in (a) and the gate current in (b) for a front-gate scan from inversion ($V_{G1}>0$) to accumulation ($V_{G1}<0$). Although such devices should maintain a zero potential during the $V_{G1}$ scan, the difficulty of injecting holes in the structure when passing from depletion to accumulation provokes this potential variation. The dynamic character of the effect is evidenced through the potential value decrease for higher scanning speeds (SS). Additionally, the body potential variation is associated with the front-gate current, and more specifically with a distinct spike observed in the characteristic. This peak is also enhanced with the scanning speed and appears during the return of the body potential to its equilibrium value, when the electrodynamic conditions allow for injection of holes in the silicon film.

![Figure 2.8](image)

**Figure 2.8:** a) Body potential and b) Front-gate current versus front-gate voltage for three scanning speeds measured in the double gate FD-SOI MOSFET. The applied front-gate voltage swept the device from inversion to accumulation. The inset of (b) shows a schematic of the measured device [27].
Bawedin et al. [27], proposed a semi-analytical model to describe the effect, proving that it is provoked by two different carrier injection mechanisms. The current is related with the body potential through the following formula [27]:

\[
\frac{I_G}{C} = -\frac{V_B}{\Delta t}
\]

where \(I_G\) is the gate current of the operating gate, \(V_B\) the body potential variation, \(t\) the time and \(C\) an equivalent capacitance.

The same effect was also observed during the \(V_G\) scan under quasi-static conditions in SOI wafers tested in the pseudo-MOSFET configuration. The out-of-equilibrium body potential is extensively discussed for quasi-static measurements by Benea et al. [28] in 2018. \(V_B\) measurements require a third probe placed on the Si film. To accurately monitor the body potential the SMU of the probe contact should be set to “I-mode” in which, a zero current condition is imposed. An example of the out-of-equilibrium body potential versus \(V_G\) in the pseudo-MOSFET is presented in Figure 2.9. Observe that \(V_B\) manifests itself for both scanning directions due to the metal contacts, contrary to the FD-SOI transistors in which only one sweep direction induces \(V_B\).

![Figure 2.9: Drain current, gate current and out-of-equilibrium versus gate voltage for the forward (a) and reverse (b) scanning direction, measured in the pseudo-MOSFET configuration. The wafer has an 88nm thick Si film and 145nm thick BOX [28].](image)

2.2. Implementation of transient voltage ramps in the pseudo-MOSFET

All the \(V_B\) experiments in the pseudo-MOSFET configuration were done in quasi-static conditions. To really explore the dynamic conditions for the out-of-equilibrium body potential in this thesis, transient experiments are designed, with a linear \(V_G\) ramp applied to the gate.
A 5x5mm² silicon mesa was etched from an SOI with 88nm Si film over 145nm BOX. On this sample, we repeated the measurements as in [28] and plotted the drain current, gate current ($I_G$) and body potential versus gate voltage in Figure 2.10. $I_G$ shows a variation when the device is in depletion. When the film enters weak inversion a spike is measured and then $I_G$ returns to zero, similarly to what is observed in SOI MOSFETs. The potential follows the linear variation applied to the gate and at a given $V_G$ returns to the equilibrium value ($V_D/2=50$mV). Notice the positive values of $I_G$ for a forward $V_G$ scan (from $V_G=-10V$ to $V_G=10V$) and the negative values for the reverse scan (from $V_G=10V$ to $V_G=-10V$). This behaviour is characteristic of the pseudo-MOSFET configuration and its origin was explained in [28], [29]. Although it was initially suggested [29] that $I_G$ stems from generation of carriers in the Si film actually corresponds to the rapid injection of carriers in the Si film which correlates with the amount of carriers needed for $C_{BOX}$ charging during the channel formation [28]. In chapter 5, an additional explanation, that confirms the aforementioned interpretation, is provided based on semiconductor models. As in [27], $I_G$ is associated with a potential variation as illustrated in Figure 2.10b and the equation (2.6) is true in this case also [30]. The return to the equilibrium occurs at the same $V_G$ as the maximum $I_G$ value, corresponding to the rapid injection of carriers in the Si film. Notice how both $I_G$ and $V_B$ change sign for the reverse scanning direction. Since in this case the interface is driven into accumulation, a deficit of holes arises in the film and thus the measured quantities appear to be negative.

![Figure 2.10: a) Drain and gate currents and b) body potential versus gate voltage for an 88nm Si film over 145nm BOX measured with the pseudo-MOSFET (inset of a shows the experimental configuration). The insets in b) show the charges’ signs in the device for accumulation, depletion and inversion regimes.](image)
2.2.1. Linear ramps applied to the pseudo-MOSFET configuration

Considering the state of art for transient measurements, the dynamic $V_B$ study necessitates a scan of $V_G$ that drives the device from the accumulation regime to inversion. A straightforward solution is a triangular signal with various periods ($T$) as shown in Figure 2.11. To validate the experimental set-up, the transient experiment with ramps must be comparable with the quasi-static one with the same time scales.

![Figure 2.11: Triangular signal ramps applied to the gate for the transient experiments.](image)

The Si island was probed with three pressure controlled probes for realising the source, body and drain contacts. The triangular signal of Figure 2.11 was applied directly to the substrate through the chuck of the Jandel station. For the measurements, a B1500A from Agilent analyser with two fast B1530A I-V modules were used. The drain voltage was set to $V_D=0.1V$ with a standard SMU unit. The tested scanning speed (SS) range was from 10V/s to 400V/s and it was applied at a fixed $V_G$ range (from -5V to 5V) by varying the signal period. An additional measurement with a 12s period ramp was performed for comparison with the quasi-static measurements. To match the above period during the quasi-static measurements the gate voltage step was set to 100mV, the delay time to 40ms and a medium integration time was selected (20ms) (equivalent SS≈1.667 V/s). Figure 2.12 visualises the differences between the two $V_G$ values applied during the measurement. We compare the experimental results obtained with the two methods to validate the transient measurements and we highlight the differences between them.
Chapter 2: Transient measurements in the pseudo-MOSFET configuration

Figure 2.12: Schematic of the two methods $V_G$ signals are applied during quasi-static and transient conditions.

Figure 2.13 compares the drain and gate currents versus gate voltage in transient and quasi-static experiments. While the drain current curves seem to be reasonably superposed in the inversion and accumulation regimes, a discrepancy is observed in depletion. The reason for such difference is possibly related to the different method that $V_G$ is applied. Even if the scanning speed is equivalent between the experiments, the quasi-static voltage is applied in small steps while the transient has a “fluid” linear variation. From a first site, there are two explanations that could potentially apply here: a) the change in the dynamics could potentially alter the charging/discharging effect of the traps, b) the gate current (Figure 2.13b) has higher values in all regimes. Notice how $I_G$ peak drops at higher $V_G$ for inversion and at lower $V_G$ for accumulation. The $I_G$ plateau current observed in transient when the device is in inversion or accumulation has the same order of magnitude as the drain current, potentially affecting the characteristic. Clearly, the measurement method changes the dynamics of the SOI and this change stems from different way the $V_G$ is applied.

In the quasi-static case a small voltage step is applied to the gate of the pseudo-MOSFET and $V_G$ stays constant during the integration time window. In the transient measurements the devices is in a continuously dynamic state. Additionally, in quasi-static conditions the equipment performs several measurements for each applied bias and calculates an average value for each applied voltage step to reduce noise. For the transients, only one measurement is performed. Note that, there is the option for averaging the transient values by performing several full measurements and then calculate the average curves. Even in this case though, the dynamics between each measurement point are significantly different.
Figure 2.13: a) Drain current and b) gate current versus gate voltage for transient and quasi-static measurements performed with the same scanning speed $SS \approx 1.667$ V/s. The drain voltage was kept constant at $V_D = 0.1$ V.

### 2.2.2. Impact of the scanning speed on the currents

For the dynamic phenomena one expects to obtain a different behaviour based on the frequency of the applied signal. The effect of the scanning speed on the drain current versus gate voltage characteristics is depicted in Figure 2.14 for the forward scan in (a) and for the reverse in (b). The empty symbols Figure 2.14a correspond to the $|I_D|$. For all the tested scanning speeds, the double conduction characteristic (hole current in accumulation and electron current in inversion in one measurement) of the pseudo-MOSFET is present. However, for scanning speeds higher than 100 V/s the curves seem to lose their shape. An increase in the threshold voltage is evidenced for the forward scan direction, while $V_T$ decreases for the reverse one. A similar effect (inverse behaviour) is observed for the flat-band voltage. Notice how the opposite trend is observed in the reverse scanning direction ($V_T$ decrease and $V_{FB}$ increase), creating a hysteresis which seems to increase with $SS$. At lower scanning speeds, the transient effects seem to be reduced. More elements for the understanding of the transient response are obtained through the gate current response.
Chapter 2: Transient measurements in the pseudo-MOSFET configuration

Figure 2.14: Dependence of the scanning speed of the drain current characteristics a) for the forward and b) for the reverse scan directions. The empty symbols in (a) correspond to negative $I_D$ values and since it is represented in a semi-log scale they were taken in absolute value. The tested SOI has $t_{Si}=88\text{nm}$ and $t_{BOX}=145\text{nm}$.

The gate current versus gate voltage curves for the same scanning speeds as in Figure 2.14 are shown in Figure 2.15. As illustrated in [28], an increased scanning rate results in higher gate current values. $I_G$ was identified and connected with the BOX capacitance charge/discharge [28]. The plateau of the current is a function of SS. Unlike the static measurements, here the values are significantly amplified, reaching several $\mu\text{A}$ for the highest SS. Notice that the values of the transient $I_G$ for SS>$20\text{ V/s}$ are comparable with the $I_D$ at a given $V_G$. Since the sum of all terminals’ currents should be zero ($I_D+I_G+I_S=0$), the increase of $I_G$ will affect the shape of the measured $I_D$. Hence, the increase of $V_T$ for the forward scan stems from the compensating $I_G$. The opposite is true for the reverse scan in which $V_T$ is reduced since $I_G$ is negative. Considering the large size of the device, this effect could be associated with the large oxide capacitance. In order to verify this hypothesis, we compare the $I_G(V_G)$ responses for two different SOI samples with the same $t_{Si}$ but different $t_{BOX}$ ($t_{BOX}=145\text{nm}$ in Figure 2.15a and $t_{BOX}=190\text{nm}$ in Figure 2.15b). Both wafers show similar behaviour but the $I_G$ plateau values are different.
Chapter 2: Transient measurements in the pseudo-MOSFET configuration

Figure 2.15: Transient $I_G$-$V_G$ curves for various scanning speeds. SOI with a) $t_{Si}=88\text{nm}$ and $t_{ox1}=145\text{nm}$ and b) $t_{Si}=88\text{nm}$ and $t_{ox2}=190\text{nm}$.

The experimental results show indeed an $I_G$ plateau value proportional to the frequency of the applied signal (or inversely proportional to the period) in accumulation or inversion, similarly to a capacitive induced current: $I_G \sim \omega C$. To identify whether the last apply here, the inverse $I_G$ values measured on the plateau were traced with respect to the signal period in Figure 2.16. The values were monitored at $|V_G|=4.9\text{V}$ of the forward scan and then fitted with a line. The ratio of the capacitances ($C_{145\text{nm}}/C_{190\text{nm}}=1.31$) seems to be in agreement with the ratio of the slopes from the fitting ($a_{190\text{nm}}/a_{145\text{nm}}=1.28$). This confirms that the BOX capacitance is responsible for the plateau current.

To further support this argument we fit the plateau values with an analytical model. To do so, we start with the fact that $C_{BOX}$ is associated with the inversion current. To model $I_G$ we start from the general definition of the current:

$$ I_G = \frac{dQ_{inv}}{dt} = \frac{dQ_{inv}}{dV_G} \cdot \frac{dV_G}{dt} \quad (2.8a) $$

where $Q_{inv}$ is the inversion charge and $dV_G/dt$ is the scanning speed. In fully depleted MOSFETs, the inversion charge is modelled based on the Lambert W function [31] (described in the appendix E):

$$ Q_{inv,acc} = C_{BOX} \frac{n_k T}{q} \text{LW} \left( q \frac{V_G-V_{T,FB}}{n_k T} \right) \quad (2.8b) $$

where $n$ is the ideality factor, $V_T$ the threshold voltage ($V_{FB}$ the flat-band voltage), $q$ the elementary charge and $k$ the Boltzmann’s constant. A calculation of the charge in accumulation and inversion with $V_T$, $V_{FB}$ the values extracted from the Y-function applied to the static $I_D$-$V_G$ curves (Figure 2.13a) combined with the equation (2.7), yields the modelled $I_G$, the lines in Figure 2.16b.
Figure 2.16: \(1/I_G\) current plateau value measured in strong inversion with respect to period of the signal for the two SOI samples from Figure 2.15. The dotted lines were issued from linear fits of the experimental data (a). Same experimental point plotted with the analytical model for inversion and accumulation (inset) (b). The error bars are calculated as an average of five measured points.

The model is in good agreement with the experiments for the two BOX thicknesses tested in Figure 2.16b. The small deviation is attributed to the experimental error of \(I_G\), which reduces for higher SS as the current increases. Clearly, the large capacitance value is responsible for the plateau current that appears in the transient measurements. The \(I_G\) peak is maintained in the transient measurements with respect to the static measurements and it is enhanced thanks to the increased dynamics. The connection between \(I_G\) and \(V_B\) explained in sub-section 2.1.4 lets us assume that the increased transient response will also result in increased transient \(V_B\) response.

### 2.2.3. Effect of the transient measurement on the body potential

From the experimental point of view, there are practical problems related to the monitoring of the transient body potential. The accurate measurement of \(V_B\) requires a constant zero-current condition on the body contact. While source/monitor units (SMU) can be programmed to impose zero current values, remote-sense and switch units (RSU) cannot source and impose a zero current condition simultaneously. As demonstrated earlier, the large die surface enhances the capacitive effects under fast transients. Considering that recent studies for Si films show an impedance value of \(Z\approx10\,\Omega\) at 40 Hz [30] in depletion, there is the need for an adapted experimental set-up that matches the above value. This ensures the zero-current condition necessary for \(V_B\) monitoring with an oscilloscope.

A schematic of the new system is depicted in Figure 2.17. The triangular \(V_G\) signal is now sourced by an arbitrary waveform pulse generator (Agilent 33250A) directly connected to the
The comparison between the transient and quasi-static body potential is depicted in Figure 2.18. The static drain current is also presented as reference. The transient out-of-equilibrium body potential shows an increase in value with the scanning speed. On the reverse scan, the value is slightly increased. In both cases, the return to the equilibrium happens at higher $|V_G|$, as expected from the transient $I_G$ which showed the same trend (Figure 2.13b). During inversion or accumulation, both static and transient $V_B$ signals return to the equilibrium $V_D/2$ value. The transient $V_B$ shows a small shoulder during the forward and reverse scan during the drop. These results validate our experimental set-up for dynamic $V_B$ measurement.
Chapter 2: Transient measurements in the pseudo-MOSFET configuration

Figure 2.18: Drain voltage and body potential versus gate voltage. For the transient experiments, an SS=0.416 V/s was chosen. The equivalent sweep period in the quasi-static experiment is $T=24s$.

The effect of the scanning speed on the transient $V_B$ response is traced in Figure 2.19. The raw data as captured by the oscilloscope are presented in Figure 2.19a. Evidently, the traces are very noise due electronic circuit (constructed on a circuit board) which probably creates open loops. At this stage of the development we search for an easy fix for this issue. Thus instead of improving the electronics, we filtered the data as explained in the appendix A. This step was necessary for reducing the measurement noise and reveal the trend of the out-of-equilibrium body potential for various scanning speeds. The dynamic $V_B$ character is verified in transient measurements also, since the values of the body potential increase with SS. As for $I_G$ (Figure 2.15a), the return to equilibrium occurs at higher $V_G$ values. For SS=100V/s or higher, a shoulder appears during the return to the equilibrium and it is more pronounced during inversion. Previously in this chapter, the body potential drop was connected with the carrier injection. The body potential drop was associated with the injection of carriers in the Si film. The appearance of the shoulder signifies that the injection of carriers might occur in two steps probably due to the damage caused by the contacts.
Chapter 2: Transient measurements in the pseudo-MOSFET configuration

Figure 2.19: Raw data in (a) and filtered curves in (b) of the transient body potential measured with the new experimental set-up depicted in Figure 2.17. Drain voltage was set to 100mV.

2.3. Conclusions

In the literature, the pseudo-MOSFET configuration with pressure controlled probes usually aimed to the fast SOI characterization and a wide range of measurements and methods were adapted for the estimation of important parameters such as mobility and threshold voltage. The majority of the developments were focused on quasi-static curves. An out-of-equilibrium body potential was reported during quasi-static measurements, similar to what is observed in double-gate FD-SOI MOSFETs. Some papers showed also the possibility to extend the pseudo-MOSFET to sensing applications exploiting both $I_D$ current and out-of-equilibrium body potential versus $V_G$ but they were only measured in quasi-static conditions. To really profit from the transient body potential response, $V_B$ must be monitored in an experimental set-up adapted for transients. Here, the transient response of the device was studied with triangular ramps with various frequencies applied directly to the back-gate of the SOI.

The analysis started with a comparison between the quasi-static and transient $I_D$ and $I_G$ currents. During the transient measurements and for scanning speeds lower than 20V/s, the measured $I_D$ is similar to the quasi-static one. For higher scanning speeds a deformation of the drain current is observed. This change in the shape of $I_D$ is related to the huge displacement current $I_G$ which appears during the transients. The $I_G$ plateau current, present during the transient experiments, is associated with the BOX capacitance. A simple analytical model derived from the inversion charge equation of SOI MOSFETs confirmed the origin of the $I_G$ plateau.
The voltage amplifier of the set-up ensures the accurate potential measurement thanks to its huge input impedance, ensuring a zero-current condition for the body contact. Most importantly, it demonstrates the ease of potential measurements compared to the currents which require a full analyser. This is an indication for easy system integration and development of portable devices based on the transient $V_B$.

This chapter was focused on the implementation of the transient set-up for $V_B$ monitoring. Before moving towards the applications, it is essential to understand the origin of the out-of-equilibrium body potential to optimise it later for device sensing. Having the experimental findings as a reference, we proceed to TCAD simulation in the next chapter to really get an insight on the mechanism that provokes the effect.
Chapter 2: Transient measurements in the pseudo-MOSFET configuration

References


Chapter 2: Transient measurements in the pseudo-MOSFET configuration


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Chapter 3: Transient TCAD simulations with a novel pseudo-MOSFET structure

Table of contents of the chapter

3.1 Introduction..................................................................................................................50
3.2 Simulation strategy in this thesis ..............................................................................51
3.3 Simulations with a novel structure...........................................................................54
   3.3.1 Drain current versus gate voltage response.......................................................54
   3.3.2 Contact specifications and transient \( V_B \) response.......................................56
3.4 Comparison with experimental results.......................................................................58
   3.4.1 Transient gate current .......................................................................................58
   3.4.2 Transient body potential ...................................................................................59
3.5 Body potential dependence on the contact properties.............................................60
   3.5.1 Contact size effect on \( V_B \) ............................................................................60
   3.5.2 Contact insertion inside the silicon film............................................................63
   3.5.3 Effect of the silicon thickness on \( V_B \) ...............................................................65
   3.5.4 Impact of the BOX thickness on the out-of-equilibrium response.................65
   3.5.5 Effect of the substrate .......................................................................................66
3.6 Impact of channel-related parameters on the dynamic response .........................67
   3.6.1 Effect of the excess silicon ...............................................................................67
   3.6.2 Effect of the channel length ............................................................................68
3.7 Effect of electrical parameters on the \( V_B \) response...............................................69
   3.7.1 Effect of the mobility .......................................................................................69
   3.7.2 The effect of the interface state densities on the \( V_B \) .....................................70
3.8 Conclusions................................................................................................................73
While the pseudo-MOSFET contacts are metal-semiconductor junctions, they are frequently characterized as ohmic contacts. Although this approximation is a practical solution in certain cases, it leads to simulation difficulties. This chapter proposes an innovative simulation structure for transient simulations of the pseudo-MOSFET, focused on the recreation of the out-of-equilibrium body potential.

3.1 Introduction

As previously seen, the pseudo-MOSFET technique was developed for wafer characterization. The models and methods developed are mainly focused on the extraction of useful electrical parameters for the SOI [1]. However, the contacts with pressure-controlled probes are not fully understood and therefore cannot be easily simulated. Previously published pseudo-MOSFET articles aimed on specific problems such as D\text{it} [2]–[4], surface potential [5] or noise [6] modeling. They used valid assumptions to achieve their objectives, but they did not provide a full description of the contacts. An extensive simulation study of a 3D pseudo-MOSFET was realised with metal contacts of various workfunction values [7]. A comparison between the simulated and the experimental curves of the above study is illustrated in Figure 3.1. While this approach accurately simulates the two currents in the pseudo-MOSFET, it completely eliminates the depletion region, in which the transient body potential appears.

![Figure 3.1: Drain current and transconductance versus gate voltage: a) measurements with a classic pseudo-MOSFET and b) simulations with a 3-D structure with metal contacts [7].](image)

On one hand, the ohmic contact behaviour observed experimentally has been attributed to defects under the probes [2], [8] or phase transformation induced by nanoindentation in the silicon film [9]. On the other hand, other drain-current-focused studies investigate the effect of the Schottky contact [10] or use it in simulations [11]. Within this uncertain context, an
implementation of ohmic contacts with pressure controlled probes allowing both electron and hole transport is not straight-forward in commercial simulation tools.

In this chapter, we explore a novel architecture for TCAD simulations of the pseudo-MOSFET (section 3.2), with focus on the transient response (section 3.3). The simulation results are benchmarked with experiments in section 3.4. Sections 3.5 and 3.6 are dedicated to the study of the effect of some geometrical and physical parameters on the simulated $V_B$.

### 3.2 Simulation strategy in this thesis

Our objective is to identify a structure which can recreate the injection of both carrier types in the pseudo-MOSFET configuration with a single simulation. The first approach tested in this thesis was the use of metal contacts with various workfunction values in 2D structures simulated with Synopsys-Sentaurus TCAD [12] (Figure 3.2). Lombardi’s model with doping dependence was used for the mobility and Schottky boundaries were applied to the contacts. Two simulations are required, one for the drain current $I_D$ and one for the body potential $V_B$. For the later, a zero current condition was applied on the electrode on the right contact, named body in this case.

*Figure 3.2: Schematic of a 2D SOI with Schottky boundaries as source and drain/body contacts.*

Figure 3.3 illustrates the simulated drain current in (a) and body potential in (b) versus gate voltage calculated using the structure in Figure 3.2. One can notice that, even perfect metal/silicon contacts, without any Fermi level pinning [13], are not able to recreate the two currents (of electrons and holes) observed experimentally in the pseudo-MOSFET. Depending on the workfunction of source and drain, either a current of holes or electrons is formed. In the case that the metal workfunction being close to one of the silicon, the two types of currents is provided and the simulation shows an ambipolarity as in the experiments. However, the current values are low compared to the ones measured with the pseudo-MOSFET response (in the order of magnitude of 100pA in Figure 2.3a). Additionally, Figure 3.3b confirms that the metal
contacts are not suitable for our purpose since the $V_B$ response shows a potential increase but not a return to the equilibrium value, unlike the experimental results (Figure 2.9b).

Figure 3.3: Simulated drain currents (a) and body potential values (b) versus gate voltage for the 2D structure in Figure 3.2 with two Schottky contacts with various workfunction values as source and drain terminals. The contacts were placed on the top Si surface.

A second simulation approach would be the combination of simulations with $N^+$ and $P^+$ doped-regions as source and drain to recreate separately the effect of electrons and holes, adding the two simulated curves yields the full characteristic. This strategy is effective for describing the static currents for example, $I_D-V_G$ or $I_D-V_D$ as shown in [14]. As previously said, the transient phenomena occurring in the depletion region which spreads from the end of accumulation to the beginning of strong inversion cannot be captured through this approach. Indeed, for $V_B$, it is mandatory to fully reproduce the response of the pseudo-MOSFET under transient conditions with a single structure. However, the idea of $P^+$ and $N^+$ doped regions is interesting and a combination might describe accurately the depletion region, where $V_B$ manifests itself. Based on that, another approach to describe the transient response was firstly introduced by our group [15] with $P^+$ and $N^+$ regions simultaneously defined inside the silicon film. While a recreation of the potential was achieved the shape of the potential did not capture the experimental $V_B$ variation correctly. Here, we start the highly doped regions and we proposed a novel architecture to identify the problems, solve them and provide physical insight for the origin of the transient body potential.
Novel simulation structure

Normally, the pseudo-MOSFET has a 3D geometry which demands more computational resources and time. Therefore, we preferred a 2D planar geometry in this thesis and our aim was to understand the transient phenomena rather than looking for one-to-one fitting with the experimental curves.

Figure 3.4 shows the simulated structure based on SOI with an 88nm Si film thickness on a BOX of 145nm thickness. In order to obtain a simulated structure that approaches the experimental one each pressure controlled probe was defined as a highly doped silicon, with carrier concentration $N_D=10^{20} \text{cm}^{-3}$, divided in two regions, one $P^+$ and the other $N^+$. The contacts are placed on top of the Si film as in the pseudo-MOSFET configuration. To keep a reasonable amount of calculation points while we maintain a relatively dense mesh, the distance between the inner edges of the contacts $L_{ch}=1 \mu m$ (instead of 1mm in the experimental set-up). The contacts are placed on top of the device to mimic the pressure contacts of the experimental configuration. The total length of the simulated device is made of the contacts length $L_C$, the distance between their inner edges $L_{ch}$ and 10% of $L_{ch}$ (supplementary length added on the left and right of the contacts). The addition of the latter is an attempt to simulate more accurately the pseudo-MOSFET configuration in which excess of Si is present “outside” the contacts. Additionally, the substrate effects were considered by the addition of bulk silicon region under the BOX with a thickness of a $t_{sub}=1.2 \mu m$. This value was chosen to exceed the space charge region which for the lightly doped silicon of the wafers used, was calculated to $\approx 900nm$. The simulations in this chapter are based on this structure and all of its geometrical parameters will be examined here one by one in the next sections.

Figure 3.4: Schematic of the pseudo-MOSFET experimental configuration and novel simulation structure, with doped source and drain, to emulate the source and drain contacts obtained experimentally with controlled pressure probes.
Another important aspect of the structure is the sequence of the highly doped regions that replace the pressure contacts. Thus in the next section, all the possible combinations are examined in terms of drain current and body potential. The final selection of the structure will be based on the benchmark between the simulated data and the experimental results.

### 3.3 Simulations with a novel structure

For the simulations of this chapter, the drain voltage $V_D$ was set to 0.1V and the source was grounded ($V_S=0V$), while a linear ramp was applied to the gate electrode, scanning from accumulation ($V_G<0$) to strong inversion ($V_G>0$) with a slope of 20 V/s. Default models were selected for the contacts: ohmic boundary conditions between electrodes and highly doped regions were applied. For the carrier mobility, the Lombardi model with doping dependence (for the inclusion of the vertical field) was used in all the simulations.

#### 3.3.1 Drain current versus gate voltage response

The first group of contacts (Figure 3.5a) contains the highly doped N$^+$ and P$^+$ regions which are mirrored with respect to the center of the device, named NP-PN and PN-NP respectively. Figure 3.5b illustrates the corresponding simulated $I_D$-$V_G$ curves. Clearly, this contact sequence benefits one type of carriers over the other. NP-PN contacts produce a very steep subthreshold slope for holes while PN-NP structures a very steep slope for electrons. This improved switching performance is accompanied also by higher ON-current. This behaviour originates from the highly doped regions of the contacts which induce band bending of the undoped Si film underneath. This way, an N$^+$ region creates a barrier for the holes along the structure leading to a degraded subthreshold slope. The same is true for the effect of P$^+$ regions on the electron current. So, none of these two structures is appropriate for both e$^-$ and h$^+$ in the experimental pseudo-MOSFET.
Chapter 3: Transient TCAD simulation with a novel pseudo-MOSFET structure

Figure 3.5: Schematic of the simulated structures with mirrored doping regions with respect to the centre of the device, b) simulated $I_D-V_G$ for mirrored contacts, $V_D=0.1V$ and $L_C=0.5\mu m$.

The second possible arrangement of the contacts corresponds to alternating highly doped regions (Figure 3.6a): PN-PN or NP-NP. Figure 3.6b, shows the corresponding $I_D-V_G$ curves, which are clearly similar to the experimental ones: both electron and hole currents are visible and they have similar subthreshold slopes. The difference between the ON current values for holes and electrons is very small. The ratio of these ON currents was found to be around 3 ($I_{ON,electrons}/I_{ON,holes}\approx3.45$), similar to the ratio of electron and hole mobility ($\mu_{electrons}/\mu_{holes}\approx3.11$). Note that, in the pseudo-MOSFET also $I_{ON}$ for electrons is higher than for holes but, additionally to the effect of the mobility on the channel conductivity one should also consider the difference in the series resistance for the two carrier types (see chapter 2). The alternating contacts show similar trends with the experimental pseudo-MOSFET characteristics in terms of $I_D-V_D$ curves presented in the appendix B. Therefore we will use alternating contacts for the $V_B$ evaluation.

Figure 3.6: a) Schematic of the simulated structures with alternating doping for the contacts. b) Simulated $I_D-V_G$ for alternating doping contacts, $V_D=0.1V$ and $L_C=0.5\mu m$. 
3.3.2 Contact specifications and transient $V_B$ response

In the experiments, $V_B$ is monitored with a third probe placed between the source and drain contacts. In the simulations, a similar approach is not applicable since third probe would definitively introduce another “barrier” for the carriers halfway between the contacts affecting the conductivity of the structure. This is one of the drawbacks of simulating a 2D architecture compares to the 3D in experiments. Hence, for the $V_B$ monitoring a zero-current condition was imposed to the right contact of the structure (similarly to Figure 3.2). As a result, two individual simulations are required for the whole description of the response: 1) the right contact is used for the body potential with the-zero current condition and 2) the right contact is used for the drain current with a $V_D=0.1\text{V}$.

In Figure 3.7, the simulated transient body potential and gate current are presented for the alternating contacts for the forward and the reverse scan directions. Interestingly, both structures with alternating contacts can reproduce the out-of-equilibrium body potential and the displacement $I_G$ current. However, each one of them is accurate for either forward or reverse scanning direction. Since the carriers can only be injected through the source contact, each structure will be appropriate for only one direction simulation. To clearly illustrate this, we consider the results of the NP-NP structure of Figure 3.7a. The carriers injected in the Si film under the N$^+$ part of the source contact are blocked by the depletion region due to the space charge region in the Si film under the P$^+$ part of the contact. Thus, lack of e$^-$ creates an out-of-equilibrium $V_B$ response in the forward scan. However, for the reverse scan direction, the injection of holes (or evacuation of electrons) in the film, governed by the P$^+$ type region, is not affected by the N$^+$ type region (Figure 3.7b) since it is not blocking the access of holes to the rest of the Si film. So no out-of-equilibrium is observed in the reverse scan with this structure.

Thus, only one scanning direction can be reproduced per simulation structure. While this outcome is not ideal, it opens new opportunities on the theoretical understanding of the transient body potential through simulations.
Before we move forward, we first evaluate the relation between $I_G$ and $V_B$ in the simulations. The connection of the out-of-equilibrium body potential with the $I_G$ displacement current is well defined in FD MOSFETs [16]:

$$\frac{I_G}{C} = \frac{\Delta (V_G - V_B)}{\Delta t} \Leftrightarrow \frac{\Delta V_B}{\Delta t} = \frac{\Delta V_G}{\Delta t} \frac{I_G}{C} \Leftrightarrow I_G \propto \Delta V_B$$

(3.1)

where $C$ is an adjustment capacitive coefficient. Figure 3.8a presents the $I_G$ and the derivative of $V_B$. The two traces have a similar shape but the values are very different since $I_G$ was not normalised by any capacitive coefficient $C$. Regardless of the mismatches between 3D experimental structure and the 2D simulation with only two contacts, the relation (3.1) remains true. This further confirms that the simulated effect corresponds to the out-of-equilibrium body potential.
Chapter 3: Transient TCAD simulation with a novel pseudo-MOSFET structure

Additional insight is provided through $V_B$ when plotted in a log scale (Figure 3.8b). The trace reveals that the carrier injection (corresponding to the peak of $I_G$) is a two-step process. Firstly the abrupt drop of $V_B$ ($\sim V_G=2V$) corresponding to the return to the equilibrium is evidenced. This drop is associated with the injection of carriers for $C_{BOX}$ charging, as explained in chapter 2 and proven in [15]. Secondly, an exponential decrease of $V_B$ is observed as the gate voltage increases. This seems to be in agreement with the exponential increase of the inversion charge during the inversion regime.

![Figure 3.8: a) Simulated $I_G$ and derivative of $V_B$. b) Simulated $I_G$ and $V_B$ in log scale for $SS=20V/s$ produced by NP-NP structure with $V_G$ scan from accumulation to inversion.](image)

As the last step of validation of the proposed simulation structure the calculated curves will be benchmarked with the experimental ones in the next section.

3.4 Comparison with experimental results

For the validation of the simulation with the experimental set-up we will focus on the out-of-equilibrium body potential and the transient gate current. The following analysis starts with $I_G$ since its plateau region was identified as a capacitive induced current in chapter 2 and it should be easy to correlate with the simulation results.

3.4.1 Transient gate current

The comparison is restricted to the forward scan. A triangular ramp scanning from -10V to 10V was applied to a NP-NP structure to recreate the curves. For the simulation in this section, the largest contacts ($L_C=0.5\mu m$) were selected to amplify the transient effects (the selection of $L_C$ was made to get a strong transient response and it will be justified later in this chapter). The $I_D-V_G$ curves for various scanning speeds are depicted in Figure 3.9. The scanning speed values were chosen to match the experimental ones. The simulated curves (Figure 3.9a) exhibit the
same trend as the experimental ones (Figure 3.9b). However, the simulated values are significantly lower compared to the real measurement. Considering that no $V_D$ is applied in the simulation, the gate current corresponds to the displacement current, associated with $C_{BOX}$, and it is therefore, proportional to its area. Thus, the simulated curves are severely impacted by the significantly smaller simulated area. To support this argument, we normalize the simulated and experimental curves with respect to the corresponding total silicon areas and plot them in Figure 3.9b. Observe how the curves are almost perfectly superposed at the equilibrium regions, verifying the above assumption. However, the $I_G$ seems to follow a different path during the increase when compared to the experiments. This highlights the difference between the metal probes and the simulation contacts with $P^+$ and $N^+$ doped regions. Note that, a fine tune of the contact doping and length might lead to a perfect superposition of the two curves.

![Figure 3.9: a) Simulated gate current with respect to gate voltage, for various scanning speeds and b) comparison between simulated and experimental current densities. The inset in (b) presents the curves for SS=20V/s, which have a different scale with respect to the other scanning speeds.](image)

### 3.4.2 Transient body potential

One of the most interesting experiments of the last chapter was the effect of the scanning speed on the transient phenomena. Thus, we recreated it with simulations.

As said previously, in the simulation environment, adding a third contact between source and drain induces an extra barrier for the carriers in 2D and it changes the configuration. Thus the drain is replaced by the body contact. The evolution of $V_B$ curve with respect to $V_G$ for various scanning speeds is presented in Figure 3.10 for both the experiments preformed in chapter 2 and the simulations of this chapter. Clearly the simulations reproduce well the experimental data. The increase of the scanning speed translates into an increase of the out-of-
equilibrium response. Like in experiments, the simulated body potential also drops to higher $V_G$ as the SS increases. This was anticipated from the evolution of the $I_G$ in the previous section.

Contrary to the experiments, the simulated curves do not show any shoulder during the return to the equilibrium for high scanning speeds. This is probably related to the contact configuration in the 3D experiment and the 2D simulation. Indeed, a major difference between simulations and experiments is the excess silicon “outside” the contacts. As the drop is connected with the carrier injection, it seems possible that the injection happens in two stages in the experiments and is most likely associated with the large distance that the carriers have to travel beyond the body contact. While there is not enough evidence to support this argument here, devices with metal contacts described in the next chapter will support this assumption.

![Figure 3.10: Body potential with respect to gate voltage for various scanning speeds a) measurements and b) simulated results.](image)

### 3.5 Body potential dependence on the contact properties

Now that the novel simulation structure is validated, we exploit the strengths of simulations and explore the effect of various geometrical parameters on the occurrence of the out-of-equilibrium body potential.

#### 3.5.1 Contact size effect on $V_B$

In the experimental configuration, different diameter contacts can be equipped in the Jandel station with the pressure controlled probes. In our experiments, the installed probes had a diameter of 30μm, which is significantly bigger than the simulated ones. To test whether or not the contact size could affects the simulation, the out-of-equilibrium body potential $V_B$ and the displacement current $I_G$ are plotted in Figure 3.11a and Figure 3.11b respectively. For very
short contacts the body potential does not manifest itself but it increases drastically with $L_C$. The associated $I_G$ increases similarly with the body potential. The $I_G$ peak, which is related to $V_B$ increases in value and shifts towards higher $V_G$ values for longer contacts. Previous studies showed that the current corresponds to the charge of BOX capacitance [17], confirmed also experimentally in chapter 2. Notice that the contact length also changes the total length of the device hence, to isolate the influence of the device length from capacitive effects, we included in the graphs a simulation with $L_C$=0.3μm but with extended silicon area on the sides of the device so the area can match the area of the structure with $L_C$=0.5μm. The simulated curves show that the out-of-equilibrium body potential also depends weakly to the total capacitance of the device since we notice a small increase of the $V_B$ for the same contact length but larger device area.

![Figure 3.11: Simulated a) $V_B$-$V_G$ and b) $I_G$-$V_G$ curves for NP-NP structure for various contact sizes and areas.](image)

However, it seems that $V_B$ originates from the contact, since devices with different areas and the same contact length have comparable potential response while an increase of 0.2μm of contact length on the same SOI has almost two time stronger $V_B$ signature. It is evident that the plateau $I_G$ current is a function of the device area only, since devices with constant area and different $L_C$, have the same $I_G$ plateau values in strong inversion and accumulation. This further supports the modeling of chapter 2 in which we have connected the plateau of $I_G$ with the BOX capacitance. The body potential depends strongly on the contact length as illustrated in Figure 3.11a.

The increase of the $V_B$ value is associated with the nature of the emulated contact which seems to affect the undoped Si under them. Figure 3.12 shows the space charge region...
distribution in the Si channel for four \( V_G \) values, two of which correspond to the linear increase (out-of-equilibrium) and two on the drop of \( V_B \) (return to the equilibrium). Under specific conditions, a space charge region is created under the inner highly doped contact and it blocks the instant injection of carriers in the rest of the silicon film, like an electrostatic barrier. As the contact length increases the space charge region is increasing proportionally. As a result, the body potential increases, following the \( V_G \) variation. The increase of \( V_G \) modifies the space charge region under the \( N^+ \) region of the contact and at a given \( V_G \) value, the barrier drops and allows the rapid injection of carriers in the film resulting in a spike on the displacement current and a sharp drop of \( V_B \). This argument implies that the threshold voltage (\( V_T \)) of the device increases with \( L_C \) which is noticed also on the \( I_D-V_G \) curves (Figure 3.13).

Figure 3.12: Space-charge region contours of a simulated structure with \( t_{Si}=88\text{nm} \) and \( L_C=0.3\mu m \) (as in Figure 3.11). The gate voltages correspond to the linear increase and the drop of the body potential. The white line is the junction line.

Figure 3.13 presents the drain current characteristics for the simulated structures with different contact length. Notice how the threshold voltage increases with \( L_C \). This is in agreement with the Figure 3.11a since the \( V_B \) drop is associated with the carrier injection for the formation of the inversion channel. A similar effect was simulated with metal contacts in [10].
Chapter 3: Transient TCAD simulation with a novel pseudo-MOSFET structure

3.5.2 Contact insertion inside the silicon film

As demonstrated in [8], the pressure-controlled probes are damaging the silicon at the area of impact and also affect electrical parameters such as access resistance and mobility. On the contrary, in the simulations all the interfaces are perfect and well defined. In an attempt to implement some of the experimental aspects, the contact depth $T_{\text{depth}}$ was investigated in our structure. $T_{\text{depth}}$ is defined as the depth at which the contacts penetrates inside the Si film measured from its top surface. A schematic of the simulated structures for this comparison is presented in Figure 3.14.

![Figure 3.14](image)

**Figure 3.14:** Schematic representation of contacts penetration in the silicon film to mimic the experimental pseudo-MOSFET with pressure controlled probes.

Figure 3.15 illustrates the simulated $V_B-V_G$ (Figure 3.15a) and $I_G-V_G$ (Figure 3.15b) curves for contact insertion of 0nm, 22nm, 44nm and 66nm in the Si film. The contact length was kept constant at 0.1μm. The case of 0nm insertion of contact has already seen previously (Figure 3.13).
3.11) and for the short contact length the out-of-equilibrium body potential was not visible. However, the simulated results reveal that as the contact approaches the BOX, the dynamic phenomena are significantly enhanced even for this short length. The simulation suggests that the origin of the mechanism, which prevents the instant carrier injection, is related to the electrostatic interaction between the voltage imposed by \( V_G \) through the BOX and the source contacts (space charge region formation under the contacts). The results of the simulations are an additional proof that the “barrier”, which blocks the carriers, in our structure stems from the space charge under the contacts. As the \( N^+ \) region approaches the Si/BOX interface, the depleted area underneath blocks the carrier transport. Considering the fixed potential on the \( N^+/p \) Si interface under the contact, it is also harder to impose favourable conditions for the Si under it to become conductive. Consequently, the Si film remains depleted for higher \( V_G \) values and the \( V_B \) strengthens.

![Figure 3.15: Simulated a) \( V_B-V_G \) and b) \( I_G-V_G \) curves for NP-NP structure for \( L_C=0.1\mu m \) and various contact depths.](image)

Until now, we presented two parameters directly related to the contact (\( L_C \) and \( T_{\text{depth}} \)). However, the space charge region is also controlled by the gate voltage applied to the substrate. Consequently, if the voltage drop in the bulk of the wafer varies, this will significantly affect the response. Thus, the impact of the silicon film and BOX thickness are included and will be discussed in subsections 3.5.3 and 3.5.4.
3.5.3 Effect of the silicon thickness on \( V_B \)

Figure 3.16 depicts the simulated body potential and gate current versus gate voltage for various silicon film thicknesses. For this simulation, the contact length was fixed at \( L_C=0.3 \mu m \), to ensure that the full response is reproduced within the same \( V_G \) range as in the previous experiments. As the film thickness decreases, the transient response is amplified both in potential and current. The increase is similar to the one observed in section 3.5.2. Since the same outcome is achieved for thinner films and for contacts approaching the BOX/Si interface, one can conclude that the major impact stems mainly from the contacts. This further supports the previous explanation, based on space charge region. The last parameter to be examined for the proof of the suggested theory arrived from the simulations with various BOX thicknesses in the next section.

![Simulated body potential and gate current](image)

*Figure 3.16: Simulated a) \( V_B-V_G \) and b) \( I_G-V_G \) curves for NP-NP structure for \( L_C=0.3 \mu m \) and various Si thicknesses.*

3.5.4 Impact of the BOX thickness on the out-of-equilibrium response

To demonstrate the influence of the BOX thickness \( (t_{BOX}) \) on the dynamic out-of-equilibrium phenomena, a structure with \( L_C=0.5 \mu m \), to assure that we have a strong \( V_B \) signature, was considered. The BOX thicknesses were set to 30nm, 70nm, 145nm and 200nm. Figure 3.17a depicts the evolution of \( V_B \) in the studied structures.

The out-of-equilibrium \( V_B \) response is stronger and occurs at a wider \( V_G \) range as the BOX thickness increases. This result was anticipated for the \( V_B \) response and agrees with the explanation based on the space charge region in the Si between \( N^+ \) and BOX interfaces. As the BOX thickness increases, the control of \( V_G \) over the Si region weakens and consequently the lowering of the “barrier” through the BOX becomes more challenging. As a result, \( V_B \) drops...
for higher voltages. The response of the gate current (Figure 3.17b) is slightly more complex to understand since the displacement current values are defined by the BOX capacitance which changes radically. This is evident through the plateau current in the equilibrium regimes; which is increasing as \( t_{\text{BOX}} \) decreases (capacitance increases) for the same SS. Lastly, for the forward scan in this simulations, \( t_{\text{BOX}} \) affects \( V_G \) at which the device is driven into accumulation. For thinner BOX the plateau is reached at higher \( V_G \) values. A possible explanation for that is; as the capacitance increases, more charge is needed under the BOX and since electrons are minority carriers in the substrate, more time is required for them to reach the other end of the capacitor.

![Figure 3.17: Simulated a) \( V_B-V_G \) and b) \( I_G-V_G \) curves for NP-NP structure for \( L_e=0.5\mu m \) and various BOX thicknesses.](image)

**3.5.5 Effect of the substrate**

To illustrate the importance of the voltage drop in the low doped bulk gate material on the phenomenon of interest, the bulk of the structure under test was removed and the results are presented in Figure 3.18a. \( V_B \) seems to have stronger values when the substrate was included and also drops for higher \( V_G \) values. Additionally, during the increase, the linear behaviour seems slightly distorted for the structure with the substrate. This indicates that the slope of \( V_B \) is also affected by the bulk capacitance. Concerning \( I_G \), Figure 3.18b shows that the step for \( V_G<8V \) regime stems from the substrate. \( I_G \) peak is shifted slightly towards smaller \( V_G \) values, as anticipated from the \( V_B \) response. The plateau current stays unaffected since it is only defined by the BOX capacitance.
Chapter 3: Transient TCAD simulation with a novel pseudo-MOSFET structure

3.6 Impact of channel-related parameters on the dynamic response

3.6.1 Effect of the excess silicon

The extension of the silicon film was set in the configuration in order to emulate more accurately the experimental configuration where the probes are in the center of the die, far from the edges. A schematic illustrating this parameter is depicted in Figure 3.19.

Figure 3.19: Schematic of two structures with different excess Si part beyond the contacts.

The influence of the additional Si part seems to be negligible for the transient phenomena, as illustrated by Figure 3.20. As presented in Figure 3.20a, although the body potential has slightly increased values for bigger devices, the $V_B$ drop is fixed at a certain $V_G$ value. Similar behaviour is noticed for the displacement current. We can conclude that the excess silicon area...
can increase the transient behaviour since it is connected to the total capacitance of the device but it seems to have small influence on the body potential response.

![Figure 3.20: Simulated a) $V_B$-$V_G$ and b) $I_G$-$V_G$ curves for NP-NP structure for $L_C$=0.5μm and various excess silicon lengths aside of the emulated contacts.](image)

### 3.6.2 Effect of the channel length

The simulation results in Figure 3.21 depict the effects of the channel length on the dynamic phenomena. For this simulation, the contact length remains at $L_C$=0.5μm while the channel length was modulated from 1μm to 3μm. As expected from the previous results, a similar effect as the excess silicon is evidenced. However, there is a noticeable deviation on the $V_B$ drop with the channel length. As the channel length increases, the slope of the $V_B$ drop decreases slightly. For the practical application of this structure, this is a favourable outcome since the effect of increase of Si area for sensing will not affect the transient response strongly.
Figure 3.21: Simulated a) $V_B$-$V_G$ and b) $I_G$-$V_G$ curves for NP-NP structure for $L_C=0.5\mu m$ and various channel lengths. Extension regions 0.1-$L$.

Since we have illustrated the effect of the technological parameters on the body potential signature we can now continue investigating the effect of electrical parameters (mobility and interface state density).

## 3.7 Effect of electrical parameters effect on the $V_B$ response

### 3.7.1 Effect of the mobility

This section shows the effect of the mobility on the occurrence of the body potential. To isolate the effect of the top Si film, the following simulations were performed in a structure without silicon substrate and the bias was applied directly under the BOX. The definition of a mobility value in Sentaurus TCAD demands the selection of the constant mobility model. This means that the rest of the mobility models have been deactivated. Figure 3.22 depicts the transient body potential in (a) and the transient gate current in (b) for various electron and hole mobility values. For these simulations, the selected mobility values correspond to the default values proposed by Centaurus and to the experimentally estimated ones from the data of chapter 2. One additional value for holes and electrons was simulated as an intermediate step. The body potential response in Figure 3.22a strengthens as the mobility decreases. In the case of reduced electron mobility the response increases for the same $V_G$ and the return to the equilibrium occurs at higher $V_G$. When the hole mobility is reduced, the body potential exhibits the linear increase at lower $V_G$ values. Notably, the simulated curves indicate that the starting point of the linear increase is a function of the holes and the drop a function the electron mobility, while the slope itself is independent of the mobility values. The $I_G$ peak seems to
increase in value when the carrier mobility decreases and shifts towards positive $V_G$ for lower electron mobility values. Clearly, the out-of-equilibrium response is a combined holes and electrons effect that depends on their transport from the contact towards the rest of the silicon film. Finally, the phenomenon manifests itself regardless of the activated mobility models (constant mobility here and including the vertical field dependence for the rest of the simulations), showcasing that any dependence on the vertical electric filed component is negligible for the appearance of $V_B$.

Figure 3.22: Simulated body potential (a) and gate current (b) with respect to gate voltage and for various electron and hole mobility values. The scanning speed was set to 20V/s.

3.7.2 The effect of the interface state densities on the $V_B$

Another parameter that can benefit from a TCAD analysis compared to experiments is the interface trap density. For SOI with thin Si films, the interface states on the top can strongly affect the performance of the wafer [18]. While imposing an exact value of interface state densities is almost impossible experimentally, their effect can easily be captured through TCAD simulations. For the analysis of this section, only the two Si interfaces of the film are considered and the substrate/BOX one was omitted. In each boundary both donor and acceptor types of traps were defined with the same properties described in [2]. Figure 3.23 depicts the body potential and corresponding $I_G$ curves with respect to the applied gate voltage for various interface trap densities at the top Si. For relatively low trap densities, the body potential follows the same path for its increase and drop while weakens in value. As the traps density reaches $10^{12}\text{cm}^{-2}\text{eV}^{-1}$ the $V_B$ shape starts to be distorted and a second peak seems to appear. Additional the return to the equilibrium seems to occur at lower $V_G$. Similarly, the gate current has a slight decrease in the maximum value for low trap density and a small increase in value during
depletion for higher densities. This is very promising for sensing applications since $V_B$ seems to be sensitive to the top interface.

![Graphs showing body potential and gate current versus gate voltage for various interface trap densities.](image)

**Figure 3.23:** Body potential (a) and gate current (b) versus gate voltage for various interface trap densities at the top of the Si film. The scanning speed was set to 20V/s.

Since in the pseudo-MOSFET configuration the conduction takes place on the Si/BOX interface, we examine also the effect of the traps here. Figure 3.24 illustrates $V_B$ and $I_G$ versus $V_G$ for various interface traps densities at the Si/BOX substrate. While the trend on the body potential and gate current is similar to traps placed on the top interface, the effect is more pronounced when the defects are placed on the back interface. Considering that the conductive path on the inverse MOSFET structure is formed close to the back interface, this result was anticipated. However, the previous studies in this chapter indicate that the $V_B$ response is provoked by the creation of a space charge region which blocks the injection of carriers in the Si film. Consequently, there are two possible explanations for this tendency: 1) the space charge region formed under the N$^+$ region of the contact, weakens towards the Si/BOX, establishing the effect of traps more pronounced and 2) the traps actually release carriers into the Si film compensating for the lack of carriers in the channel and suspending the out-of-equilibrium response.
Lastly, the combined effect of the traps is illustrated in Figure 3.25 that depicts the body potential and gate current curves simulated for various interface trap placed on both top and bottom interfaces. The effect is enhanced in this case, as expected. However, one can observe that if the Si film/BOX interface quality is low, the $V_B$ shape deforms for the lower density of traps ($5 \times 10^{11} \text{ cm}^{-2}\text{eV}^{-1}$) and might lead to a total suppression of the effect for higher values. Finally, the dynamic character of the out-of-equilibrium body potential combined with the dynamic response of the traps and the interface coupling in thin films demands an extensive study on the other parameters, such as SS and Si film thickness to fully capture the effect. Here, we only showed a quick presentation of the effect of interface traps densities in order to identify them in the experimental curves during the development steps later. A more extensive study of the density of states impact is necessary to understand in depth the mechanisms involved.
Conclusions

In this chapter, a novel TCAD simulation structure for the study of the out-of-equilibrium body potential was validated. The pressure controlled probes of the pseudo-MOSFET were emulated thanks to two highly doped P$^+$ and N$^+$ regions used for each contact and placed on top of the Si film. Using these contacts, the simulations can accurately reproduce the $I_D-V_G$ curve, from accumulation to inversion, with a single device.

Special attention is required on the contact definition since the sequence of the highly doped regions (mirrored or alternating N$^+$P$^+$ ones) strongly affects the simulation results. For this reason two groups of contacts were benchmarked using $I_D-V_G$ curves to identify which structure behaves similarly to the experiments with the pseudo-MOSFET configuration. While all the contacts reproduced both holes and electrons current as in pseudo-MOSFET, the mirrored sequences (PN-NP and NP-PN) show a drain current which favours one type of carrier over the other, by producing steeper subthreshold slopes. On the other hand, alternating highly doped P$^+$ and N$^+$ regions (NP-NP and PN-PN), produce $I_D-V_G$ curves very similar with the experimental data and they were preferred for the out-of-equilibrium body potential study.

The simulations with NP-NP and PN-PN contacts allowed to obtain the $V_B$ signature. However, each sequence reproduced only one of the scanning directions. Thus one should consider the appropriate structure for the study of phenomena appearing in the forward or reverse scan direction. The simulations strongly support that the origin of the out-of-equilibrium body potential is the space charge region under the P$^+$ or N$^+$ region which blocks...
the carriers from being injected in the Si film, similarly to a barrier that is modulated through $V_G$. Even if in the experiments the probes are metallic and not highly doped $P^+N^+$ silicon, this simulated structure reproduced well the measured curves. Both the $V_B-V_G$ and the $I_G-V_G$ show the same dependency on the scanning speed as in the experiments despite that the experimental device architecture is 3D within the mm size, while the simulated one is 2D with a channel length of 1$\mu$m. The displacement $I_G$ current is in perfect agreement with the accumulation and inversion regimes, while the $I_G$ peak seems to be adjusted through the properties of the contact (e.g. its length).

A simulation analysis of the impact of each technological/geometrical parameter was presented to further understand the body potential in the pseudo-MOSFET structure. It is evident that parameters that affect the properties of the contact such as the contact length, BOX and Si thicknesses or contact distance from the Si/SiO$_2$ interface modulate strongly the occurrence and intensity of the transient $V_B$. Contrary to the previous ones, parameters concerning the properties of the Si channel, like length of the Si film, leave the transient response relatively unaffected in depletion. For example, a change in the length of the device will affect the equilibrium displacement current in inversion or accumulation according to the BOX capacitance charging established in chapter 2, but only slightly the $V_B$ response. These results confirm that the barrier that limits the carrier injection is electrostatically controlled by the contacts and the applied voltages for a given physical structure. More specifically, for an $N^+P^+$ source contact in the forward configuration, the space charge region under $P^+$ side blocks the injection of electrons into the rest of the silicon film and prevents the inversion layer creation. When this $P^+$ region approaches the Si/BOX interface (either for thinner Si film or when the contact penetrates in the film), a higher $V_G$ is required to reduce the electrostatic barrier leading to $V_B$ enhancement. Similarly, thicker BOX, results in a $V_B$ increase since a higher voltage drop occurs between substrate and Si film and less potential is “available” for the barrier modulation inside the silicon film. Additionally, the dependence of $V_B$ to the electrons and holes mobility, fits well this interpretation. Lower mobility values strengthen $V_B$ and extend the $V_G$ range where $V_B$ manifests itself. This suggests that slower carriers require more time for their transport to the Si film leading to an increased potential response.

This chapter provided useful insights on the understanding of the transient body potential. The results show a strong dependence on the properties of the contact for the occurrence of $V_B$ in FD-SOI, while the size of the structure itself seems to have only a minor role. Additionally, small structures suppress the displacement current, which is excellent news for applications.
based on the out-of-equilibrium body potential since a miniaturization of the device in later development steps will produce weak displacements currents while maintaining a strong potential response.

Many parameters could be interesting to analyse for device optimization (i.e. doping level) however, the objective was not to fine-tune the structure but to provide the understanding before moving forward to the applications. In the next chapter, having in mind the impact of the technological parameters provided through these simulations, we focus our attention on the fabrication of SOI devices with deposited metal contacts and test their out-of-equilibrium body potential.
References


Chapter 3: Transient TCAD simulation with a novel pseudo-MOSFET structure


Chapter 4: SOI devices with deposited metal contacts

Table of contents of the chapter

4.1. Introduction......................................................................................................................... 80
4.2. Issues with metal contacts on SOI .................................................................................... 80
   4.2.1 Probes with controlled pressure in the pseudo-MOSFET configuration.................... 80
   4.2.2 The effect of the metal contacts on SOI ................................................................. 82
4.3. Fabrication process for SOI with metal contacts ............................................................... 84
   4.3.1 Sample preparation ...................................................................................................... 84
   4.3.2 Drain current response for deposited metal contacts ................................................. 86
   4.3.3 Body potential response with deposited metal contacts ........................................... 89
   4.3.4 Cr contacts: Lift-off versus lithography and etching .................................................. 90
   4.3.5 Annealing effect on the $V_B$ response .................................................................... 92
4.4. Geometry optimization of the device .............................................................................. 94
   4.4.1 BOX thickness impact on $V_B$ ................................................................................. 95
   4.4.2 Silicon film thickness impact on the out-of-equilibrium body potential ................ 96
   4.4.3 The effect of the distance between the probes .......................................................... 98
   4.4.4 Contact shape impact on $V_B$ .................................................................................. 100
4.5. Is the body potential a pressure related effect? .............................................................. 104
4.6. Conclusions .................................................................................................................... 105
This chapter focuses on the practical fabrication of SOI devices with deposited metal contacts. This is a huge step on the development of the sensor, since it moves from the pseudo-MOSFET configuration towards practical devices.

4.1. Introduction

As already discussed in chapter 2, the pseudo-MOSFET is a great platform for SOI electrical testing and development. However, it still remains an electrical characterization configuration, dependent on a particular probe station [1] and not an actual device adapted for applications. In this chapter, the limitations of such a configuration are surpassed thanks to the development of a pragmatic SOI device with deposited metal contacts. While deposited metal contacts have already been studied previously [2]–[6], with various metals and alloys, they are mainly focused on the current response. After a quick review of the issues related to metal contacts (probes or deposited metal) on SOI and of their electrical behaviour (in section 4.2), we proceed to our fabricated devices in section 4.3. The main challenge here it to maintain the dynamic body potential variation with deposited metal contacts. The last sections of the chapter (4.4 and 4.5) show the effect of some geometrical parameters on the $V_B$ response and provides additional elements for future optimizations.

4.2. Issues with metal contacts on SOI

4.2.1 Probes with controlled pressure in the pseudo-MOSFET configuration

This section presents the main issues related to the use of contacts directly placed on SOI substrates. While the pseudo-MOSFET configuration facilitates the parameter extraction for SOI, it induces also variability on the extractions due to the damage caused by the pressure-controlled metal probes. Figure 4.1a, illustrates the damage provoked by the pressure control probes on a 200nm silicon film over 400nm of buried oxide measured with an atomic form microscopy (AFM) topography. Observe how different probes leave different footprints on the silicon when placed on the film. Also the pressure of the contact, significantly increases the impacted area of the probe and the depth [7]. In Figure 4.1b, the extracted series resistance and mobility based on the $Y$-function method (explained in chapter 2) are presented [7]. The series resistance decreases as the pressure increases, leading to more accurate mobility extraction. For this reason, the pressure on the contact was associated with the ohmic behaviour of the contacts in the pseudo-MOSFET. Keep in mind that re-positioning of the probes will increase the damage on the silicon film leading to variability in the parameter extraction [8].
Chapter 4: SOI devices with deposited metal contacts

Later, another interpretation of how the pressure-controlled probes affect the electrical response was suggested, based on nanoindentation of the silicon film due to high pressure areas [9]. The explanations could eventually support the variation in resistance and mobility. However, if also the transient body potential response depends on nanoindentation, deposited metals could fully suppress the phenomenon. Thus the deposited metal contacts, which will eliminate any variability for the pseudo-MOSFET configuration, could be problematic on the occurrence of the $V_B$. Besides the applied pressure though, the contact layout could also affect the electrical response.

Due to the unconventional size and shape of the pseudo-MOSFET configuration, the W/L ratio was substituted by the geometrical factor $f_g$ (discussed in chapter 2). This is the result of the current distribution inside the silicon film and is related to the geometry of the contacts [10]. Figure 4.2a, illustrates a top view of the simulated current density distribution in the silicon film of a 3D structure. While the current seems to follow a straight line between the two contacts, as we move away from the center of the circles the current diminishes but also extends around the contacts. Obviously, the distribution is affected by the geometry of the contacts and the silicon film size. Figure 4.2b, shows the effect of the distance between the contacts in the drain current and transconductance versus gate voltage characteristic curves. As the distance increases, the ON current value decreases, which is attributed to the edge effect due to the proximity of the contacts to the boarders of the silicon mesa. Those elements indicate that the transition from the pseudo-MOSFET configuration to an actual device might not be as simple.
as a direct replacement of the pressure-controlled probes with a deposited metal in the center of the device but, other parameters such as the contact layout should also be assessed.

Figure 4.2: a) Simulated 3D current density distribution (iso-current line every 50A/μm²) around the contacts in the pseudo-MOSFET configuration b) Drain current and transconductance curves simulated for various distance between the contacts [10].

4.2.2 The effect of the metal contacts on SOI

Metal on low-doped semiconductor usually behaves like Schottky junctions [11]–[13]. We remind that the workfunction of the semiconductor is the energy between the vacuum and the semiconductor Fermi level [11]. The formation of an ohmic contact requires the metal workfunction to be smaller than the one of the n-type semiconductor (the opposite stands for a p-type semiconductor). If the above condition is true, then the band bending at the interface allows free carriers in the silicon interface under zero bias conditions. However, in the pseudo-MOSFET universe, it is repeatedly reported that the contacts with metal probes on low doped Si have an ohmic response [1], [3], [7], [9]. While the experimental drain current versus drain voltage curves support this, evidence of the Schottky behaviour can be seen on drain current versus gate voltage curves obtained with samples with different metals deposited. Figure 4.3 illustrates I_D-V_G curves in similar SOI structures with deposited a) Cr/Au [6] and b) Ti/Al [4] contacts. Notice the effect of the deposited metals on the hole and electron currents. The difference in workfunction values favour the conduction of one type of carrier over the other, producing a curve with either higher hole or higher electron current. Cr/Au contacts seem to favour holes which give a two order of magnitudes higher current compared to electrons, while Ti/Al produce a curve where the electron current is superior. One can assume that according to the applied voltages, the maximum ON current is actually limited by the Schottky current provided by the contacts. To demonstrate this we refer to [14], where simulation of two
Schottky junctions connected in series (one is forwardly biased and the other reversely biased) were analysed. As illustrated in Figure 4.4 a and b, a device with metal contacts will form two Schottky diodes connected with the opposite polarity. As a result the forward current of the whole system will be limited by the reverse current of the inversely biased diode (Figure 4.4c). The structures in [14] are similar to the devices in Figure 4.3 and they produced similarly shaped characteristics supporting the previous argument. Note that, there are several reports in the literature with deposited metal contacts in which metal deposited contacts such as square patterns [4] an HgFET [15], and a structure with concentric circles, known as the Corbino pseudo-MOSFET was proposed [2] and then accurately modelled [16] to solve the issue of the $f_g$ factor (see chapter 2). All the above information considered, we proceed to the fabrication of the metal contact SOI devices.

![Figure 4.3: a) Drain current versus gate voltage curves produced by “pseudo-MOSFET-like” configurations with deposited a) Cr/Au [12] and b) Ti/Al stacks [10].](image)

![Figure 4.4: Schematic of a double Schottky diodes for the conductance of electrons in (a) and holes in (b). Simulated current density of the double Schottky diode configuration (c) [14].](image)
4.3. **Fabrication process for SOI with metal contacts**

According to the findings of chapter 3, the presence of “barriers” under the contacts induced the out-of-equilibrium state. The question we would like to answer here, is how critical is the choice of metal for maintaining the response in devices deposited contacts. To do this we selected chromium (Cr) and gold (Au) contacts for the low p− doped silicon film used in this study ($N_A=10^{15}\text{cm}^{-3}$ gives a workfunction of $\phi_{\text{Si}}=4.91\text{eV}$). Chromium was selected to test the Schottky-type contacts since $\phi_{\text{Cr}}=4.5\text{eV} < \phi_{\text{Si}}=4.91\text{eV}$ while gold has $\phi_{\text{Au}}=5.1\text{eV} > \phi_{\text{Si}}=4.91\text{eV}$ and should yield ohmic contacts, according to the theory.

4.3.1 **Sample preparation**

There are two options to choose from for the fabrication process of the devices. The first one is a lift-off process in which the top chemical oxide already existing on the top of the SOI provided by SOITEC will be maintained. The second one is a lithography and etching process which could be easily adapted for industrial production but the chemical oxide of the SOI will be removed and a native one will regrow naturally when the sample will be exposed to ambient air at the end of the process. Obviously, the native oxide is of a lower quality than the chemical one. A schematic representation that compares the two processes is given in Figure 4.5.

The silicon film of the SOI has a thickness of 70nm laying on a 145nm thick buried oxide. 5mm by 5mm silicon mesas are obtained with a lithography step and reactive ion etching. Afterwards, the wafers are rinsed with de-ionised water and dried with $\text{N}_2$.

Then the samples were baked at 120°C in an oven in ambient atmosphere so, the absorbed water in the top $\text{SiO}_2$ evaporates. After, a primer layer (Hexamethyldisilazane [17]) is deposited on the already hot sample and the wafer is placed in the oven for a second time. Then an AZ1505 photoresist layer is spin coated at 4000 rpm (expected resist thickness of 500nm) followed by a 1.5 min soft bake on a hotplate at 100°C. Note that, at this point the visual inspection under an optical microscope is crucial after each step to ensure that the resist is homogenous, well aligned and defect free (absence of dust or other particles). In case of any issue, the resist should be removed and the process has to be restarted. Then a second photolithography defines the patterns in which the metal will be deposited. In our case, for a relatively dark mask and reflective substrate, the expose time during lithography was set to 25s. After exposure, the sample is submerged in an AZ developer solution (50% diluted with de-ionized water) for 10-12 sec. This step requires special attention since, a short development time will leave residual resist compromising the contact quality and a long development time
Chapter 4: SOI devices with deposited metal contacts

will certainly affect the boundaries of the resist, resulting in rough contact edges and huge variability between the dies. Then the samples go through a hard bake on the hotplate at 120ºC. After the hard bake, the samples are submerged in a 5% HF solution for 5 to 7s to remove the top SiO$_2$ from the exposed areas. The samples are transferred in the deposition chamber of the sputtering tool and the metal is deposited. Finally, the wafer is submerged in acetone and in an ultrasonic bath for 2 min and the metal patterns are revealed after lift-off. Note that it is essential for the samples to be placed at a certain angle, with the metal layer facing downwards, so that the residual material does not stick on the SiO$_2$ on top of the mesas or the exposed BOX.

The second process option (bottom of Figure 4.5) is lithography and etching after metal deposition. In this case, the SiO$_2$ top layer was removed right away with a 5% HF bath, prior to the metal deposition. Then, a lithography step followed by wet etching (Cr etchant for ~5min) allowed to finalize the contact fabrication.

Figure 4.5: Major steps of the fabrication processes followed. Lift-off on top and lithography and etching on the bottom.

It has to be stated that, contrary to the Cr contacts which are fabricated with the optimised protocol presented above, the SiO$_2$ layer for the Au/Ti contact devices was removed from the whole top surface. A thin (~5nm) Ti layer was deposited to ensure adhesion of Au to Si surface. Then the photoresist was deposited followed by the metal deposition. Finally the patterns where revealed with lift-off.
4.3.2 Drain current response for deposited metal contacts

As a first step, the contact layout was chosen to mimic the probe placement of the pseudo-MOSFET configuration in order to have comparable devices with previous results in chapter 2. Metal pads were deposited in the centre of the silicon surface with a distance \( d \) between the contacts. The metal pads are either circular or squares with 100\( \mu \)m diameter or side and they are positioned at various distances between them: 0.3mm, 0.5mm and 1mm. They serve as source, drain and body contacts. The gate voltage is applied on the bulk of the SOI with a B1500 Agilent analyser. The source contact is grounded and a 0.1V bias is applied on the drain terminal. To accurately monitor the body potential, a zero current condition is imposed on the body probe [18]. The performance is evaluated through quasi-static drain current measurements first.

Figure 4.6: Schematic of the SOI wafer with deposited metal contacts a) cross-sectional view and b) top view.

Figure 4.7, illustrates the drain current measured with the tungsten carbide (WC) pressure controlled probes of the pseudo-MOSFET in comparison with Cr and Au/Ti contacts deposited on top. For positive voltages, a relatively high ON current is observed for all the cases (\( \geq 1\mu \text{A} \)). Current is higher for Cr contacts, followed by Au/Ti contacts and the pseudo-MOSFET. As the gate voltage decreases, the film is driven into depletion and all the currents fall into a region where \( I_D \) is in the nano-ampere range. Note the degraded subthreshold slope for Au/Ti contacts, which is a result of a lower quality top oxide after the re-growth of the native SiO\(_2\) compared to the chemical oxide made in SOITEC. This can potentially explain the lower ON current compared to Cr contacts. Contrary to Au/Ti contacts, Cr contacts have a minimum current value of 100pA, as in pseudo-MOSFET. For negative voltages, where the silicon film is supposed to be in accumulation mode, the pseudo-MOSFET probes produce higher current values compared to the deposited metals. While in Cr contact, the current increases to some hundreds of nano-amperes, devices with Au/Ti contacts remain depleted. This suggests that
Au/Ti contacts behave like ohmic contacts only for electrons. Cr contacts allow a weak hole current, even though it is at least one order of magnitude smaller than the one measured with the pseudo-MOSFET probes. The aforementioned behaviour was encountered in the literature as briefly illustrated in the sub-section 4.2.2 and it seems to originate from the workfunction of the deposited metal.

Figure 4.7: Drain current versus gate voltage characteristic curves in semi-log scale for pressure-controlled probes and deposited Cr and Au/Ti contacts. The wafer has a 70nm thick silicon film on 145nm thick BOX layer.

To further understand the response of the device for the various metals tested we examine the drain current versus drain voltage curves. Figure 4.8 illustrates the drain current versus gate voltage for deposited Cr contact for a) positive and b) negative gate voltages. For $V_G=1\,\text{V}$, the devices with Cr pads are depleted and the $I_D$-$V_D$ curve show a Schottky behaviour. When the device is in inversion $V_G>V_T\approx2\,\text{V}$, the $I_D$-$V_D$ curves show an ohmic behaviour. This is a typical pseudo-MOSFET response as seen in chapter 2, where for positive gate voltage and when $V_G<V_T$, the Cr contacts behave like Schottky diodes (an equivalent behaviour is observed for negative gate voltage and $V_G<V_{FB}$).
Figure 4.8: Drain current versus drain voltage characteristics for Cr pads measured for a) positive and b) negative gate voltages.

Figure 4.9, depicts the I_D-V_D curves for SOI with Au/Ti contacts for a) positive and b) negative gate voltage. For V_G>0V the contacts produce a fully linear response for low V_D. Negative gate voltage induces very low current values. This correlates with the I_D-V_G curve (Figure 4.7), also showing low current values for V_G<0, which correspond to a reverse current of a Schottky diode.

Figure 4.9: Drain current versus drain voltage characteristics for Au/Ti pads measured for a) positive and b) negative gate voltages.

Theoretically, the type of contact between a metal and a semiconductor is defined by the difference between the semiconductor and metal workfunction values [11]–[13]. As previously said, the low doped p-type Si film used has a theoretical workfunction of ~4.91eV. When compared to the Cr workfunction (ϕ_Cr=4.5eV [19]), the contacts should exhibit a rectifying behaviour. On the contrary Au/Ti contacts, on the same silicon film, should yield a not
rectifying ($\phi_{Au} \geq 5.1eV$ [19]) behaviour. The Ti workfunction is neglected in this calculation since, for 5nm deposited layer, Ti is expected to diffuse into the Au grain boundaries [20] and not to affect the electrical response [21] of the contact. Note that, if the Ti layer is not employed the Au contact show very poor adhesion and they can be displaced or removed even under a N$_2$ flow. Evidently, the $I_D$-$V_D$ curves in Figure 4.8 present a more complex behaviour, with an ohmic response that depends, not only on the workfunction difference but also on the applied $V_G$. This indicates that the contact type is also affected by the actual carrier concentration in the Si film under the metal/semiconductor interface and is controlled by $V_G$, as we will see later with the numerical simulations in chapter 5. For now, the discussion is focused on the effect of the deposited metal on the $V_B$ response.

### 4.3.3 Body potential response with deposited metal contacts

Figure 4.10a shows the body potential response versus gate voltage measured in the pseudo-MOSFET and devices with deposited Cr and Au/Ti contacts with the same measurement conditions. Compared to the WC pressure probes, Cr shows higher maximum value for the body potential and an extended range of $V_G$ where it appears. On the other side, devices with Au/Ti contacts do not exhibit any out-of-equilibrium response. Figure 4.10b, illustrates the gate current monitored in the same devices as in Figure 4.10a. As for $V_B$, $I_G$ has the same signature for devices with Cr contacts and pressure WC contacts while, Au/Ti shows a current value close to zero. A correlation with the contact behaviour in the previous section shows that the body potential response is only present when the contact behaves like a Schottky. This is confirmed with all the measured curves: 1) for the $I_D$-$V_G$ characteristics, $V_B$ is visible in the depletion region where the contact has a Schottky behaviour 2) the $I_D$-$V_D$ curves for Au/Ti contact showed a purely ohmic contact and no $V_B$ response.
4.3.4 Cr contacts: Lift-off versus lithography and etching

Starting from this point only sample with Cr contacts will be used, that are appropriate for \( V_B \) study. The major differences between the fabrication processes is that in the lift-off process, the original SiO\(_2\) layer, which meets the factory standards of SOITEC) is maintained while, in the lithography and etching, the chemical grown SiO\(_2\) is removes and a native oxide is re-grown (Figure 4.5). Figure 4.11 depicts the a) drain current and b) body potential versus gate voltage curves of devices with deposited Cr contact fabricated with the two fabrication flows. In \( I_D-V_G \) curves, a wider gate voltage is required for film inversion in the devices fabricated with lithography/etch. Additionally, the subthreshold slope is greatly degraded in these samples, most likely due to the increase of interface states densities because of the native oxide regrowth. In the accumulation regime, both devices produce an \( I_D \) current of about 100nA, which is obtained for lower \( V_G \) for the devices produced with a lift-off process. For \( V_G > 0 \text{V} \), lift-off devices produce an order of magnitude higher ON-current. Therefore, in terms of \( I_D \), lift-off produces devices with better conductive properties. Unlike the current measurements, \( V_B \) response is enhanced with the second fabrication process, with a maximum value reaching almost 4V. The out-of-equilibrium response is extended in a \( V_G \) range between -14V and -2V, compared to the restricted range obtained for devices fabricated with lift-off. From the practical point of view, a large \( V_G \) interval is undesirable since, the pulse generator and oscilloscope used for the transients are limited to the range of -5V to 5V and thus more specialized instruments are required for the dynamic experiments. It is suspected that a surface modification during the process might be responsible for the difference in the electrical properties.
behaviour. To check this, an atomic force microscopy (AFM) topography was performed on the samples.

**Figure 4.11**: a) Drain current and b) body potential versus gate voltage for the same SOI but with Cr contacts fabricated with lift-off or litho/etching process.

Figure 4.12, illustrates the AFM surface topography of a fresh wafer (as obtained from the factory) and of a sample after lithography and etching. The height profiles are extracted along the cutlines indicated in the topographic maps. The bare SOI wafer shows a very smooth surface, with an average roughness of 0.8nm and root mean squared average of 1nm. In contrast, after Cr etching, a network of patterns and dots/particles are observed throughout the whole image. The height of the patterns is of some nanometers while the height of the dots is over 30nm. Roughness is of 2.5nm and the root mean square is of 4.1nm. The topography difference between the samples cannot just be related to the re-growth of the native SiO$_2$ in the second case. Indeed, the native oxide growth should be homogenous on the whole surface area and not show such patterns. Consequently, the explanation is elsewhere. For the lithography/etching process, the metal is deposited directly on the silicon surface. As explained in [22], Cr mixes with silicon even if an SiO$_2$ is present. Thus, residual Cr can remain on the surface even after etching and thus, explain the non-homogenous topography of Figure 4.12b and the increased roughness of Figure 4.12b. Note that if Cr diffuses in the silicon, this is undetectable by an AFM topography and more sophisticated techniques are required such as Auger electron spectroscopy combined with depth profiling or secondary ion mass spectrometry. However, such study exceeds the purpose of this thesis so, we simply concluded that there is residual Cr remaining on the surface after etching and it probably modifies the electrical characteristics (for example by inducing interface state densities). It could also increases the complexity for sensing applications since, a compound SiO$_2$/Cr layer should be
considered. In the next section we wanted to evaluate the effect of the annealing on the electrical response.

Figure 4.12: AFM topography of a) an SOI wafer as recovered from the factory and b) after etching the excess of Cr fabricated with the lithography and etching process. c) Height profile obtained from the bare SOI following the cutline in figure a). d) Height profile obtained from the fabricated device following the cutline indicated in figure b).

4.3.5 Annealing effect on the $V_B$ response

An annealing step was performed to explore its effect on the electrical response of the device, especially $V_B$. For this study, devices with Cr contacts, fabricated by lithography and etching and devices with Au/Ti were used. The wafers were baked in an oven at 300°C under vacuum for an hour. For the wafers with Au/Ti contacts, $V_B$ response was suspended before annealing. After annealing their behaviour show a slightly improved conductance but the body potential still does not manifest itself. Thus, the discussion is focused on the effect of annealing on devices with Cr contacts. Figure 4.13 depicts the $I_D-V_G$ curves measured in devices with Cr contact before and after annealing. Observe the higher ON current for the annealed devices on both hole and electron currents. Moreover, the current in the depletion region is increased by one order of magnitude and $V_G$ range to obtain the depletion regime narrows, like in SOI wafers tested with the pseudo-MOSFET [23]. Figure 4.14 illustrates the $I_D-V_D$ curves measured in the annealed devices. For $V_G>0V$, the curves exhibit a fairly linear response while, before
annealing (Figure 4.8) the behaviour is “Schottky-like” for low $V_G$. A similar effect is observed for the accumulation mode of the film ($V_G < 0V$), with lower current values. These $I_D-V_D$ curves suggest an improved ohmic contact after annealing but is this beneficial for the out-of-equilibrium body potential?

Figure 4.13: Drain current versus gate voltage characteristics measured in devices with Cr contacts fabricated with lithography and etching process before and after annealing.

Figure 4.14: Drain current versus drain voltage characteristics measured in devices with Cr contacts fabricated with lithography and etching process after annealing for a) $V_G > 0V$ and b) $V_G < 0V$.

Figure 4.15 shows the body potential and the associated gate current versus gate voltage for devices with Cr before and after annealing. Undoubtedly, there is a huge decrease on the body potential response after the thermal process. Note that the vertical scales for $V_B$ are not the same before and after annealing. The potential presents a very small fluctuation around the equilibrium value of 50mV (which corresponds to half of the voltage between the source and drain terminals). Similarly, the gate current is diminished after thermal treatment, as expected.
The potential build-up corresponds to a deficit of carriers. Since $V_B$ is not present, one can conclude that the carriers are injected immediately when needed in the film, and the device stays in the equilibrium state. Although, annealing is generally beneficial for contact improvement in terms of $I_D$, eliminates completely the $V_B$ response.

**Figure 4.15:** a) Body potential and b) gate current versus gate voltage characteristics measured in devices with Cr contacts fabricated with lithography and etching process before and after annealing.

The conclusion of the analysis of the technological splits tested is that the material selection and the thermal treatment of the samples have an eminent role on the emergence of the transient body potential. Although, a low resistance ohmic contact is favourable for $I_D$, it obviously leads to the suppression of the transient body potential. The above studies, indicate that $V_B$ arises only when the contact has a Schottky behaviour, illustrating the need for a barrier to block the carriers and thus drive the silicon film into the out-of-equilibrium state.

In the next section, the influence of the device geometry on the out-of-equilibrium body potential response is examined.

## 4.4. Geometry optimization of the device

For all the above reasons, the lift-off process is preferred for the next fabricated sensors. Keep in mind that, lift-off might not be optimal for mass production and the fabrication process needs to be adapted for the development of a real product, but here it serves well the research purposes. The transition from the pressure-controlled probe station to these actual devices with deposited metal contacts allows for additional possibilities of device optimization in terms of the geometry. The aim of this study is to maintain a profitable $V_B$ response. However, we will evaluate carefully the effect of each geometrical parameter on the occurrence of the transient...
body potential. This benchmark is done with devices with Cr contacts, fabricated with the lift-off process and measurements on the wafers in the pseudo-MOSFET configuration.

### 4.4.1 BOX thickness impact on $V_B$

For the fabrication of the desired device, one should carefully select the substrate. BOX thickness variation modifies the BOX capacitance and, as seen in chapter 2 and 3 for the pseudo-MOSFET, can significantly affect the transient effects. A comparison of the drain current and body potential response between two SOI devices with deposited Cr contacts and two BOX thicknesses is depicted in Figure 4.16. The $I_D-V_G$ characteristics show higher inversion current and lower threshold voltage for the thin BOX layer. The thinner oxide allows a better electrostatic control of the gate due to the smaller voltage drop on the oxide. $V_B$ maintains its shape in the two wafers and shows a steeper slope for thinner BOX. Moreover, the response seems to be stronger for $t_{\text{BOX}}=30\text{nm}$ compared to the 145nm. This contradicts the simulation results of chapter 3 (Figure 3.17), where the inverse response was obtained through TCAD. There are two assumptions that explain the effect. For the first, one should observe the slope during the body potential increase (Figure 4.16b) which changes with the BOX thickness. This slope is associated with the capacitive coefficient [24] of the device in depletion, which could include also the a capacitance term associated with $D_{it}$. As explained in sub-section 3.7.2, $D_{it}$ on the Si interfaces can change the slope of the linear increase of $V_B$ explaining the unexpected result of Figure 4.16, since the two wafers have different top SiO$_2$ layers. The second explanation is found in the contact quality, since simulations in chapter 3 showed that the contact can strongly affect the $V_B$ response. To support this assumption, the two wafers are also compared with the pseudo-MOSFET configuration on dies without deposited Cr.

![Figure 4.16](image)

*Figure 4.16: a) Drain current and b) body potential versus gate voltage for devices with Cr contacts fabricated with lift-off for two SOI wafers with different BOX thicknesses.*
Chapter 4: SOI devices with deposited metal contacts

Figure 4.17 presents the $V_B$ response measured in the same wafers as in Figure 4.16 in the pseudo-MOSFET configuration prior to metal deposition. While devices with deposited contacts show a large variation in the maximum value, the curves produced in the pseudo-MOSFET exhibit a comparable maximum value in $V_B$ between the tested wafers. This suggests that the body potential dependence on the contact itself might even be superior to the BOX capacitance. In the simulations of chapter 3 the contacts are considered to be perfect with smooth, well defined boundaries while, in reality this is impossible due to imperfections and lattice mismatch, Cr/Si intermixing, etc. Although the simulated and experimental results support the interpretations of this contradictory result based on $D_n$ or the contact quality, further investigation is needed to conclude on the reason for this discrepancy.

![Graph showing $V_B$ response vs gate voltage for SOI wafers with different BOX thicknesses.]

*Figure 4.17: Body potential versus gate voltage for two SOI wafers with different BOX thicknesses, measured with the pseudo-MOSFET (the pressure was set to 80g).*

4.4.2 Silicon film thickness impact on the out-of-equilibrium body potential

The second wafer parameter to test is the Si film thickness impact on $V_B$. Figure 4.18 presents a comparison of the drain current and body potential response between an SOI with and two different Si film thicknesses. The $I_D-V_G$ characteristics show a steeper slope and smaller hysteresis in the thick Si film. Thin films also have increased threshold and flat-band voltages compared to the thick layers. This behaviour is in agreement with the pseudo-MOSFET reports [23], where an increased threshold voltage was attributed to the thin film and the Schottky contact [25]; the larger hysteresis was due to top interface traps [23]. The body potential response seems to be greatly enhanced in thin silicon films. Considering the $V_T$ increase in thin Si films, the increase of $V_B$ was expected since the device inverts at higher
voltages and thus a larger carrier deficit is defined for the same $C_{\text{BOX}}$. Additionally, the two measured $V_B$-$V_G$ seem to have similar slopes in the linear increase region which is agreement with the fact that the slope is mostly related to $C_{\text{BOX}}$. Observe also that the results agree with the simulations presented in chapter 3.

![Figure 4.18: a) Drain current and b) body potential versus gate voltage for devices with Cr contacts fabricated with lift-off for two SOI wafers with different Si film thicknesses.](image)

Once more, we benchmark this outcome with the pseudo-MOSFET curves obtained with the same wafers as in Figure 4.18 without Cr contacts. The results are illustrated in Figure 4.19. The results are consistent with what was observed in devices with deposited Cr pads and the simulations in chapter 3 since the same trend was observed. Clearly, thinner Si film produces a stronger potential response and thus could be beneficial for applications. Also, thinner films are expected to be more sensitive during detection due to stronger coupling. One can conclude that the contact quality seems have a minor effect over the Si film thickness. Once again, the body potential slope during the linear increase seems to be constant for the tested wafers, showing small or no dependence on $C_{\text{Si}}$. 

![Figure 4.19: Pseudo-MOSFET curves obtained with the same wafers as in Figure 4.18 without Cr contacts.](image)
Figure 4.19: Body potential versus gate voltage for two SOI wafers with different Si film thicknesses, measured with the pseudo-MOSFET. The pressure was set to 80g.

Since the contacts are the key element on the origin of the out-of-equilibrium $V_B$, the attention is focused on the contact layout in the next two sub-sections.

4.4.3 The effect of the distance between the probes

In the pseudo-MOSFET the major part of the resistance in inversion stems from contact between the probes and the silicon film [26]. However, for sensing applications the distance between the contacts will increase significantly due to an adjustment of the layout to implement a PDMS chamber for restraining the liquid species. This will probably affect also the response of the device. In a first step, we investigate the effect of the distance between two Cr pads placed in the center of the device for three samples with contact distances of 0.3mm, 0.5mm and 1mm. The experimental body potential and gate current are illustrated in Figure 4.20. The body potential seems to have similar response in the samples where the distance between the contacts is of 0.5mm and 1mm, while there is a discrepancy when the contacts are close to each other. This indicates that the current distribution in the silicon film can induce the $V_B$ response since the distance between the probes is comparable to their size. The gate current shape seems to be unaffected by the distance between the probes while it only presents a small shift which is in agreement with the point where $V_B$ returns to equilibrium in the $V_B-V_G$ curves. This behaviour can be attributed to the variability between the devices. To avoid the variability issue a similar experiment was repeated in the same sample with four circular contacts placed on the center of the device.
Figure 4.20: Body potential (a) and gate current (b) for three devices with two Cr circular contacts placed in the center of the device at a distance of 0.3mm, 0.5mm and 1mm between them. The SOI has $t_{Si}=70\text{nm}$ and $t_{BOX}=145\text{nm}$.

Figure 4.21 illustrates the body potential and the gate current monitored in one device with four metal pads placed on the silicon film. The distance between the pads is of 1mm. While pad P1 was grounded and kept as source, the other pads were used alternatively as terminals for $V_B$ monitoring. In this experiment, the body potential always returns to equilibrium at the same $V_G$ value and the gate currents are perfectly superposed. Such a behaviour verifies once again that the gate current corresponds to the inversion charge required by the BOX capacitance as in [8]. $V_B$ follows the same linear increase regardless of the pad. The deviation between the experimental curves in the $V_B$ appears before the return to the equilibrium and seems to be more abrupt for larger distance between the probes. This implies that the lack of carriers is not filled instantaneously in the silicon film and the carriers need time to travel from source to the body contact. This is a consequence of the high time constant of the Si film in depletion [27]. As a result, carriers are injected in the film, the same way for the three cases (since the source contact is exactly the same), but they also need to travel from source to each $V_B$ contact. For large distance between the probes, the carriers require more time to reach from one contact to the other and hence, the drop seems more sudden and linear. However, when the contacts are close to each other, the electrons charge “partially” the film (between source and body contact) but they are also transferred to the distant parts of the silicon, provoking the small shoulder on the $V_B$ shape. In every case, the return to equilibrium ($V_B=0$) occurs at constant $V_G$, as indicated also from $I_G$ (Figure 4.21) which is unaffected by the probe placement. In this context, one expects also to see an effect related to the shape of the contact, which is discussed in the next sub-section.
4.4.4 Contact shape impact on $V_B$

The aim of this section is to verify whether or not the out-of-equilibrium still appears regardless of the contact layout shape. Figure 4.22 portrays a comparison of the body potential for devices with circular (100μm radius) and square (100μm sides) contacts and with various distances between the contacts. For 1mm distance between the probes, the two traces are almost perfectly superposed. However, as the distance reduces to 0.5mm and 0.3mm, a discrepancy between the responses appears. For 0.5mm and 0.3mm, the distance between the pads is comparable to their size, thus the electric field distribution in the film might affect $V_B$ causing a discrepancy between the two measurements. In any case, if the contacts are placed at a certain distance from each other, the $V_B$ response seems quite reproducible.

Figure 4.22: Body potential versus gate voltage for circular and square pads for various distances between the contacts.

For the purpose of sensing, the contacts should be placed on the edges of the silicon mesa, enabling the placement of a chamber in the center of the device for the liquid species under detection. Would $V_B$ response still be present in this case? The layouts tested are illustrated in Figure 4.23. The sensing results will be shown later in chapter 6. Here, we focus on the $V_B$
response and how it is affected by these particular contact layouts. Although, contact shape seems to be important only when the distance between the pads is relatively small, the electrical performance of the devices with the sensing contact layout was evaluated again, since the contact size and distance significantly increase. Notice that in some cases, the contacts are comparable to the mesa size (e.g. the ribbons on the left in Figure 4.23). This might highlight additional effects on $V_B$ such as the contact resistance. As previously, the benchmark will be based on the drain current and body potential measurements. To provide comparable results, the body potential and the drain current was measured with the same Cr pad in two $V_G$ sweeps in which the two terminals were exchanged. For the layouts named “Circles” and “Triangles” two different pad sizes were tested with 100μm and 500μm radius or side, which correspond to the small and big circles in the next comparison.

![Figure 4.23: Contact layouts adapted for sensing applications.](image)

Drain current versus gate current measurements for the layouts depicted in Figure 4.23, are illustrated in Figure 4.24a. Regardless of the contact layout the devices show a small current of holes for negative $V_G$ and a stronger electron current for positive $V_G$. The current values are comparable with the ones obtained with the three Cr pads in the centre of the device. While the electron current seems to be relatively unaffected by the layout, except for the ribbon contacts, hole currents vary a lot with the shape and size of the pads. To further identify the origin of the above observation, the transconductance $g_m$ is plotted in Figure 4.24b. While the maximum of the transconductance appears at the same $V_G$, indicating relatively constant threshold voltage [28], its value and decreasing slope after $V_T$ shows a dependency on the contact layout. Note that, this effect is not so evident on the electrons current which seemed to be well superposed previously. As discussed in chapter 2, the $g_m$ decrease at high $V_G$ is associated with the attenuation factor $\theta$ and the maximum value with the mobility $\mu$. Both of these quantities affect the series resistance (see sub-section 2.1.1).
Chapter 4: SOI devices with deposited metal contacts

Figure 4.24: Drain current (a) and transconductance gm (b) versus gate voltage measurements for the devices with the layouts shown in Figure 4.23.

The extracted series resistance versus the metal pad area is plotted in Figure 4.25 in a semi-logarithmic scale. We remind that $f_g$ depends on the contact layout and for an accurate extraction it should be estimated experimentally [29]. For this demonstration we set $f_g=1$ and the second order attenuation factor ($\theta_2$) was neglected as in pseudo-MOSFET. The resistance was calculated from equation (2.3). The resistance reduces exponentially with the area of the metal contact with the logarithmic fit showing great linearity with the extracted values. This indicates that $f_g$ seems to have roughly the same value for all the layouts. In this case, even if $f_g$ real value differs from the unit, the trend between the resistance and area should be maintained. The values range from $5k\Omega$ for the small circle layout to $1k\Omega$ for ribbons. The extracted resistance is lower than the one for the pseudo-MOSFET (chapter 2) and an order of magnitude higher compared to FD-SOI MOSFETs [30], highlighting that the current limitation in the structures are the metal contacts.
Figure 4.25: Extracted series resistance values extracted from the $I_D$-$V_G$ curves in Figure 4.24 versus the area of the contact in semi-logarithmic scale.

The body potential versus the gate voltage for the tested structures of Figure 4.23 is depicted in Figure 4.26a. Although, the body potential potential maintains roughly its shape for the various devices and the linear increase seems to follow the same slope, different maximum values were obtained for each contact layout. For larger pads the maximum value is lower than for the smaller pads. For a comparison with the resistance values, the maximum value of $V_B$ is added to the data in Figure 4.25 and presented in Figure 4.26b. Similarly to the resistance, the maximum value of $V_B$ seems to reduce exponentially with the area of metal pad. This result agrees with the previous observations: when the conductivity improves, $V_B$ seems to decrease or even disappear (for example with Au/Ti contacts or after annealing). Observe how $V_B$ reduces with the area of the contact, similarly to the resistance. Note that, the variability on the $V_B$ response for devices with metal contacts and the fact that the maximum potential value is correspond to the reading of a single point (compared to the resistance which was extracted based on a fitting), lead to a reduced linearity of 0.6. However, if the third and fourth points of the graph in Figure 4.26b are are excluded from the fitting the linearity reaches the value of 0.9.
4.5. **Is the body potential a pressure related effect?**

The results suggest that the $V_B$ signal is strongly depended on the contact (conductivity, layout, etc…). While a major development step was realised in this chapter by depositing metal contacts, one might still relate $V_B$ with the pressure applied on the probes placed on the metal pads during the electrical measurements. While the Jandel station with pressure-controlled probes was avoided, probes still press the Cr pads on the Si mesa. To answer this inquiry, we tested one device with the Cr pads wire-bonded to external aluminium (Al) pads. Then the measurement probes were placed on the external Al pads. In Figure 4.27, drain current and body potential curves of the device are presented. The measurements was repeated three times with the probes connected to the Cr metal pads of the device. Then the measurements was performed three more times, with the probes connected to the aluminium pads which are wire bonded with the Cr pads of the device. The measurements were repeated three times to show repeatability of the measurement both with the probes on the device or the aluminium pads used in wire bonding. Both current and body potential curves are perfectly superposed. This result, along with the simulations of chapter 3, proves that the origin of the body potential is purely electrodynamic and not related to the pressure applied on the silicon film. Thus, the device could be directly integrated into a circuit for the next steps of development of the sensor.
Figure 4.27: Drain current (a) and body potential (b) versus gate voltage for six consecutive measurements of an SOI wafer with 16nm/145nm Si/BOX thicknesses. The three first measurements are made through Al pads wire-bonded to the Cr pad of the device and the three latter by directly probing the deposited Cr on the SOI.

4.6. Conclusions

A pragmatic sensing device requires integrated contacts which do not depend on a certain measurement equipment (such as Jandel station for the pseudo-MOSFET configuration). The replacement of the pressure-controlled probes by deposited metal pads was a mandatory step for applications. In this chapter, we showed the technological transition from the pseudo-MOSFET configuration to an actual SOI device with deposited metal contacts that could be used for sensing applications. Previous studies illustrated the effect of metal contacts deposited on SOI but they mainly focused on the classic current measurements and their optimization, while the novelty of this work arises from the analysis of the transient body potential.

The effect of technological parameters on the occurrence of \( V_B \) in SOI devices was investigated. Two metals with workfunction values selected to yield ohmic or Schottky contacts with the Si film were tested. The effect of the annealing was also considered to improve the contact performance. In all the cases the conclusion is the same: 1) ohmic contacts are beneficial to \( I_D \) but suppress \( V_B \), 2) improved contacts increase the \( I_D \) and decrease the \( V_B \) response and 3) contacts with Schottky behaviour are needed to drive the device into an out-of-equilibrium state. While deposited Au/Ti contacts show greater conductivity, Cr contacts proven to be the best candidates for strong potential response similar to SOI measured with pressure probes. Additionally, conductivity improvement through annealing of Cr lead to suspension of the \( V_B \) signal.
Since the contacts seem to have a dominant role in the occurrence of $V_B$, we studied different layouts in terms of distance between the probes and metal pad size or shape. An important conclusion was that the shape of the deposited pads should be considered if the contacts are in proximity to each other.

However, for detection shown in chapter 6 of this thesis, the pads need to be placed at the maximum distance possible on the die in order to optimise the sensing area in the middle and put a PDMS chamber in the center of the device for restraining the liquid. In this configuration, the body potential signal retain its shape for all the tested layouts, but exhibited different maximum values depending on the contact layout especially for large pads. The resistance and body potential values can be tuned to fit the sensor circuit in later development stages. Finally, the origin of the body potential is not the pressure applied on the Si, which was mandatory for the next steps of development.

In addition to the development of the transducer, the above study also provides elements concerning the origin of the body potential. As revealed by drain current versus drain voltage measurements, contacts with the expected purely ohmic behaviour did not produce a $V_B$ signature. Contrary, theoretically rectifying contacts show a Schottky behaviour for low $V_G$ and a $V_B$ signature. Note that even in this case, when $V_G$ increases, $I_D-V_D$ becomes linear. For high $V_G$ the device is in a steady state and $V_B$ returns to its equilibrium value. All these confirm that a barrier is mandatory for $V_B$ to be produced, as seen with TCAD simulations in chapter 3. Clearly, the state of the Si region under the contact strongly affects how the metal/semiconductor junction behaves creating the barrier for the carrier injection. Additionally, the “barrier”, seems to originate from the contact itself and to be enhanced when it forms a Schottky junction with the Si film. This will be an important building block for the modeling of $V_B$ in the next chapter.
References


[17] “Hexamethyldisilazane reagent grade, ≥99% | Sigma-Aldrich.”


Chapter 5: Origin and modeling of the out-of-equilibrium body potential

Table of contents of the chapter

5.1 State of the art ........................................................................................................... 112
  5.1.1 Potential modeling in thin films ................................................................. 112
  5.1.2 Quasi equilibrium approximation ............................................................ 115
  5.1.3 Non-ohmic contacts on 2D structures ..................................................... 117
  5.1.4 Transient effects in p-i-n silicon diodes .................................................... 119
5.2 Numerical simulations .......................................................................................... 120
  5.2.1 Potential equations and $V_B$ response .................................................... 120
  5.2.2 Benchmark with transient experiments ..................................................... 122
  5.2.3 Potential distributions and $V_B$ origin ...................................................... 123
  5.2.4 $V_B$ dependence on geometrical and physical parameters ..................... 126
5.3 Equivalent circuit model ....................................................................................... 132
5.4 Circuit model and device parameters ............................................................... 135
  5.4.1 Impact of device area, as captured by the equivalent circuit .................... 135
  5.4.2 Impact of contact area, as captured by the equivalent circuit .................. 136
  5.4.3 Impact of $t_{\text{BOX}}$ variation on the modeled curves ............................... 137
  5.4.4 Model response $t_{\text{Si}}$ variation .............................................................. 137
  5.4.5 Model response on $V_T$ ............................................................................ 138
5.5 Conclusion ............................................................................................................. 139
Chapter 5: Origin and modeling of the out-of-equilibrium body potential

The aim of this chapter is to build a model combining the experimental and simulated conclusion obtained until now and to explain the origin the out-of-equilibrium body potential in SOI devices with deposited metal contacts.

5.1 State of the art

The development of a sensor on an SOI with metal contacts based on the out-of-equilibrium body potential reading requires the understanding of the origin of this dynamic effect. Until this point of the thesis, we verified that an electrostatic barrier is created under the contact and that it blocks the rapid injection of the carriers needed for the film inversion. Previous reports [1] verified that the amount of carriers, associated to the $I_G$, correspond to the $C_{BOX}$ charge. However, all the above findings give elements regarding the out-of-equilibrium body potential but not a full description of it. To give a straightforward answer to what really provokes the out-of-equilibrium body potential, we need to understand the physics and support it through modeling. The development of semiconductor-device models is a wide and multidisciplinary subject which aims to construct compact models used later for circuit simulations [2]. Even if they are mainly built for practical purposes, they also provide extensive insight on device operation [3], through the assumptions and basis on which they are established. However, the assumptions in our case are not clear, since highly doped regions replaced the pressure controlled probes in TCAD and metal contact simulation seem not to reproduce the $V_B$ signature. Additionally, the phenomenon occurs during large-signal experiments and it is anticipated to suppressed in small signal measurements [1], [4]. In this context, it seems that approximations and modeling techniques form the literature do not directly apply on our case and the path towards the description of the out-of-equilibrium body potential might not be straightforward. Thus, in this section, some modeling techniques applied to fully depleted (FD)-SOI transistors and the pseudo-MOSFET will be presented, along with some elements concerning the transient modeling. However, one should not consider this as a thorough review of the literature but as a simple “tool-box” with elements needed for the modeling next.

5.1.1 Potential modeling in thin films

Devices on FD-SOI show improved performance over the partially depleted (PD) ones [5]. As a result, modeling of such devices rapidly emerged. FD and PD metal oxide filed effect transistors (MOSFETs) have the unique property of two independent gates [6]. Note that, FD-SOI MOSFETs show reduced floating body effects but they are not immune to them [7]–[12]. Additionally, the improved electrostatic control of the two gates enables for channel doping
Chapter 5: Origin and modeling of the out-of-equilibrium body potential

decrease. A particular case of a double-gate MOSFET is the symmetric FD-SOI MOSFET which corresponds to a structure with two identical gates connected to the same biasing point. Such a device has a symmetrical potential distribution with respect to the center of the silicon thickness, as shown in Figure 5.1. The potential in this structure was modelled by Taur in [13], starting from Poisson equation for electrons:

\[ \Delta V = \frac{q}{\varepsilon_{Si}} \cdot n_i \cdot e^{qV/kT} \]  

where V is the local potential, q the elementary charge, \( \varepsilon_{Si} \) the silicon permittivity, \( n_i \) the intrinsic carrier density, k is Boltzmann’s constant and T the temperature. It is worth noting that for the undoped Si film, only the mobile charges are considered (more precisely only the inversion charge), while the doping concentration \( N_A \) is neglected.

\[ \begin{align*}
\psi_0 & = 0 \\
V_g & = V_t
\end{align*} \]

\[ \begin{align*}
\psi_0 & = 0 \\
V_g & = V_t
\end{align*} \]

**Figure 5.1:** Taur’s model of a symmetric FD-SOI MOSFET with undoped silicon film a) for zero gate bias and b) for gate voltage equal to threshold [13].

Considering the symmetry of the structure, the electric field was considered always equal to zero in the centre of the silicon film thickness. This is a boundary condition for the differential equation (5.1), which drastically simplifies the solution and yields an elegant analytical form for the surface potential, \( \psi_s \):

\[ \frac{q(\psi_s - \psi_0)}{2kT} = -\ln \left[ \cos \left( \sqrt{\frac{q^2 \cdot n_i}{2\varepsilon_{Si} \cdot kT}} \cdot e^{qV_0/kT} \left( W / 2 \right) \right) \right] \]  

where W is the thickness of the silicon film and all the other parameters have their usual meaning. \( \psi_0 \) is the potential in the center of the silicon film and it can be calculated through the
Si/oxide interface by applying Gauss’s law. It should be stated that double gate SOI-MOSFETs were rigorously modelled by various groups as described in [14]; it was extended to junctionless structures in [15] and later to asymmetric structures in [16].

However, in this thesis we based our devices on the SOI wafers and not a double-gate transistor. The floating top interface along (which might also have different quality to the Si/BOX interface) with the different thicknesses of the top SiO\(_2\) and BOX of the SOI, makes the modeling of the potential more complex. For depleted SOI wafers, Rodriguez et al. [17] proposed a more sophisticated analytical model to calculate the surface potential at the Si/BOX interface. A schematic of their model is presented in Figure 5.2. They demonstrate that the top interface quality strongly affects the expression of the potential and they propose two models, for passivated and non-passivated films accordingly. For passivated wafers, the approximation of zero electric field was employed yielding the surface potential as [17]:

\[
\psi_2(x) = -\frac{2kT}{q} \ln \left[ e^{-\psi_2/kT} \cos \left( e^{\psi_2/kT} \cdot \frac{q^2 \cdot n_i}{2\varepsilon_{Si} \cdot kT} \cdot (x - t_{Si}) \right) \right] 
\]

where \(\psi_2\) is the potential on the floating silicon interface of the SOI wafer and \(x\) the vertical dimension (along the thickness of the structure). Notice that equations (5.2) and (5.3) are equivalent to each other. \(\psi_2\) is again calculated through Gauss’s law applied to the Si/BOX interface. However, for non-passivated films, the potential is pinned at a specific energy level in the top Si surface. As a result, the previous approximation does not stand and the equation becomes more complicated to solve. Finally, a solution was proposed by including the top and bottom boundary conditions for the Si film.
Interestingly, in the same work [17], the proposed solutions are merged in:

$$\psi(x) = \frac{2kT}{q} \ln \left[ \frac{\varepsilon_{Si}}{2kT \cdot n_i} \frac{E_m}{\sinh \left( \frac{q \cdot E_m}{2kT} (x - t_{Si}) + \lambda \right)} \right]$$

(5.4a)

where the $E_m$ and $\lambda$ parameters are described by the following equations:

$$E_m^2 = E_{S2}^2 - \frac{2kT}{\varepsilon_{Si}} n_i \cdot e^{\psi_S/kT}$$

(5.4b)

$$\lambda = \text{arcsinh} \left( \frac{\varepsilon_{Si}}{2kT \cdot n_i} E_m \right)$$

(5.4c)

The passivated-SOI case corresponds to the mathematical condition of $E_m^2 \approx E_{S2}^2$ in equations (5.4). Notice how the complexity of the solution depends on the applied boundary conditions. Additionally, the above approaches all focus on static conditions.

### 5.1.2 Quasi equilibrium approximation

Only a small percentage of the modeling publications include non-quasi-static effects, the majority of which are focused on single-gate MOSFETs [18]–[22] and/or small signal modeling [20]–[23]. In almost all of these cases, the transient effects are considered through the addition of the continuity equation:
\[ \Delta J = -q \frac{dn}{dt} \]  

(5.5)

where \( t \) is the time, \( n \) the mobile charge density, \( q \) the elementary charge and \( J \) the current density. Roughly, this equation describes the variation in time of the carriers in order to reach the equilibrium state in a given structure. Any deviation from the equilibrium state is described with the help of the quasi-Fermi levels [24]. For SOI transistors, the transient effects were modelled in [25]. Clearly, the addition of this second equation (5.5) in the mathematical system increases the complexity. Thus in [25], the quasi-equilibrium approximation was considered. Figure 5.3 illustrates the Fermi and quasi-Fermi level variations across the thickness of a Si film. In equilibrium conditions (Figure 5.3a), the carrier concentration is fully described by the Fermi level. However, in transient conditions, the quasi-Fermi levels deviate from the equilibrium value as shown in Figure 5.3b and it rises across the thickness of the silicon film. To simplify the simulation process, one can consider the quasi-equilibrium approximation in which the quasi-Fermi level is constant across the Si film thickness, as illustrated in Figure 5.3c. This approximation was proven very successful for modeling the transient effects of SOI transistors, accurately describing the inversion charge under dynamic conditions in [25]. Also, this approximation is reasonable from the physics point of view, since in FD-SOI structure the drift diffusion current is negligible in the vertical direction. Consequently, no quasi-Fermi potential variations are expected across the Si film.

Figure 5.3: Potential distribution in a thin Si film of an SOI across its thickness in equilibrium conditions (a), transient conditions (b) and the quasi-equilibrium approximation in (c) [25].

All of the above studies describe the behaviour of the film and the contacts are considered to instantly provide the inversion charges in the transistor channel. However, chapter 4 illustrated that the state of the contact can severely affect the SOI response. In the literature, the contact effect was captured in some special cases as shown in the next sub-sections.
5.1.3 Non-ohmic contacts on 2D structures

As previously mentioned, the description of the pseudo-MOSFET contacts is not straightforward. A study on FD-SOI wafers with the effect of the Schottky barrier on the pseudo-MOSFET electrical response was reported [26] explaining its possible influence on the extracted $V_T$. Figure 5.4 presents the band structure of an SOI probed in the pseudo-MOSFET configuration for the flat-band condition and after $V_G$ is applied, considering a Schottky junction. Observe how the Schottky barrier induces band bending in the silicon under the contacts. According to the findings in [26], the Schottky barrier will severely increase the threshold voltage as the Si film thickness decreases and as the Schottky barrier increases. This can be easily understood, we remind that for thin Si film the two Si interfaces are electrostatically coupled. As a result, if the energy level varies due to the Schottky contact, the electrical behaviour of the whole device will be affected. This effect is illustrated better through the minority carrier distribution in the silicon film (Figure 5.5).

![Figure 5.4: Energy levels of an SOI wafer in the pseudo-MOSFET configuration considering a Schottky junction a) for flat-band conditions and b) after $V_G$ is applied at the device [26].](image)

![Figure 5.5: Minority carrier distribution in a SOI film with Schottky junctions as contacts. The carrier distributions in calculated for two back-gate voltages (5.6V are represented with full lines while 4.7V with dotted lines) [26].](image)
The minority carrier concentration profile along the channel is presented for two $V_G$ values applied to the back-gate of an undoped SOI with 35nm Si film thickness in Figure 5.5. Observe how the gate voltage affects the concentration under the source contact. Regardless of the applied voltage, the carrier concentration under the source is always lower than in the rest of the film. Also, the carrier concentration seems to reduce close at the edge of the region under the contact, as we approach the rest of the Si film. According to the authors in [26], for $V_G=4.7V$ the carrier concentration under the source is below the doping concentration of the film and thus this part of the silicon is depleted. At threshold, for $V_G=5.2V$, the minority carrier concentration is higher than the doping level, the device is in inversion and the contact behaves like ohmic. Thus, the inversion of the SOI depends on the contact. Note that, it is necessary to consider a Schottky contact for phenomena that take place in depletion as illustrated in [27], for the accurate estimation of the carrier lifetime during depletion in SOI wafers measured with the pseudo-MOSFET.

A similar dependence of the contact type on the back-gate voltage was observed in graphene/MoS$_2$ systems. In these multilayer structures, graphene is deposited on MoS$_2$ (Figure 5.6a) and the contact type showed a dependence on the applied voltage on the substrate used as back-gate [28], similar to the SOI with Schottky contacts. As observed by the drain current versus drain voltage (Figure 5.6b), the contact type is different for $V_G=-10V$ and $V_G=42V$. Remember that a similar dependency was observed in the pseudo-MOSFET (chapter 2), TCAD simulation (chapter 3 in the appendix B) and for the metal contact SOI (chapter 4). For the graphene/MoS$_2$ structure this property is attributed to the variable Schottky barrier of the graphene (Figure 5.6c), which reduces as the back-gate voltage increases. This modifies the amount of carriers that can be injected in the conductive channel and affects the device performance.

In the general case of Schottky contacts the barrier height depends on two materials and on the process but, it stays fixed during device operation. Note that, the theoretical value corresponds to the difference between the semiconductor and metal workfunction values. However, the real value can vary significantly [29] due to Fermi level pining. In the SOI with metal contacts only the properties of the Si film can be modified by the applied voltage, as we will see later in the next sections of this chapter.
Chapter 5: Origin and modeling of the out-of-equilibrium body potential

Figure 5.6: a) Schematic of a MoS$_2$ with graphene deposited on the top interface. b) Drain current versus drain voltage curves for negative (on the top) and positive (bottom graph) $V_G$ applied to the substrate c) graphene Schottky barrier modulation by the back gate [28].

Resuming with silicon devices, the research on the transient effects on Schottky junctions is very limited. In the next session, we discuss briefly the transient modeling of a silicon diode as an example.

5.1.4 Transient effects in p-i-n silicon diodes

The last state-of-art result that we will refer to is a transient effect observed in p-i-n diodes. While the structure is not identical with the ones in this thesis, the similarities of the responses between this devices and ours is remarkable and they should be mentioned. In the reality, the devices are non-ideal components and variations can occur during switching, if the carrier transport time is significantly big. Ma and Lauritzen [30] developed a model that included the transient recovery of a p-i-n diode when a fast potential signal is applied.

Figure 5.7a presents the model schematic of [30] and Figure 5.7b the forward recovery waveform of the studied diode. In our case, the Schottky diode for $V_G>0$ is forwardly biased. Thus we should focus on the forward recovery in [30]. Their model by solving Poisson equation and for the forward recovery, they only considered the drift term of the current. Observe how their modelled curve follows a linear increase that leads to a maximum similar to the experimental $V_B$ of the pseudo-MOSFET. This peak later drops to the equilibrium value like $V_B$ measured in chapter 2.
5.2 Numerical simulations

5.2.1 Potential equations and $V_B$ response

The aim of this sub-section is to verify whether the Poisson and continuity equations used for semiconductor modeling can recreate the transient potential response. For the static potential $V$, we only calculate the contribution of electrons and we exclude $N_A$ as in [13] and [17] since the Si film was essentially undoped. All the studied cases in the literature consider the continuity equation for simulation of the transient effects and the quasi-Fermi potential is included as explained in [24]. The final forms of the equations are:

$$\Delta V = \frac{q}{\varepsilon} n_0 \cdot e^{\frac{V-U_c}{kT}} \quad (5.6a)$$

$$\nabla \cdot \left( \mu \cdot n_e \cdot \nabla(U_c) \right) = -n_e \frac{q}{kT} \frac{d(V-U_c)}{dt} \quad (5.6b)$$

where $V$ is the local potential, $U_c$ the quasi-Fermi potential, $\mu$ is the electron mobility, $n_e$ and $n_0$ are the local and the equilibrium minority carrier density concentrations, respectively. The equations were solved numerically in FlexPDE solver [31]. Note that, equation (5.6b) is the continuity equation (5.5) as we programme it in the differential equation solver to facilitate the simulations and reduce calculation times.

The simulation domain consists of a 70nm Si film over 30nm BOX, to fit the experimental structure. The structure has a source contact with a length $R$ and a silicon channel length of $L$; the total device length is $R+L$. A schematic is presented in Figure 5.8. To accurately compensate for the large mesa size, the equations (5.6) were solved in the cylindrical domain.
Chapter 5: Origin and modeling of the out-of-equilibrium body potential

as shown in the schematic. Following this technique, the problem is projected from 3D to 2D, with a reasonable number of points where the coupled equations were solved. For the boundary conditions, a $V_S - |V_{SB}|$ voltage was applied on the source contact with $V_S = 0$ at all times since source is grounded in all of the experiments. The additional voltage $|V_{SB}|$ is added to emulate the Schottky barrier, similar to the Schottky conditions of commercial simulation tools [32]. A gate voltage $V_G = SS \cdot t$ was applied to directly to the BOX; not substrate was included in the numerical solution of this chapter. A “zero flow” condition was selected for the potentials for the rest of the boundaries such as the floating Si part, the vertical Si and BOX boundaries on the sides of the structure. The transient body potential was taken equal to quasi-Fermi level at 0.9$L$ ($V_B = U_c @ 0.9L$) as indicated in the schematic. As a first step of verification, the dependence of the measured potential with the scanning speed (SS) is simulated and benchmarked with the experimental results.

![Figure 5.8: a) Top view of the simulation domain used in FlexPDE in cylindrical coordinates and b) cross-sectional view of the cutline shown in (a).](image)

Figure 5.9 illustrates the results of the numerical simulations with FlexPDE partial differential solver, for various scanning speed values. The curves show the same shape and dependence on SS as the ones shown in the previous chapters. Thus, one can conclude that the equations (5.6) are capable to reproduce the effect. Note that, no generation-recombination phenomena or channel doping concentration ($N_A$) are included in the differential equations, proving that the effect is not related to them. In the next sub-section, we benchmark the evolution of $V_B - V_G$ with SS in numerical solutions with experimental curves obtained with the transient measurements (as in chapter 2) and SOI devices with deposited metal contacts (from chapter 4).
5.2.2 Benchmark with transient experiments

The wafer used for this experiment is an SOI with a p-type lightly doped Si film (Na=10^{15} \text{cm}^{-3}). Cr was deposited following the lit-off process, as explained in chapter 4. The contact layout corresponds to 500\text{μm} side square placed in the angles of the Si mesa which has a 5x5cm^2 area. The source contact was kept grounded and the body contact was connected to the voltage follower used in chapter 2. The gate voltage was applied directly to the substrate through the chuck with an arbitrary pulse generator. For the gate current measurements the body contact was left floating and the measurements performed with a B1500 analyser and the B1560A fast I-V modules similarly to the transient measurements in chapter 2.

![Figure 5.10: Schematic of the experimental device measured in transient conditions.](image)

The experimental curves for various scanning speeds are traced for the transient body potential and gate current in Figure 5.11. The body potential shows similar response to the one produced with numerical simulations in FlexPDE (Figure 5.9). As the scanning speed increases...
the transient response is enhanced and the body potential reaches higher values. This is also accompanied by an increase of $V_G$ corresponding to the return to the equilibrium value for $V_B$.

The gate current in Figure 5.11b, shows the characteristic peak at the transition to the inversion regime and then its value drops in a SS dependent plateau. This is in perfect agreement with the transient $I_G$ in the pseudo-MOSFET (chapter 2) and all the explanations provided in chapter 2 are also valid here, for the metal contact SOI devices.

![Figure 5.11: Experimental $V_B$ (a) and $I_G$ (b) versus $V_G$ for transient conditions, with the same scanning speeds. As in chapter 2, the fluctuation on $V_B$ is a result of the data treatment presented in the appendix A.](image)

Now that, the metal contact SOI show similar transient characteristics as the numerical solutions of the simple equations (5.6). We analyse the potential distribution in the simulated domain to identify the origin of the out-of-equilibrium body potential.

### 5.2.3 Potential distributions and $V_B$ origin

The metal contact SOI transients have been benchmarked with the numerical solutions of the simple equations (5.6) and they show good agreement. We analyse the potential $V$ and quasi-Fermi potential $U_c$ distributions in the simulated domain to identify the origin of the out-of-equilibrium body potential in Figure 5.12. The potentials are plotted for two applied voltages, one during the linear increase (out-of-equilibrium) and one after the return to equilibrium, for comparison. To facilitate the description, we define two regions for the Si film of the structure. The first one corresponds to the Si part under the source contact, hereafter referred as Schottky diode region. The second one is the rest of the Si film which is named as MOS capacitor region in the analysis below. For $V$, one observes two constant potential values along the two regions, one under the source contact and one the rest of the Si film. The potential should be continuous and thus, it smoothly changes value from the Schottky diode region to
the MOS capacitor one, at the boundary between them. This variation extends to some hundreds of nanometres in the MOS capacitor, across the boundary. The quasi-Fermi potential $U_c$, is zero under the source contact. As we reach the boundary with the MOS capacitor, $U_c$ increases rapidly until it reaches the maximum value in the Si film. Then it stays constant along the full device length. This means that the body potential builds close to the boundary between the Schottky diode and the MOS capacitor regions. Considering the static potential, which is lower under the source contact, it is now obvious that the barrier originates from the electrostatic conditions imposed by the Si/metal interface and the coupling with the Si/BOX interface.

The last quantity, plotted in Figure 5.12, is the difference between the potentials, $V-U_c$. Notice how a valley with a minimum is formed close to the boundary under the contact for the transient conditions. This shows that a deficit of carriers close to the boundary of the MOS capacitor is defined. Clearly, the carriers provided by the contact are insufficient to charge the MOS capacitor and they are drained aggressively towards the Si film. However, this reduces the minority carrier concentration at the boundary and increases the resistance of this part of the device. For the equilibrium conditions (Figure 5.12b), the film is inverted and $U_c$ is zero along the whole length of the Si film. At this point we encourage the comparison with Figure 5.5 extracted from [26]. Notice how the potential has a similar shape as Figure 5.12. In the equilibrium conditions, even if $V_G$ is not sufficiently high to invert the Si film under the source contact, the necessary carriers are injected in the film in a slow rate until the device reaches a steady state. As a result, the effect is not captured because sufficient time is provided to the carrier to charge the BOX capacitance.

![Figure 5.12: Potential distributions along the Si/BOX interface under the Schottky diode and MOS capacitor regions. The selected $V_G$ values correspond to a) out-of-equilibrium (for $V_G=0.7V$) and to b) equilibrium ($V_G=1.4V$) conditions.](image-url)
Chapter 5: Origin and modeling of the out-of-equilibrium body potential

As shown in Figure 5.12, beyond 3.5μm, V and U_C are constant. Consequently, V_B shows not distance dependence on distance when monitored in a sufficient distance from source. The potential profile across the Si film thickness, presented in Figure 5.13, shows that both V and U_C are constant across the Si film depth. This verifies that the quasi-equilibrium approximation [25] (discussed earlier in sub-section 5.1.2), stands for the wafers tested in this chapter. Combining the above findings, one concludes that as long as the potential is traced at a point sufficiently far from the Schottky/MOS boundary, no dependence on distance is expected on the simulated value. Keep in mind that, in the fabricated devices the distance between the contacts are from 300μm to 4mm, which correspond to the range in which V_B reaches the plateau. For shorter devices (L<1μm), the modulation with the distance should also be considered.

Assuming a “step-like” behaviour of U_c between the two regions, with U_c=0 under the source contact, the Schottky diode is always in the equilibrium state and it is not affected by the rest of the device. On the contrary, the charge for the MOS capacitor is provided by the Schottky and can be in an out-of-equilibrium state if the carriers are not injected in a sufficiently high rate. The bias of the Schottky diode should correspond to the static value V. Since for the equilibrium conditions the Si film is depleted, a linear potential distribution can be considered across the Si film thickness. Solving Poisson’s equation (5.7a) and applying Gauss law on the boundary conditions on the Si/BOX interface we calculate the surface voltage under the source contact, V_surf, as

$$V_{surf} = \frac{C_{Si} \cdot (V_S - |V_{Si}|) + C_{BOX} \cdot V_G}{C_{Si} + C_{BOX}} \tag{5.7}$$
where $C_{Si}$ and $C_{BOX}$ are the Si film and BOX capacitances. This result will be used in the modeling approach later in this thesis (section 5.3). Before that, the dependence of the out-of-equilibrium on various physical parameter is presented. The aim of this investigation is the validation of the method and setting the reference for the comparison with the curves issued from the equivalent circuit model later.

5.2.4 $V_B$ dependence on geometrical and physical parameters

As in chapter 3, in the next sub-sections, the dependence of geometrical parameters such as $t_{Si}$, $t_{BOX}$, $R$, $L$ and physical ones, mobility and Schottky barrier height, are presented.

In this section, a large number of the numerical simulations show similar trends as the TCAD simulations, in chapter 3. To avoid a tedious presentation, the attention is focused only on the particular elements brought by the FlexPDE simulations, like the Schottky barrier, contact radius $R$ and carrier injection direction. Any discrepancy with TCAD will also be discussed. After, the parameters for which a one-to-one comparison between FlexPDE and TCAD is possible, are grouped together and presented briefly at the end of this sub-section.

Analysis of the Schottky barrier effect on $V_B$

To emulate a Schottky contact in the FlexPDE numerical solver an additional voltage was added ($-|V_{SB}|$). Note however that, no “limitations” on the current injection were imposed here. This strategy was sufficient to recreate the out-of-equilibrium potential response, unlike the TCAD simulations with metal contacts performed in chapter 3. This forced us to artificially create a barrier with our TCAD simulations structure. The reason for that seems to be the much smaller TCAD structure which could potentially be capable of recreating the effect, if physical parameters such as the mobility are tuned to unrealistically small values. A more detailed explanation is presented in the Appendix D. Regardless the fact that only a potential condition was defined for the Schottky contact, $|V_{SB}|$ is expected to describe accurately the effect of a Schottky barrier.

Figure 5.14 depicts the dependence of $V_B - V_G$ curves for various Schottky barriers. As $|V_{SB}|$ value increases, the body potential response exhibits higher maximum values. Additionally, the out-of-equilibrium regime expands: the linear increase starts at lower $V_G$ and the drop occurs at higher gate voltages.
Figure 5.14: Numerical simulations of the body potential versus gate voltage for various Schottky barrier heights calculated in FlexPDE solver. $V_B$ was calculated as $U_C$ at 0.9$L$. The scanning speed was set to 5V/s.

Comparing the results from Figure 5.14 with TCAD simulations in chapter 3 (sub-section 3.5.1), a similar behaviour of $V_B$ was observed when the length of the PN contact increases. At first, this outcome seem bizarre, but in reality it corresponds to the effect seen here. In the FlexPDE simulation, $|V_{SB}|$ increase defines the barrier by partially controlling $V_{surf}$ in equation (5.7). In TCAD simulation this barrier is modified by the extension of the depletion region under the P$^+/N^+$ regions of the contact, thus the effect on $V_B$ is similar for both. This can be further supported by the dependence of $V_B$ on the contact radius $R$ in the FlexPDE calculations.

$V_B$ dependence on the contact size

Figure 5.15 illustrates the influence of the contact radius $R$ of the simulated structure (Figure 5.8) on the $V_B$ response. As the contact radius increases the body potential weakens and the $V_G$ range where it occurs shrinks. Although this is the exact opposite outcome with what was presented in TCAD simulations, it agrees with the experimental data of chapter 4 (section 4.5). The discrepancy between the simulations originates from the different manner that the barrier is formed. For the P$^+/N^+$ regions, the bands in the undoped part are bended due to the difference in the doping. As a result, this barrier is imposed by the structure itself. In the FlexPDE simulations, there is no space charge region defined “artificially” as in TCAD. A depleted region is formed at the boundary under transient conditions due to the insufficient amount of carriers provided by the contact. Consequently, under dynamic conditions an equivalent to a space charge region occurs naturally in the structure with the Schottky contacts. When comparing with the experiments, an improved description of $V_B$ is made with FlexPDE at this point. The physical meaning behind this behaviour is the conductivity of the Source.
contact. Since the resistance of each element is inversely proportional to the area, a larger contact will provide more carriers in Si film leading to a $V_B$ decrease. This also verified by our models later in this chapter (section 5.3).

Figure 5.15: Numerical solution of the body potential versus gate voltage for various source radii (calculated with FlexPDE solver). The scanning speed was set to 5V/s and the Schottky barrier at 0.1V.

All the scientific findings until this point, strongly signify that the origin of the transient out-of-equilibrium in the studied structure is related to the contact. To cover the topic spherically we present how the carrier injection direction could affect the response, next.

**Direction of the carrier injection**

In this sub-section, the geometry of the source contact on the occurrence of the out-of-equilibrium is tested. For that reason, the source contact, which is initially vertical to the Si, is placed at an angle by keeping the point at the boundary between the Schottky and the MOS capacitor regions constant and moving the other point ($y=0$), deeper in the silicon, to $0.75\cdot t_{Si}$ and $0.5\cdot t_{Si}$ and at the Si/BOX interface. Lastly, a parallel carrier injection was tested as the extreme case in which the Schottky diode region is completely bypassed. The structures are schematically illustrated in Figure 5.16.

Figure 5.16: Schematic of the various structures of the source contact to test the effect of the carrier injection on the occurrence of the body potential.
Figure 5.17 depicts \( V_B \) obtained numerically in the structures described in Figure 5.16. For these simulations, \(|V_{SB}|=0\) V and SS=5V/s were chosen. This ensures that the solver converges for most of the structures. The curves show an increase in the out of equilibrium \( V_B \) as the carrier injection changes from parallel to the SOI, to vertical. In the first four cases this is explained by considering equation (5.7). When the contact has a certain angle, \( V_{surf} \) is \( x \) depended and its value changes as we approach the boundary. Consequently, \( C_{Si} \) has a stronger effect on \( V_{surf} \), on the thinner parts of the source region. The carriers injected from the Schottky contact correspond to the integral from \( y=0 \) to \( y=R \) and their number is definitely smaller than in the vertical case. Thus the out-of-equilibrium body potential is enhanced as the angle increases. Very interesting is the parallel case, in which the Schottky diode is not controlled by \( V_G \). In this structure, the potential on the boundary is fixed and is not modified by \( V_G \), keeping a constant value defined by the boundary condition. As a result the carriers are injected at a constant rate which is not sufficient for changing the MOS capacitor as \( V_G \) increases. Consequently, \( V_B \) just increases indefinitely and the film never reaches an equilibrium state within the simulation time. This shows that the electrostatic “barrier” that block the instant carrier injection from source to the rest of the Si film depends on the \( V_G \) applied on the bulk.

It is worth mentioning that both FlexPDE and TCAD simulations produce equivalently the \( V_B \) response and each one deals with different problems that stem from the difficulties of simulating an “astronomically large” (for semiconductors standards) structure. Indeed the experimental structure is in the millimetre range and its contacts are ~50-500\( \mu \)m. In order to
avoid repeating the same explanations as in chapter 3, here we briefly present the rest of the geometrical parameters tested with FlexPDE (also tested in chapter 3 with TCAD) along with the effect of the mobility.

Figure 5.18 illustrates the dependence of $V_B$ on $t_{Si}$ in (a), $t_{BOX}$ in (b), silicon length $L$ in (c) and electron mobility in (d). For the three first parameters, the effect is identical to TCAD simulations and experiments in chapter 4. Thinner films, thicker BOXs and longer devices enhance the out-of-equilibrium response. The detailed explanations for the effect of each parameter remain the same in chapter 3 (sub-sections 3.5.3, 3.5.5, 3.5.6 and 3.6.1). A minor discrepancy is observed when comparing the dependence on the electron mobility in TCAD and FlexPDE. While in TCAD, the electron mobility affected the body potential drop and the hole mobility modified the $V_G$ at which $V_B$ starts to increase, here we observe that both, the increase and drop, to depend on the electron mobility. A major difference in the numerical solving of the equations (5.6) is that $V_B$ appears at positive $V_G$ only while in TCAD the linear increase starts for $V_G<0$. Thus, it is clear that TCAD simulation will have a dependence on hole mobility in that region. In any case though, lower carrier mobility increases the transient response, as in TCAD.
Chapter 5: Origin and modeling of the out-of-equilibrium body potential

Figure 5.18: Numerical solution of the body potential versus gate voltage in FlexPDE solver. The dependence on $t_{Si}$ is depicted in (a), on $t_{BOX}$ in (b), on the Si length $L$ in (c) and on the electron mobility in (d). The scanning speed was set to 5V/s for all the simulations and the Schottky barrier to 0.1V. Exception is (b) in which the barrier is set to 0.05V so the simulation converges for all the structures. Other parameters are: $t_{Si}$=70nm, $t_{BOX}$=30nm, $L$=18μm and mobility $\mu_0$=500cm$^2$/V/s, unless differently stated in the graph.

All the differences between the TCAD simulations and the solution from FlexPDE are pointed out. Each method has a different approach to emulate the $V_B$ response and this imposes several limitations. Nevertheless, in both simulations, $V_B$ is well described, a very good agreement between the methods is observed and each one provided different elements necessary for the understanding of the out-of-equilibrium response.
5.3 Equivalent circuit model

As previously shown by the potential distribution of Figure 5.12, the voltage drop occurs between the Schottky diode region and the MOS capacitor. Thus we can image a two-component equivalent circuit to describe the phenomenon, as illustrated schematically in Figure 5.19. In the model, the region that is under the contact is replaced by a vertical Schottky diode which is forwardly biased through the gate voltage. Considering the voltage drop in the BOX, the bias that the Schottky diode sees on its semiconductor side is $V_{surf}$ that is given by the equation (5.7). This diode is then connected to the MOS capacitor which is accurately modeled with the Lambert function (see Appendix E). Based on this circuit and the physical understanding that we gain from the simulations, the out-of-equilibrium body potential response should appear when there is a difference between the currents of the two components.

![Figure 5.19: Schematic of the two components modeled. The Si/BOX under the contact is replaced by an equivalent Schottky junction.](image)

To model the experimental Schottky diode current we start from the equation [33], [34]:

$$I_{Sc} = A_{Sc} \cdot A^* \cdot T^2 \cdot e^{-\frac{q|V_{Sh}|}{kT}} \cdot \left( e^{\frac{qV_{Surf}}{kT}} - 1 \right)$$  \hspace{1cm} (5.8)

where $A_{Sc}$ is the area of the Schottky diode, $V_{surf}$ is the potential on the Si/BOX interface, as calculated previously and $A^*$ is the effective Richardson constant. The other parameters have the usual meaning. The ideality factor of the Schottky diode was considered equal to one at all cases.

For the calculation of the MOS capacitor current we employ the inversion charge based on the Lambert W function [35], [36] equation:

$$Q_{inv}(t) = A_{MOS} \cdot C_{BOX} \cdot \frac{n k T}{q} \cdot LW\left( e^{\frac{q(V_G-V_T)}{n k T}} \right)$$  \hspace{1cm} (5.9)

where $A_{MOS}$ is the area of the capacitor and $LW$ is the abbreviation for the Lambert W function, $n$ is the ideality factor of the Si film and the rest of the parameters have the usual meaning. The inversion current ($I_{inv}$) is the derivative of the inversion charge $Q_{inv}$ (eq. 5.9) with respect to time ($I_{inv}$=$dQ_{inv}/dt$). So, by substituting the areas with the experimental values for the Schottky
(A_{Sc}=2.5\cdot10^{-7}m^2) diode and MOS capacitor (A_{inv}=2.5\cdot10^{-5}m^2), we can calculate the two currents and compare them in the same plot.

Figure 5.20 illustrates $I_{inv}$ and $I_{Sc}$ for the two SS tested. While $I_{Sc}$ is perfectly superposed for the two scanning speeds, $I_{inv}$ value increases with SS. This was expected from the equations (5.8) and (5.9) since $I_{Sc}$ does not show any other dependence in SS except the one which is included in $V_G=SS\cdot t$. On the contrary, $I_{inv}$ is calculated through the derivative with respect to time and with a fast analysis we can observe that SS contribution appears independently of $V_G$:

$\frac{dQ_{inv}}{dt}=(\frac{dQ_{inv}}{dV_G}) \cdot (\frac{dV_G}{dt})=(\frac{dQ_{inv}}{dV_G}) \cdot SS \quad (5.10)$

The device behaviour can now be explained from a physics point of view, if we analyse the currents. The Schottky diode current is smaller than the inversion one for low $V_G$. Since the carriers are injected through the Schottky diode and the diode is not capable of providing electrons needed in the MOS capacitor, a carrier deficit is defined. This deficit increases until the intersection point of the two currents ($I_{Sc}=I_{inv}$). Although, for higher $V_G$ the Schottky diode current is now sufficient to charge the MOS capacitor, the real current continues to increase because it needs to compensate for all missing carriers during the regime $I_{Sc}<I_{inv}$, until the equilibrium point is reached. Then the current rapidly drops to the $I_{inv}$ value and the device is in equilibrium. The equilibrium points were calculated by integrating the difference between the $I_{inv}$ and $I_{Sc}$ to give equal areas before and after their intersection point. The integration yielded $V_{G5}=0.72V$ and $V_{G10}=0.77V$ for the SS=5V/s and 10V/s respectively.

The calculation of the body potential was based on the potential distribution shown in Figure 5.12 and the equivalent circuit. The potential drops on the boundary between the Schottky diode and the MOS capacitor. At the same time, this potential increase is the result of the carrier deficit due to the Schottky diode. Thus, the potential increases according to the difference between the inversion charge needed and the charge provided by the contact. Similar to the formula in [10] we calculate the body potential as the charge difference between the Schottky contact and the MOS capacitor divided by an equivalent capacitance $C$ as:

$V_B = -\frac{Q_{Sc} - Q_{inv}}{C} \quad (5.11)$

where $Q_{Sc}$ is the integral of equation (5.8). The modeled body potential is plotted in Figure 5.20b. The body potential shape is recreated by equation (5.11) for values that correspond to the experimental structure and conditions. The body potential increases with SS as in the
Chapter 5: Origin and modeling of the out-of-equilibrium body potential

experiments. The return to the equilibrium occurs at the $V_G$ voltage corresponding to the equilibrium points in Figure 5.20a.

![Figure 5.20: Schottky and inversion currents (a) and calculated body potential with respect to the gate voltage for SS=5V/s and SS=10V/s. The equilibrium point is presented with dotted lines. The Schottky barrier was set to $|V_{SB}|=0.3V$.](image)

In order to verify the influence of the Schottky barrier, Figure 5.21a depicts $I_{inv}$ and $I_{sc}$ for two $V_{SB}$ values. In chapter 4 we calculated the Schottky barrier of our devices at 0.36V, thus here we tested 0.3V and 0.4V for $V_{SB}$. As expected from the equations, since $|V_{SB}|$ is a parameter only appearing in $I_{sc}$, $I_{inv}$ stays unaffected, while the Schottky current shifts towards positive $V_G$. As $|V_{SB}|$ increases, so does the carrier deficit since the intersection point shifts to positive voltages. Consequently, the return to equilibrium is reached at higher $V_G$. This is depicted also in the body potential curve which shows a strong increase with $|V_{SB}|$.

![Figure 5.21: Schottky and inversion currents (a) and calculated body potential with respect to the gate voltage, for $|V_{SB}|=0.3V$ and $|V_{SB}|=0.4V$. The equilibrium point is presented with dotted lines. The scanning speed was set to 5V/s.](image)
Although, this simplified model captures well the transient body potential, it has also several limitations. This becomes evident when comparing the modeled curves which always follow the same path during the body potential linear increase, with the simulated (FlexPDE) curves that follow different paths for various scanning speeds or barrier heights. A possible explanation for this is that the voltage modulation under the source contact close to the boundary that is not captured by our equivalent circuit. Remember that for the calculation of $V_{surf}$ we considered $U_c=0$ under the whole region of the contact. Additionally, the effect shows a dependence on mobility, which is not included in any of the semiconductor component equations used. Lastly, the FD-SOI film for low $V_G$ has no mobile charges. Regardless of the limitations, the model reproduces quite well the dependences on $SS$ and $|V_{SB}|$. The question is: does this model describe also well the impact of the geometrical parameters for device engineering?

5.4 Circuit model and device parameters

The proposed model includes directly all the geometrical parameters that concern the studied structure. In the next sub-sections, these parameters will discussed along with the dependence on $V_T$.

5.4.1 Impact of device area, as captured by the equivalent circuit

To test equation (5.11) for various die areas, we plot the modeled curves for a 4x4mm$^2$, 5x5mm$^2$ and 6x6mm$^2$ dies in Figure 5.22. In the model, the capacitive coefficient $C$ was chosen to be equal to the BOX capacitance. Even if this seems to be a good order of magnitude, the real capacitive coefficient in depletion is smaller as described in [37]. Although in equation (5.11) $C$ is considered as constant coefficient, in reality a capacitive value depends on the capacitor area and on the thickness of the dielectric material. To accurately illustrate the effect of the $A_{MOS}$ on the modelled $V_B$, the curves are produced for $C$ constant in (a) and for $C=A_{MOS}\varepsilon_{ox}/t_{BOX}$ in (b). Starting from the case with constant $C$, the potential starts increasing for the same $V_G$ but has different slopes in the linear region and exhibits higher maximum values for larger dies. Most importantly, the return to the equilibrium occurs at higher $V_G$ since the need for inversion charge (and therefore the deficit of carrier) is bigger for larger $A_{MOS}$. One can observe that, when the capacitive coefficient dependence on $A_{MOS}$ is included, $V_B$ follows the same path during the linear increase but once again the $V_G$ value for return to the equilibrium is higher as the $A_{MOS}$ increases. This implies that $C$ should be adapted with the die size.
Chapter 5: Origin and modeling of the out-of-equilibrium body potential

5.4.2 Impact of contact area, as captured by the equivalent circuit

To illustrate how the model captures this dependence on the Schottky diode area, \( V_B \) model is traced for three \( A_{Sc} \) values in Figure 5.23. Smaller contact areas provoke higher \( V_B \) maximum values and a return to equilibrium at higher \( V_G \). A comparison with Figure 5.15, shows a similar trend between simulations and the model. This result is also in agreement with the experimental results in chapter 4 (Figure 4.26), where large contacts (ribbon layout) produced significantly smaller \( V_B \) signals when compared to smaller ones (small circles) which exhibited almost twice higher \( V_B \) maximum values.

Figure 5.22: Modeled body potential versus gate voltage for various Si mesa areas for a constant capacitive coefficient \( C \) in (a) and for \( C=A_{MOS}\varepsilon_{ox}/t_{BOX} \) in (b). The scanning speed was set to 5V/s and Schottky barrier to 0.4V.

Figure 5.23: Modelled body potential versus gate voltage for various Schottky contact areas. The scanning speed was set to 5V/s and Schottky barrier to 0.4V.
5.4.3 Impact of t_{BOX} variation on the modeled curves

Similar to the analysis on A_{MOS}, t_{BOX} is a parameter of the capacitive coefficient. Figure 5.24 illustrates the evolution of V_{B} with BOX thickness for constant capacitive coefficient in (a) and for C=A_{MOS} ε_{ox}/t_{BOX} in (b). In both cases, V_{B} is enhanced and returns to equilibrium at higher V_{G}. While in Figure 5.24a, the linear increase shows different slopes, in (b) V_{B} follows always the same path. Showing again that C_{BOX} is associated with the equivalent capacitance but the exact value of C should be carefully selected to include any size dependent effects, as in Figure 5.24b. Lastly, the Si film thickness is evaluated.

![Graph a) and b)](image)

*Figure 5.24: Modeled body potential versus gate voltage for various BOX thicknesses for constant capacitive coefficient C in (a) and for C=A_{MOS} ε_{ox}/t_{BOX} in (b). The scanning speed was set to 5V/s and Schottky barrier to 0.4V.*

5.4.4 Model response t_{Si} variation

Figure 5.25 depicts the dependence of the modeled V_{B} with t_{Si}. A thicker silicon film shows a weaker potential response. The return to the equilibrium occurs at lower V_{G}. Observe how the intervals between the V_{G} values were V_{B}=0 are not equal. Considering that the return to the equilibrium corresponds to the rapid injection of carriers for the inversion of the MOS capacitor it could be described as a V_{T} reduction. A non-linear decrease of V_{T} with t_{Si} was also observed in [38] and the response seemed to be parabolic. Additionally, regardless of the t_{Si} value, V_{B} follows the same path during the linear increase. Lastly, the MOS capacitor equation also shows a dependence on V_{T}. While the threshold voltage is a function of the gate material, it appears independently in the proposed model and its effect is examined next.
Figure 5.25: Modeled body potential versus gate voltage for various Si film thicknesses. The scanning speed was set to 5V/s and Schottky barrier to 0.4V.

5.4.5 Model response on $V_T$

Figure 5.26 illustrates the effect of the MOS capacitor threshold voltage on the modeled $V_B$. The body potential signal starts to increase at lower voltages for lower $V_T$. Considering that the potential variation corresponds to a lack of carriers and $V_T$ is the value at which the film inverts, a lower $V_T$ translates to a higher carrier deficit at given $V_G$ and thus, a stronger $V_B$ signal for that given $V_G$. The return to equilibrium stays relatively unaffected by $V_T$ since the Schottky contact is (almost) independent of the inversion state of the film. Finally, this parallel displacement is very similar to the experimental and numerical results for the SS increase. Thus, one can imagine a transient term added (or subtracted) to $V_T$ that could potentially model the transport mechanisms which are not captured by our equivalent circuit model.

Figure 5.26: Modeled body potential versus gate voltage for various Si film threshold voltage values. The scanning speed was set to 5V/s and Schottky barrier to 0.4V.
5.5 Conclusion

This chapter focuses on the understanding of the physical mechanisms that provoke the out-of-equilibrium body potential in SOI with metal contacts. The Poisson and continuity equations used previously to model undoped thin film SOI devices were solved with a partial differential equation solver (FlexPDE).

The numerical results obtained with FlexPDE are in a good agreement with the TCAD simulations in chapter 3. Although, mobility and contact radius show a counterintuitive impact on the body potential, the difference is attributed to the highly doped P+ N+ regions used as contacts in TCAD. Note that, contact radius simulations in FlexPDE are in agreement with the experiments. The potential distributions in the silicon film reveal that the effect originates from the difficulty to inject electrons from the source to the Si film, due to an area of low carrier concentration under the Source contact. To model this behaviour, the source region was considered as Schottky contact placed on top the SOI. On the Si side, the diode is polarized through the gate voltage, after excluding the voltage drop on the BOX. The rest of the device is well understood and modelled as a MOS capacitor using the Lambert W function for the calculation of the inversion charge.

The V_B response was then recreated with an equivalent electronic circuit consisted by a Schottky diode and a MOS capacitor. The circuit model contains all the geometrical parameters of the device and the benchmark with the FlexPDE numerical simulations show that it provides an accurate description of the effect. This can be seen in the resume of the V_B dependency on the physical and technological parameters is provided in Table5.1. The green arrows signify an increase in the respective quantity while the red ones a decrease.
Table 5.1: Summary of the $V_B$ dependence on physical and technological parameters as evaluated experimentally, in TCAD and Flex-PDE simulations and by our equivalent circuit model.

<table>
<thead>
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<th>Physical and Technological Parameters</th>
<th>Experiments</th>
<th>TCAD simulation</th>
<th>Flex-PDE</th>
<th>Model</th>
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</table>

This outcome is a start towards a compact model that can vastly accelerate the circuit design in the next development stages of a pragmatic sensor. At its current state, the model is not perfect. The major drawback is that the two components used are considered completely independent while in reality, the voltage continuity mandates a modulation of the static and transient potential at the Schottky/MOS capacitor boundary. This means that any transport effects from one region to the other are not captured by this model.

Although the calculated curves in FlexPDE show that the potential increase should start at lower $V_G$ as SS or $|V_{\text{Si}}|$ increases, in the circuit model curves, $V_B$ follows always the same path. This discrepancy is attributed to the compromise made during the model development in which the diode is independent of the MOS capacitor. In reality, the potential of the MOS capacitor affects the potential distribution under the source contact. This creates a space charge region at the boundary between the two components which provokes the carrier transport from one region to the other. Finally, a fast solution to this problem could be the implementation of an additional transient term added to the MOS capacitor threshold voltage in the Lambert W function.

Our technology and understanding of the $V_B$ origin are now mature enough, so we can move to the pH sensing application in the next chapter.
References


Chapter 6: A novel pH sensor based on out-of-equilibrium body potential reading

Table of contents

6.1 Introduction .................................................................................................................. 146
6.2 Sensing ability of SOI substrates (pseudo-MOSFET): state of the art .......... 147
   6.2.1 $D_D$ in the pseudo-MOSFET: the starting point for sensing .................. 147
   6.2.2 Pseudo-MOSFET sensing based on the $I_D-V_G$ curves ................. 149
   6.2.3 Body potential sensing in the pseudo-MOSFET configuration .......... 150
6.3 Surface functionalization for our pH sensors ........................................................... 152
   6.3.1 Electrical response of APTES functionalization ................................ 153
6.4 Metal contact SOI devices as pH sensors: current response ......................... 155
   6.4.1 Modifications of the experimental set-up ............................................. 155
   6.4.2 Drain current response to various pH solutions ................................. 156
   6.4.3 The $I_D-V_G$ response of the sensor .................................................. 158
   6.4.4 Drain current calibration curves .......................................................... 161
6.5 Metal contact SOI devices for pH sensors: $V_B$ response ............................... 162
   6.5.1 Experimental $V_B$ response for pH detection .................................. 162
   6.5.2 Body potential calibration curves ......................................................... 164
   6.5.3 Reproducibility of the pH detection ..................................................... 165
6.6 Optimisation of the sensor through 2D TCAD simulations ............................... 167
   6.6.1 Simulated drain current response to pH ............................................ 169
   6.6.2 Simulated body potential response to pH .......................................... 170
   6.6.3 Body potential calibration curves – tuning .......................................... 171
   6.6.4 Discussion on the device tunability ...................................................... 176
6.7 Conclusion .................................................................................................................... 180
The previous chapters had as main objective the transducer development for transducer based on the out-of-equilibrium body potential. In this chapter, all the technological progress and theoretical understanding are combined to showcase and describe the performance of our sensor.

6.1 Introduction

The pioneering work of Bergveld [1], introduced a FET device into the bio-chemical detection, the ion-sensitive field effect transistor ISFET), compatible with the large scale CMOS fabrication process. ISFETs can easily be integrated into electronic systems, permitting the development of compact and portable “lab-on-chip” type of products. However, since the ‘70s, the development of microelectronics devices grew exponentially, offering new substrates for FET-sensors development, such as SOI wafers. Naturally, SOI-ISFETs or devices derived from ISFETs (like nanowires, nanoribbons, nanotubes, etc…), were developed for performance improvement, exploiting the advantages of both channel isolation and nano-scale wires, leading to ultra-sensitive devices. Additional opportunities of sensors, were exploited thanks to the unique ability of the double-gate MOSFETs to tune the operational-region of the device with the secondary gate. For example, improved sensing performance was reported in the subthreshold region of the transistors [2], [3]. While many single-gate ISFET (e.g. extended gate ISFET, etc…) have been proposed to improve the device performance [4], it has been reported that a super-Nernstian response can be achieved in an “SOI-ISFET-like structure” when sensing is done based on scanning the back-gate of [5]–[7]. Recent publications report a sensitivity up to 730mV/pH for industrial CMOS compatible devices [8] under back-gate operation. This results in signal amplification through coupling of the top and bottom gates of the device. Note that device sensitivity should not be confused with sensitivity of the membrane which is in contact with the liquid solution [9]. In the literature is reported that WO$_3$ sensing membranes can exceed the 59mV/pH limit through increase of adsorption sites on the interphase [10]. However, all the above studies, as well as others in nanowires [9], [11] or alternative materials [12]–[16], use the shift in the drain current versus gate voltage for detection. A small amount of reports propose other methods, like modification of the Schottky barrier by bio-chemical species [17]–[20] or single trap effects and noise measurements [21]. This chapter focuses on sensing based on the out-of-equilibrium body potential reading.

Section 6.2 shows the state of the art of sensing with simple SOI structures in the pseudo-MOSFET. Section 6.3 presents the functionalisation of the SOI devices with metal contacts. In the section 6.4, the response of the sensor is evaluated for the drain current measurements and...
then it is compared with the experimental body potential in the section 6.5. Lastly, some optimisation paths for the sensing capabilities of the device are illustrated through 2D TCAD simulations in the section 6.6.

6.2 Sensing ability of SOI substrates (pseudo-MOSFET): state of the art

The principle of the bio-chemical detection presented here starts with the effect of charges placed on the top SiO$_2$ layer that covers the SOI. In this section the state of the art of sensing with SOI in the pseudo-MOSFET configuration is presented. The presentation discusses the effect of D$_{it}$ and charges attached to the top interface either though chemical modification of the sensing interface or charged nano-particles.

6.2.1 $D_{it}$ in the pseudo-MOSFET: the starting point for sensing

As shown in chapter 2, SOI wafers are characterized with the pseudo-MOSFET configuration [22] and this is the inspiration for our devices with metal contacts (chapter 4). The effect of any charge variation, fixed charges or trapping/de-trapping close to the channel is known in SOI. In the pseudo-MOSFET any change close to the channel modifies its conduction. That change could be either a fixed charge in the gate dielectric or on top of it, or trapped/de-trapped charge coming from interface states (D$_{it}$). Figure 6.1a, illustrates a cross section of an SOI highlighting the three Si/SiO$_2$ interfaces and the respective surface potentials $\psi_S$ and interface state densities D$_{it}$. Note that, in static conditions, interface states are charged, acting like fixed charges thus in first approximation D$_{it}$ will affect the channel similarly the Si to any charged species on the top. However, in dynamic conditions, the traps are active and they cannot be equated to a static charge. This is also illustrated [23], where the subthreshold swing shows a different dependence than $V_T$, for various Si film thicknesses. For the purpose of this demonstration, we focus on the D$_{it2}$ of the top Si/SiO$_2$ since the charges from species under detection placed on the top oxide layer will show similar effects, (Figure 6.1b).
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

Figure 6.1: SOI wafer schematic: a) illustration of the Si/SiO$_2$ interfaces with the respective surface potentials and interface trap densities; b) effect of charged particles placed on top of the silicon film. Notice how the charge affects the silicon layer between the top oxide and the BOX.

The conduction takes place on the bottom Si/BOX interface. Thus we focus on the effect of $D_{it2}$ on $\psi_{Si}$. The mathematical model that describes the threshold voltage ($V_T$) is [23]:

$$
V_T = V_{FB} + \frac{2\varphi_F}{C_{ox}} \left( C_{it1} + \frac{C_{Si}C_{it2}}{C_{Si}+C_{it2}} \right) + \frac{qN_a Si}{2C_{ox}} \left( 1 + \frac{C_{Si}}{C_{Si}+C_{it2}} \right)
$$

(6.1)

where $V_{FB}$ is the flat-band voltage, $C_{it1}$=q$D_{it1}$ and $C_{it2}$=q$D_{it2}$ are the interfaces states capacitances for the bottom and top interfaces respectively, $C_{Si}$=\(\varepsilon_{Si}/t_{Si}\) is the silicon film capacitance, $\varphi_F$=(kT/q)ln(N$_a$/n$_i$) is the bulk potential, N$_a$ the doping concentration of the film and n$_i$ the intrinsic carrier density. Evidently, $V_T$ is mainly affected by $C_{it2}$, especially when $C_{Si}$ is large. The dependence is depicted in Figure 6.2 with experimental and simulated curves. For thinner silicon films the effect of $D_{it}$ is more pronounced especially for higher $D_{it}$ values where the curve seems to have an exponential dependence as in simulations. Thus, one can conclude that the top interface states affect the conductive channel in fully depleted FD SOI, especially when the thickness of the film is reduced. This effect is no different than the coupling of the top and bottom gates in SOI-MOSFETs reported in [24]. An effect similar to the $D_{it}$ is expected with charged molecules intentionally deposited on the top surface for sensing purposes.
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

6.2.2 Pseudo-MOSFET sensing based on the $I_D$-$V_G$ curves

The proof of concept of sensing with the pseudo-MOSFET was done using $I_D$-$V_G$ curves, and more precisely the $V_T$ shift induced by the charges intentionally placed on the top SiO$_2$ layer. In all the cases, the top silicon layer was functionalised to reach the selectivity needed. However, besides the selectivity gain, which will be discussed in the next section, the surface treatment itself charges the modified surface. A widely used substance [11], [25]–[28] for the SiO$_2$ surface functionalization is the 3-aminopropyltriethoxysilane (APTES) treatment. The amino-terminated layer obtained on the SiO$_2$ surface [29] has a positive charge, acting like a positive top-gate. Such an effect was demonstrated previously with APTES and gold nanoparticles on bare SOI [30]. Figure 6.3a, illustrates the $I_D$-$V_G$ characteristic curves of an SOI wafer before and after APTES functionalization. Evidently, the curve is shifted toward negative voltages, as expected due to the positive charges placed close to the conductive channel. Note that, these experiments were conducted with the pressure probe pseudo-MOSFET configuration so, the placement of the contacts on the silicon film creates defects that might induce a variability on the parameter extractions between different measurements [31]. Besides this variability, the SOI wafer produces quite accurate results as presented in Figure 6.3b. After a study of 15 individuals dies tested with APTES, the shift observed and by Fernandez et al. [32] seems to be quite reproducible.
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

Figure 6.3: a) $I_D$-$V_G$ curve of an SOI measured in the pseudo-MOSFET; the black curve corresponds to the unmodified die and the red one to the same die after APTES functionalization [30] b) Threshold voltage shift in 15 pseudo-MOSFET dies [32].

The threshold voltage shift imposed to the channel is proportional to the amount of charges placed on the sensing surface [32]:

$$\Delta V_T = Q_{sup} \frac{C_{si}}{C_{BOX}(C_{si}+C_{it2})}$$  \hspace{1cm} (6.2)

where $Q_{sup}$ corresponds to the charge added by the functionalization.

The studies show a change in the threshold voltage in the static $I_D$-$V_G$ curves proportional to the amount of charges placed on the top surface. However, is there any effect visible in the body potential?

6.2.3 Body potential sensing in the pseudo-MOSFET configuration

Previous studies have already demonstrated the detection of gold nanoparticles deposited on the Si surface by measuring the out-of-equilibrium body potential [33]. Figure 6.4 depicts the body potential and drain current versus gate voltage curves obtained on an 88/145nm SOI die, after APTES treatment and attachment of gold-nanoparticles. The die was measured under dry conditions, Benea et al [33] reported a shift in both body potential and drain current curves is coherent with the type of charge placed on the sensing layer. Indeed for a p` silicon channel the positive charge of the APTES induces an electron concentration increase in the film leading to lower threshold voltage. The opposite is true for the negative charges carried by the gold nanoparticles. A similar shift is induced by the charges to-be-detected between the body potential and the $I_D$-$V_G$ curves, indicating that the body potential depends on the threshold voltage of the device (which is in agreement with the model developed in chapter 5). These
experiments validate that the phenomenon could be used as a sensing technique, similar to the $V_T$ shift. The next step towards a practical sensor was to look for the quantification of the charges, in addition to the charge sign detection.

**Figure 6.4:** a) $V_B$-$V_G$ curves of 88/145 nm Si/BOX wafer in the pseudo-MOSFET configuration after various treatment steps (APTES, gold nanoparticles). b) Corresponding $I_D$-$V_G$ curves obtained during the same experiments in semi-log scale and linear scale in the inset [33].

The proof of the charge quantification through the body potential shift was also demonstrated by Benea et al. [34] with the detection of DNA strands attached to the top surface of the SOI. Figure 6.5 presents the response of the samples to DNA concentrations [34]. RNA strands were bonded on the surface after an epoxysilane (3-glycidoxypropyl) trimethoxysilane (GOPS) treatment. Afterwards, the dies was exposed to a buffer solution containing various concentration of the complementary RNA strands forming the attached DNA molecules on the device surface. Figure 6.5 a) and b) compare the shifts in the threshold voltage and the body potential respectively. The same dies were measured during different treatment states and the response of the various DNA concentrations is shown in the last three point of the graph. Evidently, both quantities shift accordingly to the DNA concentrations leading to the trace of the first calibration curve of the body potential measured in the pseudo-MOSFET configuration with pressure probes.
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

Figure 6.5: Electrical response of 88/145 nm Si/BOX for various DNA concentrations bonded with GOPS on the top silicon surface. a) Threshold voltage shift. b) Body potential shift with respect to the attached DNA concentration. [34].

In conclusion of this section, pseudo-MOSFET on SOI substrates with thin silicon films is capable of detecting charges placed on their top oxide surface and the sensing can be also done based on the body potential. In the next sections of this chapter, the performance of a pH sensor based on the out-of-equilibrium body potential reading in the SOI devices with deposited metal contacts is illustrated.

6.3 Surface functionalization for our pH sensors

Before showing the electrical measurements of the sensor, we pass to the experimental results and the sensor performance evaluation though, the binding theory of charged ions in pH solutions with APTES modified SiO$_2$ surfaces is discussed. Self-assembled monolayers are widely used functionalization layers [25], [26]. Additionally, they can modify the charge on the surface. More specifically, 3-aminopropyltriethoxysilane (APTES) is very often utilised for surface functionalization of ISFETs [27], [30], [32], [33], [35]–[37]. It was shown that without this step the sensors often have a non-linear response [37]–[39] or even completely incoherent calibration curves [36]. To avoid the above issues, a functionalized step with APTES was performed before the implementation of the liquid gate to our sensor. Moreover, any bio-chemical sensing application in wet conditions will include a buffer solution as the host for the molecule under test. This was the motivation to evaluate the sensors for solutions with various pH values. Note that, monitoring pH values in solutions is critical for a wide range of applications, from environmental monitoring [40] to DNA sequencing [41]. But what exactly is a pH value?
In aqueous solutions there is an equilibrium between water molecules (H₂O), hydrogen cations (H⁺) and hydroxide anions (OH⁻). The “power” of hydrogen cations expressed as the negative logarithm of the H⁺ activity is referred as pH value of a solution (pH=-log(α_H⁺)) [40]. Similarly, a value for the hydroxide anions can be defined as pOH value and it is complementary to pH. Solutions with pH values smaller than 7 are considered acidic with excess H⁺ and solutions with pH values greater than 7 are basic with surplus of OH⁻. In an APTES functionalized surface the ion binding mechanism was extensively discussed in the literature [35], [38], [42]. For acidic solutions the amine-terminated groups of the surface treated with APTES are getting protonated by the hydrogen cations. This increases the positive charge close to the top oxide layer, facilitating the creation of the conductive channel of electrons in the transistor. When a basic solution is used as liquid gate, then the –SiOH is deprotonated to –SiO⁻ acting like a negative biased gate and imposing a decrease of the concentration of electrons in the conductive channel. Figure 6.6 illustrates the aforementioned behaviour of the surface state in an acidic solution on the left and a basic one on the right. The schematic in the middle corresponds to a neutral solution.

**Figure 6.6:** Schematic of the binding reaction of solutions with various pH values of APTES modified SiO₂ surface. The functionalized wafer in a solution with pH=7 is depicted in the middle of the schematic. [38]

### 6.3.1 Electrical response of APTES functionalization

Considering all the above, we proceed into APTES functionalization of our devices prior to pH evaluation. The protocol used here is similar to [33]. In a cleanroom environment, the samples were cleaned thoroughly first with de-ionized water and then with ethanol. After drying in a flow of N₂ the samples were submerged in a diluted APTES solution (5ml APTES and 25ml ethanol) for 30 minutes. Finally, they were rinsed with ethanol and de-ionised water.
and annealed on a hot plate at 120°C for 30 min. To verify that the APTES treatment was successful, a control measurement was performed before and after the process. A device with three circular pads placed in the center of the device was chosen for this control measurement.

![Figure 6.7: Electrical characterization of 70nm silicon over 145nm BOX with circular chromium pads in the center of the device before, immediately after APTES and 4 days later to check the stability of the response. a) Body potential and b) drain current versus gate voltages curves (semi-logarithmic and linear scale).](image)

Figure 6.7 illustrates the electrical response for a) the body potential and b) for the drain current obtained before, immediately after functionalization and 4 days later. The positive charge attached on the top surface shifts the curves towards lower gate voltages. While 4 days later the measured curve still shows the same trend, the shift is less pronounced. This is probably attributed to the adsorption of ethanol in the SiO$_2$ layer [43]. Furthermore, the performance of the chromium pads seems to be unaffected by the APTES treatment. In any case, the APTES functionalization is successful and stable enough for the next sensing steps. Note that, the functionalized wafers were kept under vacuum at all times except during the measurements. The pH sensing experiments took place immediately after the functionalization process.
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

6.4 Metal contact SOI devices as pH sensors: current response

6.4.1 Modifications of the experimental set-up

In the literature, bio-chemical sensors were realized in wet environment with or without a reference electrode [4], [9]. Results obtained without reference electrode were either unstable or in dry conditions [4]. Indeed, the reference electrode ensures a closed electrical circuit, necessary for potentiometric sensors [44]. The performance of the reference electrode is also of a great importance. Commercial solutions of miniaturized reference electrodes are available on the market but they are costly and frequently large for integration. Considering that the goal is the development of a device compatible with the “lab-on-chip” approach, we preferred using a pseudo-reference electrode.

Pseudo-reference electrodes (pseudo-RE) consist of noble metals with or without surface coatings and they can be potentially deposited during fabrication directly on the substrate next to the device, achieving very compact packaging. Previous works [45] show a silver (Ag) pad deposited next to the device and then modified to develop a AgCl coating, acting as a pseudo-RE.

Since our device and sensing method have not reached yet this level of maturity for RE integration, we adapted the fabrication process of the reference electrode from [45] and we simply attach the wire on a standard probe placed in the standard probe holder (Figure 6.8 b). The silver wire was submerged in a 0.1M KCl solution and a 1.5V was applied with respect to a Ti wire which was the anode in the circuit. The Ag wire obtained a dark purple almost black colour after around 1 min. However, the process was 3 minutes to ensure a full coverage of the whole surface. It should be noted that, there is extended literature on the fabrication of Ag/AgCl reference electrodes [46]–[49], the majority of which follow a similar approach to the one used here.

To avoid any short circuit of the contacts through the ionic solutions, we use a chamber to restrain the liquid on the central silicon area between the metal pads which are placed in the corners of the silicon die. A polydimethylsiloxane (PDMS) sheet with 3mm diameter of circular opening was used. The pseudo-reference electrode (RE) was included in the experimental set-up. Figure 6.8 depicts the experimental set-up both a) schematically and b) in reality. The above modifications are the essential changes on the experimental set-up for transitioning to a chemical FET sensor in liquid conditions.
6.4.2 Drain current response to various pH solutions

The evaluation of sensing capabilities is mostly performed through a calibration curve produced from drain current versus gate voltage characteristics. In this paragraph, the performance of our devices is demonstrated through the drain current response to pH, before the analysis of the transient body potential.

The solutions tested in this study are pH buffer solutions for equipment calibration purchased from Sigma-Aldrich [50], with pH values of 4, 7 and 10 at 25°C. The solutions were placed in the PDMS chamber cavity with a micropipette and the potential was fixed at 0V with our homemade RE. The sensing measurements were performed immediately after the placement of the pH solution in the PDMS chamber. After, the measurements the solution were discarded, the chamber was rinsed with de-ionised water (DIW) with the help of a micro-pipette and the next solution was inserted into the chamber. The order of the solutions was pH4, pH7, pH10, pH7, pH4 and pH10, unless differently stated. Only successfully measured devices for at least three consecutive pH solutions were considered in the final results.

The device under test has three circular pads of 500μm radius placed in the corners of the silicon square. The measurements were performed with a B1500 semiconductor analyser from Agilent. The source and the reference electrode were grounded and $V_G$ was linearly swept, from negative to positive voltages and backwards with 50mV step and 100ms delay time. A 10s hold time was set at the beginning of the measurement to ensure that the scan starts when the device is in equilibrium. The integration time was set to medium (20 μs). The drain voltage was set to 0.1V for all the measurements and zero current conditions were set for the body contact. Since the difference between the drain and body contacts stems from the measurements conditions and not the device, the contacts are interchangeable and thus, we monitored both
quantities for each contact. Figure 6.9 presents a schematic of the two measurement configurations, hereafter referred to as drain (or body) placed “diagonally” or “parallel” with respect to the source contact and the silicon film. Note that, for the diagonal configuration the solution is placed between the two contacts. In this case the conductive path passes under the liquid solution to-be-detected, while for the parallel case the current follows the shortest conductive path and a large portion of it does not travel under the liquid gate.

Figure 6.9: Top view of the device under test. The two measurement configurations with the drain placed diagonally and the body contact parallel to the source with respect to the silicon. For the second experiment the drain and body contacts were interchanged.

Figure 6.10 presents the drain current characteristics of the device for the two contact configurations shown in Figure 6.9, in semi-logarithmic and linear scale. Observing the current in linear scale, the solutions have an effect on the $I_D-V_G$ curves for $V_G$ values higher than 6V. In this regime, solution with pH=4 acts like a positive gate since the drain current increases. The opposite is true for the pH=10. This behaviour is in agreement with a positive charge of the pH4 and a negative for pH10, as previously explained with the binding theory. Additionally, when the solutions are cycled (from pH=7 to pH=10 and back to pH=7), the current returns to the same value. This is a strong indicator for good reproducibility of the pH reading.

In the subthreshold region, the effect of the pH solution is not detectable. For $V_T<V_G<6V$ the curves are fairly well superposed, regardless the solution under detection. This peculiar behaviour is characteristic of our device and it will be explained in the next section.
The addition of the liquid with fixed potential will essentially transform partially the device into a “pseudo” double-gate structure, with a part of the field lines passing under the liquid while the rest stay in the “dry” region of the Si island (see Figure 6.11). However, a direct comparison with a true double-gate MOSFET is not feasible due to the difference in the architectures. The tool to identify the presence of a double conductive channel is the transconductance ($g_m = \frac{dI_D}{dV_G}$) [51]. In Figure 6.12, we plot $g_m-V_G$ based on the data of Figure 6.10. Regardless of the measurement configuration, $g_m$ has a double peak, which appears around $V_G=6$V. It is reported that such a response is due to the activation of a second channel in a double gate MOSFET [51]. In a double-gate transistor the second channel is formed on the oxide/semiconductor interface of the secondary gate. However, a channel in the top Si interface cannot be formed in our structure since the solution under test does not extend over the whole distance between the source and drain contacts. This means that a part of the Si film stays depleted while the rest of the film inverts until $V_G$ is sufficient to invert the total Si area of our device. Observe how the position of the second peak shifts with pH values. Clearly, the second peak is related to the liquid gate. Considering that double peak of $g_m$ [51], the second peak (influenced by pH) in Figure 6.12, should correspond to the activation of the channel under the liquid gate.
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

![Diagram showing current distribution](image)

**Figure 6.11:** Current distribution (red bended arrows) for the two measurement configurations discussed in Figure 6.9.

Evidently, the part of the “dry” silicon film seems to become conductive for lower voltages, which is expected, since its top potential is floating, hence the potential in the film is easily controlled by \( V_G \) compared to the one under the liquid gate. Since the pH value of the solution would correspond to different charge density value close to the top oxide, we observe the respective shift of the second \( g_m \) peak as the pH value changes. Of course, the ratio between the peaks will be proportional to the current contribution of each area and thus it appears slightly modified between Figure 6.12 a) and b) where the conductive paths are different.

In order to check the hypothesis of transport through two different channels, we used a mathematical model which consists of two independent currents added. The total transconductance of the device is calculated and plotted with respect to \( V_G \).

![Graphs showing transconductance](image)

**Figure 6.12:** Transconductance versus gate voltage characteristics of a 70nm silicon over 145nm BOX with chromium pads in the corners of the silicon film from \( I_D(V_G) \) measured diagonally (a) and in parallel (b).
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

The inversion charge in the channel is described by the Lambert W function (LW) model presented in [52], [53] (also described in chapter 5 and in appendix E). Taking into account the geometrical factor of the pseudo-MOSFET, the equation for the inversion current reads:

\[ I_D = f_g \frac{\mu_0}{1+\theta} Q_{inv} V_D \]  \hspace{1cm} (6.3a)

with \( Q_{inv} \) the inversion charge calculated based as

\[ Q_{inv} = C_{BOX} n \frac{kT}{q} LW\left( e^{\frac{q(V_G-V_T)}{nkT}} \right) \]  \hspace{1cm} (6.3b)

where \( f_g \) is the geometrical factor, \( q \) the elementary charge, \( \mu_0 \) the low field mobility, \( \theta \) the mobility attenuation factor, \( V_T \) the threshold voltage, \( C_{BOX} \) the BOX capacitance, \( k \) the Boltzmann constant, \( T \) the temperature and \( n \) the ideality factor (\( n=1 \)). To emulate a response of a structures with two conductive channels, the two currents based on equation 6.3 were simply added, with different geometrical factors (\( f_gA \) and \( f_gB \)) and threshold voltages (\( V_{TA} \) and \( V_{TB} \)).

Figure 6.13 depicts the modelled drain currents for each channel separately and for their sum. For the recreation of the curves, the attenuation factor \( \theta \) was set to 0.086V\(^{-1}\) and low field mobility \( \mu_0=100 \) cm\(^2\)V\(^{-1}\)s\(^{-1}\) as extracted from experimental data. We observe that, for \( V_{TA}<V_G<V_{TB} \) the combined behaviour actually follows the values of the first channel. For \( V_G>V_{TB} \) the contribution of the second channel starts to be comparable to the first one and thus the total current increases. A comparison with Figure 6.10 immediately shows that, the silicon under the liquid gate has a threshold voltage higher that the rest of the device. This explains why the drain current, shows a shift with pH only for high \( V_G \) while for low \( V_G \) (including in the subthreshold regime) the curves are perfectly superposed.

![Figure 6.13: Drain current versus gate voltage modelled with Lambert W function for two channels with different \( V_T \) and \( f_g \) and their sum: a) constant \( f_g \) and \( V_{T1}=0.5V, V_{T2}=1V \) b) \( V_{T1}=0.5V, f_g=0.5 \) and \( V_{T2}=1V, f_g=1 \) (effect of \( f_g \)) and c) \( V_{T1}=0.5V, f_g=0.5 \) and \( V_{T2}=1.5V, f_g=1 \) (effect of \( V_T \)).](image)
The effect is also visible in the transconductance curves. Figure 6.14 depicts the transconductance calculated numerically as the derivative of the curves in Figure 6.13. The curves in Figure 6.14a and Figure 6.14b show that the height of each peak is a function of the geometrical factor, while $V_T$ only shifts the curve to higher voltages. Benchmarking the modelled (Figure 6.14) results with the experiments of Figure 6.12, one can conclude that the difference in the height of the transconductance peaks maximum is attributed to the variation of the geometrical factor, when measuring the current diagonally or parallel. The above observations shows that drain current modulation with pH would be observed for $V_G>V_T$, which is in agreement with the experimental results in Figure 6.10. In the next paragraph we present the experimental $I_D$ calibration curves.

![Figure 6.14: Normalized transconductance versus gate voltage modelled with Lambert for two function for two channels with different $V_T$ and $f_g$ and their sum: a) constant $f_g$ and $V_{T1}=0.5V, V_{T2}=1V$ b) $V_{T1}=0.5V, f_{g1}=0.5$ and $V_{T2}=1V f_{g2}=1$ (effect of $f_g$) and c) $V_{T1}=0.5V, f_{g1}=0.5$ and $V_{T2}=1.5V, f_{g2}=1$ (effect of $V_T$).](image)

**Figure 6.14**

### 6.4.4 Drain current calibration curves

Figure 6.15 illustrates the calibration curve produced from the drain current value at $V_G=9V$, from the results presented in Figure 6.10. Figure 6.15 also compares the response between the diagonally and parallel measured current. In both cases, the values show a linear response with respect to pH value and they shift according to the binding theory. The slope for the three first points was calculated as a measure of sensitivity. The slope obtained when the current was monitored in the diagonal shows an almost 50% improvement with respect to the parallel $I_D$ measurement. This result was anticipated considering the current distribution of the electric field in the silicon film [54]. A schematic illustrating the current distribution is presented in Figure 6.11. While in the “diagonal” configuration the majority of the current passes under the liquid chamber, when the current is monitored in parallel, only a fraction of the current is affected by the liquid gate. Thus, a stronger response is expected in the first case.
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

Note that in all the cases, the Si film must be conductive (sufficiently high $V_G$) to see any effect of the pH in in the current measurements. This particularity of the architecture of the sensor is also responsible for the limitation of the detection at high $V_G$.

![Graph showing calibration curve for pH detection](image)

Figure 6.15: Calibration curve obtained by monitoring the current for $V_G=9V$ from the measurement of Figure 6.10 for the two measurement configurations.

6.5 Metal contact SOI devices for pH sensors: $V_B$ response

6.5.1 Experimental $V_B$ response for pH detection

The body potential reading was performed with the same set-up as in the current measurements in quasi-static conditions. The SMU used for measuring $V_B$ was set to zero current conditions as explained in [33]. The experimental curves obtained for the body potential are illustrated in Figure 6.16. The curves undergo a shift towards more positive or negative $V_G$ depending on the pH value of each solution. A dependence on the $V_B$ maximum value with pH is also evidenced. Additionally, the response is reproducible for the solution with pH7, which was tested before and after detection of pH10. It is worth noting that $V_B$ occurs regardless of the contact configuration, leaving additional design freedom for a sensor based on this structure. Unlike previous reports [33], [34], where $I_D$ and $V_B$ curves shifted together in the same direction, here the shift direction is opposite. While $I_D$ curves shift towards higher $V_G$ values for basic solutions, $V_B$ curves shift towards negative. Since the current behaviour is in agreement with the binding theory, the explanation of the $V_B$ response should be elsewhere.
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

Figure 6.16: Body potential versus gate voltage characteristics of a 70nm silicon over 145nm BOX with chromium pads in the corners of the silicon film a) measured diagonally and b) in parallel. The points identified in the graphs will be used for the calibration curve analysis in the next session. The insets in the graphs show the experimental configuration.

As explained in chapter 5, the emergence of the body potential is a delicate balance between the amount of charges required for film inversion and their injection form the Schottky junction at the contact level. In the structure under test, since the liquid gate is not close to the Cr contacts, one can consider that the different solutions will only affect the total charge required for silicon film inversion, without modifying the Schottky barrier. Figure 6.17, shows a cross-sectional view of the device in an equilibrium state for three solutions with different pH and the inversion carrier distribution in the silicon film. Considering pH7 as a reference, the total amount of charges required for the inversion under the liquid (Q') and in the dry region of the film (Q) would be $Q_{7, \text{Total}} = 2Q_7 + Q'_7$, which will reproduce the “reference” (for this reasoning) response. In case of an acidic solution, the required charge will be $Q_{4, \text{Total}} = 2Q_4 + Q'_4$. Assuming that the “dry” part of the silicon is unaffected, Q$_4$=Q$_7$. The inversion charge needed under the liquid is increased, for the same $V_G$, since the acidic solution acts like a positive gate: $Q'_4 > Q'_7$. As a result, $Q_{4, \text{Total}} > Q_{7, \text{Total}}$. The out-of-equilibrium response will be therefore stronger for pH4 compared to pH7: the maximum $V_B$ for pH4 is higher than $V_B$ for pH7 and the return to equilibrium appears at higher $V_G$. Following the same reasoning for basic solutions $Q_{10, \text{Total}} < Q_{7, \text{Total}}$ and consequently $V_B$ drops at lower $V_G$ and has a smaller value. The above interpretation assumes that the silicon film close to the border of the silicon layer is not a function of the liquid gate, which is reasonable given the large distance between the contacts and the liquid gate.
It has to be stated that, this behaviour is specific to our structure, originating from the double conductive paths under the “dry” and “liquid” regions. A mature version of this sensor should utilise the whole sensing area, increasing the efficiency of the device. This means, the liquid gate of a more advanced sensor will extend until the boundary between the Schottky contact and the MOS capacitor (explained in chapter 5). As a result, the boundary between the two regions will be affected by the solution leading to proportional shift to the drain current. However at this stage, the study is focused on the proof of concept.

### 6.5.2 Body potential calibration curves

Based on the curves in Figure 6.16, we can chose a specific point of the $V_B$-$V_G$ trace and follow its evolution with pH, constructing the respective calibration curves. Since the sharp $V_B$ drop is well-understood and connected with the injection carries in the silicon film [33], we choose to monitor the shift of $V_G$ for a constant $V_B$ value during the drop. Figure 6.18a illustrates the experimental calibration curves produced by the $V_G$ value at $V_B$=0.4V during the body potential drop (point identified in Figure 6.16). Once more, higher sensitivity is observed when the current path is under the liquid gate. As a first quantitative comparison between $V_B$ and $I_D$, $V_G$ for given $I_D$ values is illustrated in Figure 6.18b. A rough calculation of the slopes shows: 1) two times steeper slope for $I_D$ compared to $V_B$ in the parallel configuration and 2) slightly better response with the current method, which is ~15% higher compared to $V_B$, measured with contacts diagonally placed on the silicon film.

While the drain current produces a stronger shift in terms of $V_G$ at constant current value in the above comparison, $V_B$ has a strong potential signature for lower $V_G$ values. Note that the
A novel pH sensor based on the out-of-equilibrium body potential reading

performance of \( V_B \) could be improved by modifying the device architecture, if the liquid gate extends closer to the metal contact the \( V_B \) will change. Nevertheless, this device evolution requires also reproducible results and these aspects will be discussed in the next section.

Figure 6.18: Calibration curves of the device for different pH values, based on the \( V_G \) shift for body potential drop at \( V_B=0.4V \) (a) and for the drain current \( (I_D=3\,\mu A) \) (b) for parallel and diagonal measurement configurations.

6.5.3 Reproducibility of the pH detection

As extensively described in chapter 4, the devices had been fabricated in IMEP-LaHC cleanroom facilities starting from an industrial SOI wafer. The mask design was research oriented, aiming to the understanding of the body potential response and did not allow a reproducibility study on large statistics. A total of five architectures for devices (layouts) were successfully measured. Table 6.1 shows the layouts and the experiments conducted successfully on each die. Note that, device no.4 shows a problematic contact with the solution in the second pH4 measurement which was excluded from the analysis.

A direct comparison between \( V_B-V_G \) curves of these dies is not relevant since there is an important variability of the threshold voltage due to the different contact geometry (layout) and to process inconsistences. Additionally, the \( V_B \) drop depends on the area of the deposited Cr pad. The two aforementioned factors were discussed in chapter 4.
Table 6.1: Table of the tested contact layouts and successful measurements

<table>
<thead>
<tr>
<th>a/a</th>
<th>Layout name</th>
<th>Schematic</th>
<th>Measurement</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Circles in corners</td>
<td><img src="https://via.placeholder.com/150" alt="Schematic" /></td>
<td>pH4  pH7  pH10  pH7  -  -</td>
</tr>
<tr>
<td>2</td>
<td>Ribbons</td>
<td><img src="https://via.placeholder.com/150" alt="Schematic" /></td>
<td>pH4  pH7  pH10  pH7  -  -</td>
</tr>
<tr>
<td>3</td>
<td>Quarters of circles</td>
<td><img src="https://via.placeholder.com/150" alt="Schematic" /></td>
<td>pH4  pH7  pH10  pH7  pH4  pH10</td>
</tr>
<tr>
<td>4</td>
<td>Circles on the edge</td>
<td><img src="https://via.placeholder.com/150" alt="Schematic" /></td>
<td>pH4  pH7  pH10  pH7  -  pH10</td>
</tr>
<tr>
<td>5</td>
<td>Circles on the edge</td>
<td><img src="https://via.placeholder.com/150" alt="Schematic" /></td>
<td>pH4  pH7  pH10  -  -  -</td>
</tr>
</tbody>
</table>

In order to check the reproducibility of the response to the tested pH values with such different structures, we define a relative shift for each device and pH with respect to the response of that device to the solution of pH7. Figure 6.19, illustrates the results for $V_B$ monitored in the diagonal and parallel configuration. The error bar on the average point, corresponds to two times the standard deviation. Keep in mind that, the statistic population is difficult to obtain for accurately representing the real error on the device measurement. However, it is used as a first indicator in this thesis. Starting from the diagonal configuration, the curve shows a reasonable linearity and the error bars do not overlap. The slope is about 100mV/pH. The “parallel” response, presents also a distinguishable shift of the average value for the solutions and the devices tested. However, the linearity is less obvious compared to the curves produced $V_B$ measured on the diagonal. The higher error produced in the parallel configuration probably stems from the field line distribution in the silicon film which is very different for each architecture. While, in measurements performed with the diagonal $V_B$ a conductive path passes directly under the solution, in the parallel configuration the influence of the liquid gate is reduced. Thus, a misplacement of the PDMS chamber would easily provoke a higher error. Thus, a greater discrepancy of the shifts is observed. The sensitivity reduction
was expected, as explained previously. Not that the error for pH=7 is minor even for the “non-optimised” process used in this thesis, promising better reproducibility with an optimised fabrication process. Additionally, the super-Nernstian response (>60mV/pH), (until now explained and observed only in I_D) is depicted also in V_B.

![Figure 6.19: Average shift of V_G at constant V_B value for five devices tested in this study. The devices were tested as in Table 6.1. The shift with respect to the first solution with pH=7 and the average shift for a) the diagonal and b) parallel configuration.](image)

The super-Nernstian response stems from coupling of the top and bottom interfaces and increases the sensitivity of the device by a factor equal to the ratio between bottom and top oxide capacitances [5]–[7]. This result, unfolds new sensing opportunities with strong potential signals which still exploit the back-gate amplification effect. To further explore this optimisation possibility, the TCAD simulation method of chapter 2 is adapted to pH sensing in a 2D structure and will be presented in the next section.

### 6.6 Optimisation of the sensor through 2D TCAD simulations

The difficulties of the TCAD simulations of the real device have already been discussed in chapter 2. These limitations lead to the use of a 2D structure with contacts made by highly doped P+ and N+ regions. According to the analysis of chapter 5, the occurrence of the transient V_B with metal contacts is feasible in TCAD, but other parameters (such as mobility) need to be tuned to unrealistic values to compensate for the small simulated capacitance and still give a reasonable high V_B response. For these reason, we prefer performing the TCAD simulation for the optimisation analysis on the structure with the P+/N+ contacts.

An additional challenge here is how to emulate the effect of the solution. The simplest simulation method would be to replace the pH charges of the solution with a constant charge placed on the top interface. While in theory, this looks simple, one should individually calculate...
the total charge for each individual simulation structure (considering the size) and closely monitor its dimensions. In addition to the above, the distance from the top Si/SiO$_2$ for which the device remains sensitive cannot be estimated leading to an extra unknown value. Finally, this technique will screen any capacitive effects from the liquid-gate. A better solutions is illustrated in [55]–[57]: the effect of the solution can be emulated by a gate material with modified properties to match those of the liquid. In this thesis, we use the values and procedures described in [55]. The top-gate material has adapted hole and electron mobility in order to match Na$^+$ and Cl$^-$ velocities and the electric permittivity of the water ($\varepsilon_{\text{water}}=80$), including a band gap 1.5V. The calculation of the pH values follows the reasoning of [55] and it is illustrated in the appendix F. Note that the above approach was demonstrated for charged species in the solution (emulation of proteins, DNA, etc…), with a definition of independent areas, in the adapted gate material, with a specified amount of charge, placed close to the top surface. A more advanced emulation of biochemical species in TCAD is presented in [58], which also includes the effect of the Stern layer. Although, an extended study with charged species could be carried out for a biochemical sensor, for simplicity we only include the modified gate in the simulations for our pH sensor.

The structure used in this work is depicted in Figure 6.20. A NP-NP configuration was selected to reproduce the forward $V_B$ response. As demonstrated in chapter 3, and described in chapter 5, the “barrier” needed for the emergence of $V_B$ depends on the contact structure. Thus, to avoid any issues due to PN contacts variation and keep the barrier constant at all times, the silicon layer under the PN contacts was set to a fixed thickness of 30nm. The rest of the geometry of the channel region of the silicon film will be modified for the sensitivity study below. This way the coupling between the interfaces will effectively modify the device response, while the “barriers” themselves, will be unaffected. The solution height was set to 5 $\mu$m, contacts length to 0.1$\mu$m, top oxide layer thickness to 5nm, device length to 1$\mu$m. The silicon substrate was neglected and $V_G$ is applied directly to the BOX, since this section is focused on tuning the geometrical parameters of the device for detection with $V_B$. In the next paragraphs, the simulated results are presented. Later, the findings are grouped and the detection ability of the structure based on $V_B$ is benchmarked with the one based on $I_D$. The discussion starts from the $I_D$-$V_G$ curves.
6.6.1 Simulated drain current response to pH

Figure 6.21 illustrates the drain current versus back-gate voltage curves simulated for various pH solutions for two different wafers and the same scanning speed, SS=100V/s. Observe the shift towards positive gate voltages for higher pH values which agrees with the binding theory and the experiments presented earlier (Figure 6.10: Drain current versus gate voltage characteristics of a 70nm silicon over 145nm BOX with chromium pads placed in the corners of the silicon film a) measured diagonally and b) in parallel. Figure 6.10). Additionally, we observe a stronger response for the thinner silicon films as expected theoretically [59]. Finally, the I_D curves are expected to shift without any change on their shape. However, the subthreshold slope seems to degrade slightly. This is possibly the effect of PN contact used to simulate the sensor. The coupling of the two gates close the contact will also affect the “barrier” and thus the conductivity of the region which induces an apparent subthreshold slope degradation.

Figure 6.20: Schematic of the TCAD structure used for the sensor simulated, with the liquid gate equivalent region. NP contacts were selected for the reproduction of the forward scan response.
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

6.6.2 Simulated body potential response to pH

Figure 6.22 depicts the simulated body potential response for various pH solutions for two different wafers and a scanning speed of SS=100V/s. The body potential shifts towards right when pH is increasing. Thus, the shift is in agreement with the site binding theory explained earlier, contrary to the experimental results. As already specified, a one-to-one comparison between this simulations and the experimental results is not possible due to the difference in the architectures. In the experiments the solutions do not influence the Schottky barrier. In this simulations the solution affects the “barrier” due to its proximity to the source contact. Also, contrary to the experimental results and model, (chapters 4 and 5), the maximum value of the body potential and range are reduced for thinner silicon films. The origin of such a behaviour is on the constant silicon thickness under the PN contacts. Notice however, how the shift is increased for thinner silicon films. The effect of the silicon film on the detection capability has already been discussed in [5] and stems from the coupling of the top and bottom interfaces as explained in [60]. Considering the above, one can conclude that, the respective $V_B$ curves will depict accurately the sensing ability of the structure. However, they might not illustrate the real $V_B$ value or $V_G$ for which the effect manifests itself. Before generating a calibration curve based on this results, the monitored points on $V_B-V_G$ curves in the next section.
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

Figure 6.22: Simulated body potential response for various pH solutions for a device with a) \( t_{Si}=70\text{nm}, t_{BOX}=145\text{nm} \) and b) \( t_{Si}=30\text{nm}, t_{BOX}=145\text{nm} \). The scanning speed was set to \( SS=100V/s \).

6.6.3 Body potential calibration curves – tuning

The detection based on the transient body potential is a novel idea that was first illustrated only three years ago [33]. In contrast to a well-established drain current behaviour, where calibration curves were produced and well explained with current models in equilibrium regimes, body potential is less studied as a sensing method. Thus, in this sub-section, we explore the dependence of the sensitivity through calibration curves produced from various points of the simulated data. Considering that a \( V_B \) sensing model is not yet established, extraction of parameters based on fitting (like for the \( V_T \) monitoring) is not possible. Therefore follow the evolution of \( V_B \) with various pH solutions through monitoring of three points in different regimes (A, B and C in Figure 6.23a). Figure 6.23b presents three calibration curves produced from the data in Figure 6.22. The selected points for a wafer with \( t_{Si}=70\text{nm}, t_{BOX}=145\text{nm} \) and \( SS=100V/s \) correspond to: the \( V_B \) value at \( V_G=0.2V \), the \( V_G \) value for \( V_B =0.4V \) (during the body potential linear increase) and the \( V_G \) value for \( V_B \) the drop (see intersection of the solid lines in Figure 6.22). The selection of each point is based in the following reasoning: A) monitoring at constant \( V_G \) corresponds to the increase or decrease of the \( V_B \) value similarly to the current modulation with pH (at a given \( V_G \)) which is widely presented in the literature, B) during the linear increase of \( V_B \) with \( V_G \) at a given \( V_B \) value, the device is depleted and an enhanced response is expected [2] when following point B and C) \( V_G \) during the \( V_B \) drop, at a given potential value will correspond to the rapid injection of carriers in the film and it was tested experimentally. Monitoring point (a) produces a perfectly linear curve but the sensitivity of the device is very low (34mV/pH) and thus is excluded from
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

the discussion. The $V_G$ shift for a constant $V_B$ value in the linear increase region, on the other side, produces a fairly linear calibration curve with respect to pH values. The sensitivity is once again superior to 60 mV/pH and its value is monitored at low voltages ($V_G<V_T$). Even if the $V_G$ shift during the body potential drop is not so linear, it presents an improved average sensitivity, showing great sensing potential. Hence, in the next section, we will discuss only the calibration curves based on the $V_G$ shift during the linear increase and drop of $V_B$ for each tested sensor.

![Figure 6.23](image)

**Figure 6.23:** Body potential versus gate voltage curve for pH7 with the three monitored points indicated (a). Comparative study of the $V_B$ or $V_G$ shifts for the illustrated points on the left (b) curve. $t_{Si}=70\text{nm}$, $t_{BOX}=145\text{nm}$ and $SS=100\text{V/s}$.

**Tuning of the $V_B$ calibration curve through scanning speed**

Figure 6.24 represents the calibration curves of the $V_G$ shift at constant $V_B$, for silicon thickness 70 nm over 145nm BOX layer and scanning speeds of 10V/s, 100V/s and 400V/s. Figure 6.24a, illustrates the evolution of the curve based on the $V_B$ drop while (point C in Figure 6.23a). Figure 6.24b, during the linear increase (point B in Figure 6.23a). We notice that the obtained curves, have similar slopes regardless of the scanning speed. This result suggest that increased dynamics will not yield better sensitivity. However, constant sensitivity attained at different $V_G$ values. This could potentially make the device very versatile in terms of circuit integration and design, since the operation voltages could be tuned to fit the product specifications without compromises in terms of sensing performance.
Figure 6.24: Body potential calibration curves produced for various scanning speeds. The curves were traced for a given $V_B$ value for each structure during a) the linear increase and b) the potential drop.

The calibration curves produced from the drain current of the same structure for the three tested scanning speeds are presented in Figure 6.25 for comparative reasons. The curves are perfectly superposed, with a slope of 20mV/pH. The graph illustrates the advantage of the dynamic potential measurements. In transient, the calibration curves could be tuned to operate at a desirable $V_G$ range while, drain current stays unaffected. Note that, the experimental evidence in chapter 2 show how the gate current can modify the drain current response if the device size is large. In the experimental 5x5mm$^2$ structure, the large device area will produce huge transient currents due to the big impedance, which should be considered in later stages of the development.

Figure 6.25: Calibration curves produced from $I_D$-$V_G$ for various scanning speeds. The curves were traced at constant current, $I_D=100$nA.
BOX thickness effect on the calibration curve

The effect of BOX thickness is illustrated in Figure 6.26. The calibration curves were traced at constant $V_B$ values during the linear increase and drop, as previously. For both monitoring points, the sensitivity shows a huge increase as the BOX thickness increases. This is attributed to the back-gate signal amplification as illustrated in [5]. Contrary to SS, the above attribute was firstly observed with $I_D$ curves [59], thus $t_{BOX}$ is expected to affect the calibration curve produced from the drain current characteristics as well.

Figure 6.27a illustrate the drain current calibration curves for $t_{BOX}=145$nm and Figure 6.27b for $t_{BOX}=30$nm. The scales were selected accordingly, to visualize clearly the slope. Observe the increase in the sensitivity for the thicker BOX layer. Before explaining in detail how the measurement method amplifies the sensor performance, the effect of Si thickness is presented in the next section.

![Figure 6.26: Calibration curves produced from $V_B-V_G$ curves for SS=100 V/s, $t_{Si}=70$nm and two BOX thicknesses. The curves are traced at constant $V_B$ values during a) the linear increase b) the potential drop.](image-url)
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

Figure 6.27: Calibration curves produced from $I_D$-$V_G$ curves, at $I_D=100\text{nA}$ for $t_{BOX}=145\text{nm}$ (a) and $t_{BOX}=30\text{nm}$ (b). Si thickness was set to 70nm and SS=100V/s.

**Silicon thickness effect on the calibration curve**

Figure 6.28 illustrates the body potential calibration curves for two different silicon film thicknesses on 145nm BOX. In both cases, a thinner silicon film results in a slope increase. This is attributed to the proximity of the added charges to the conductive channel and is a result of a stronger interface coupling [60]. Comparing Figure 6.28a and Figure 6.28b, we observe also that the slope almost triples during the $V_B$ drop accompanied by a linearity lose, especially for high pH values. In Figure 6.28b, a 17% increase is observed between the two curves.

Figure 6.28: Calibration curves produced from $V_B$-$V_G$ curves for SS=100 V/s, $t_{BOX}=145\text{nm}$ and two silicon thicknesses. The curves are traced at a constant $V_B$ value during a) the linear increase and b) the potential drop.

The calibration curves, produced form the drain current characteristics are shown in Figure 6.29 for comparative reasons. As for the body potential, thinner films enhance the sensitivity
of the device. A five time increase is observed in the slope and the response seems to lose its linearity.

![Calibration curves produced from $I_D-V_G$ curves, at $I_D=100nA$ for $t_{Si}=70nm$ and $t_{Si}=30nm$. BOX thickness was set to 145nm and SS=100V/s.](image)

Clearly, the physical parameters affect drastically the response of the sensor. Over the years, different groups showed and described how each of the above parameters can affect the sensitivity in experiments based on the current measurements. In the next section, the results for the body potential are benchmarked with the ones from the literature.

6.6.4 Discussion on the device tunability

The aim of this sections is to understand the trends of the calibration curves for the tested parameters and create a guide for further development of the sensor in the future. Table 6.2, summarises the extracted sensitivities from the graphs of the above sections. Contrary to the experimental results, the body potential sensing seems to be more sensitive compared to the drain current one. The discrepancy between the simulations an experiments originates mainly from the differences between the architectures (3D experimental structure vs 2D in simulations). As previously said, in the experiments only the inversion charge under the contacts is modified by the pH solutions, while in simulations not only the whole length of the channel is affected by the solution but also the “barrier” created under the contacts.

Moreover, the PN contacts and the small dimensions of the simulated study may also play a role. As a result, a one-to-one comparison between simulated and experimental results would not be appropriate. Thus, in this section only benchmark between the simulated $V_B$ and $I_D$ calibrations curves will be illustrated.
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

Table 6.2: Extracted device sensitivities from the simulated curves.

<table>
<thead>
<tr>
<th>t_{Si}</th>
<th>t_{BOX}</th>
<th>SS</th>
<th>ΔV_G @ V_B linear region</th>
<th>ΔV_G @ V_B drop</th>
<th>ΔV_G @ I_D=100nA</th>
</tr>
</thead>
<tbody>
<tr>
<td>(nm)</td>
<td>(nm)</td>
<td>(V/s)</td>
<td>(mV/pH)</td>
<td>(mV/pH)</td>
<td>(mV/pH)</td>
</tr>
<tr>
<td>1 30</td>
<td>145</td>
<td>100</td>
<td>156</td>
<td>183</td>
<td>100</td>
</tr>
<tr>
<td>2 70</td>
<td>30</td>
<td>100</td>
<td>24</td>
<td>7</td>
<td>4</td>
</tr>
<tr>
<td>3 70</td>
<td>145</td>
<td>10</td>
<td>113</td>
<td>63</td>
<td>20</td>
</tr>
<tr>
<td>4 70</td>
<td>145</td>
<td>100</td>
<td>132</td>
<td>59</td>
<td>20</td>
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</tr>
<tr>
<td>6 30</td>
<td>90</td>
<td>100</td>
<td>90</td>
<td>19</td>
<td>62</td>
</tr>
</tbody>
</table>

As proven by Bergveld’s group [61], is given by:

$$\Delta V_T = -2.3 \frac{kT}{q} \cdot a_s \cdot \Delta pH$$  \hspace{1cm} (6.4)

where the change in the threshold voltage of an ISFET (\(\Delta V_T\)) imposed by a change in the solution pH (\(\Delta pH\)) value. Parameter \(a_s=(C_{dl}/C_s+1)^{-1}\) is the sensitivity of top membrane, with \(C_{dl}\) and \(C_s\) the double layer and buffer capacitance respectively. Note that, parameter \(a_s\) should not be confused with the extracted slopes in table 6.1, which correspond to the sensitivity of the device. As explained in [6], in a double-gate structure the sensitivity is:

$$\Delta V_T = -2.3 \frac{kT}{q} \cdot a_s \cdot \left(\frac{C_{ox}}{C_{BOX}}\right) \cdot \Delta pH$$  \hspace{1cm} (6.5a)

A quick comparison between equations 6.4 and 6.5a, shows that the threshold voltage shift is multiplied by an additional term which is the ratio between the top oxide and the BOX capacitances. In case are SiO₂, then the equation can be re-written as:

$$\Delta V_T(\text{for the same insulator}) = -2.3 \frac{kT}{q} \cdot a_s \cdot \left(\frac{t_{BOX}}{t_{ox}}\right) \cdot \Delta pH$$  \hspace{1cm} (6.5b)

If the BOX is thicker than the top oxide (which is true in most of the cases for industrial SOI) then the threshold voltage shift is amplified. To test if this equation applies here, we calculate the ratios of \(\Delta V_T\) slopes between simulated structures with different BOX thicknesses. The ratios eliminate all the other parameters, besides the thicknesses which corresponds to the term under investigation.
Table 6.3: Ratio of the capacitive amplification and sensitivity ratios for the tested wafers.

<table>
<thead>
<tr>
<th>Wafer (tsi/box) (nm)</th>
<th>$\frac{C_{ox_A}}{C_{box_A}}$</th>
<th>$\frac{C_{ox_B}}{C_{box_B}}$</th>
<th>$a_A/a_B$ of ΔV&lt;sub&gt;G&lt;/sub&gt;: linear increase</th>
<th>$a_A/a_B$ of ΔV&lt;sub&gt;G&lt;/sub&gt;: drop</th>
<th>ΔV&lt;sub&gt;G_A&lt;/sub&gt;/ΔV&lt;sub&gt;G_B&lt;/sub&gt; for I&lt;sub&gt;D&lt;/sub&gt;=100nA</th>
</tr>
</thead>
<tbody>
<tr>
<td>A) 70/145</td>
<td>4.83</td>
<td>5.50</td>
<td>8.57</td>
<td>5.00</td>
<td></td>
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The dependence on the thickness of the silicon channel shows that a thinner silicon film improves sensitivity (see again Table 6.2), for the B or C points monitored (defined in Figure 6.23a). This was simulated by Go et al. in [5]. Although it is easy to understand that a sensor with thinner film will be more sensitive since the charge placed on the top oxide layer will have greater proximity to the conductive path than in a silicon film, the response is not directly proportional to the silicon thickness or the charge under detection unless for thin Si films. This effect was illustrated for sensors by Jang and Cho in [59]. Figure 6.30 illustrates the coupling effect on double gate SOI devices for a thick and thin silicon layer. In the case of ts=84nm (Figure 6.30a), Jang and Cho reported a ~20V modulation of the back gate threshold voltage for a top gate voltage between -6V and 6V. However, one can observe that when the top Si/SiO<sub>2</sub> interface is driven into accumulation and inversion regimes the coupling effect saturates and the modulation of the back-gate voltage is no longer possible. Observe the slope of the curve which changes when the top surface reaches accumulation. This change in the slope translates to a non-linear calibration curve for a sensor. Unlike thick films, the thin ones (Figure 6.30b) show a fully linear response for the whole range of the applied voltages. This effect was firstly observe in ultrathin SOI transistors [62]–[64]. When the silicon film is very thin, a stronger coupling between the interfaces occurs and does not allow the secondary interface to saturate. The effect is known as supercoupling.
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

Figure 6.30: Back gate threshold voltage modulation versus the top gate of a double gate SOI for Si film thickness of 85nm (a) and 4.3nm (b). The BOX has a 224nm thickness [59].

Both coupling [60] and supercoupling effects are a consequence of electrostatic interaction between top and bottom gate of double gate structures. The linear relationship between the threshold voltage of the operating gate and the secondary gate is given by the ratio of capacitances. This fact was proven for SOI devices which was later adopted for sensors, extending equation (6.5) in [59]. The new form reads:

\[ \Delta V_T = -2.3 \frac{kT}{q} \cdot a_s \cdot \frac{c_{Si}c_{ox}}{c_{BOX}(c_{ox}+c_{Si})} \cdot \Delta pH \]  

(6.6a)

\[ \Delta V_T (for SiO_2 and Si) \approx -2.3 \frac{kT}{q} \cdot a_s \cdot \frac{3t_{BOX}}{3t_{ox}+t_{Si}} \cdot \Delta pH \]  

(6.6b)

where all the parameters have their usual meaning. The modified capacitive amplification factor contains now also the effect of the silicon film. The above coefficient corresponds to the coupling coefficient seen from the back gate as described in [60] and which also stands for the ultra-thin films. Equations (6.6), describe accurately the threshold voltage shift as long as the dependency is fully linear. Evidently, for thicker Si films an error is introduced as we approach the saturation of the secondary interface [59]. This explains the small discrepancy between the theoretical and simulated value for t_{Si}=70nm in Table 6.3. Nevertheless, the mechanism that improves the device sensitivity with the back-gate reading is the electrostatic coupling of the two interfaces.
6.7 Conclusion

In this chapter, the sensing capability of SOI devices with Cr contacts was validated experimentally for pH sensing and optimisations paths were analysed through TCAD simulations based on the methodology described in chapter 3.

The pH sensing required the implementation of a PDMS chamber and a reference electrode to adapt the device for “in-liquid” sensing of solutions with various pH values. Five devices were tested both in current and body potential response. All show comparable responses and good reproducibility with an average sensitivity of 100mV/pH.

The device has an unconventional configuration since the PDMS chamber (and therefore, the liquid) only covers partially its sensing surface. This results in a dual channel formation, one under the liquid and one under the “dry” Si; each of them has its own threshold voltage. The dual channel operation was explained and modeled thanks to the Lambert W function. The extraction of the classic drain current shift for the sensing was performed at a fixed high $V_G$ value, were the “wet” channel is active. The device architecture with its second channel has implications also on the sensitivity. The extracted sensitivity value from the $I_D-V_G$ shifts (134mV/pH) was superior to the one based on the $V_B-V_G$ method (117mV/pH). Note however, that the body potential signal obtained manifested itself at low $V_G$. This implies that a sensor based on the out-of-equilibrium boy potential could possibly have less power consumption.

We used the TCAD methodology described in chapter 3 in order to explore and analyse optimization paths for the sensing based on the $V_B$ response. A comparison with the TCAD simulations revealed that an ideal sensing architecture will be more sensitive in the out-of-equilibrium body potential operation than in the $I_D-V_G$ one.

The main conclusion of this chapter is the out-of-equilibrium body potential was proven to be a successful sensing technique in wet conditions. It also appears for $V_G<V_T$, leading potentially to lower power consumption which would be ideal for portable devices and “lab-on-a-chip” applications. In addition, as illustrated in chapter 2, a simple voltage follower connected to an oscilloscope is sufficient for monitoring the $V_B$ response. This is a strong indicator for easy device integration and circuit development for a commercial device. Furthermore, the relation between $I_G$ and $V_B$ in depletion, translates to a distinguishable spike of the $V_B$ derivative, which could also be exploited, depending on the reading electronics circuit.
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

The great victory for the body potential however is the freedom on tuning the device to meet the sensor specifications as revealed by the TCAD simulations. The sensitivity of the body potential response shows similar dependence on the Si and BOX thicknesses to the one reported in the literature. Furthermore, the operation $V_G$ voltage region can be optimised thanks to the adjustment of the scanning speed. This provides additional freedom for the circuit design. Lastly, the optimisation studies shows a potentially improved sensitivity when sensing with the out-of-equilibrium body potential compared to the traditional current based detection.

All these elements show a step forward in the maturity of the $V_B$ sensing technique but they need more development time to actually reach real life applications and possible competitive products.
Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading

References


Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading


Chapter 6: A novel pH sensor based on the out-of-equilibrium body potential reading


Chapter 7: General conclusion and perspectives

Table of contents

7.1 General conclusion..........................................................190
7.2 Perspectives........................................................................194
7.1 General conclusion

This thesis discusses a new detection concept for ISFET-like sensors based on SOI wafers. The new reading method uses the out-of-equilibrium body potential specific to FD-SOI transistors [1], due to the lack of carriers during a fast scan of the gate between inversion and accumulation. This measured potential provides a strong signal when the device is depleted, thus at $V_G$ values where the drain current is small, promising low power consumption during sensing. Starting from previous results of sensing with the out-of-equilibrium body potential in the pseudo-MOSFET configuration with pressure-controlled probes, this thesis aimed towards the development of a pragmatic ISFET-like sensor, with deposited metal contacts, capable of in-liquid detection with the out-of-equilibrium body potential.

Although the device is not mature enough for real-life applications, a significant amount of progress was achieved during the thesis. Two complementary axis were developed. The first concerns the technological evolution of the sensor starting from an experimental concept based on the pseudo-MOSFET configuration and moving to an integrated device. The second focuses on understanding the origin of the out-of-equilibrium body potential which will help to an efficient design and optimization of the sensing system.

A visual representation of the achievements of this thesis and the remaining objectives towards a commercial sensor is depicted in Figure 7.1. The idea was to identify the key elements from the previous works (starting point) and advance towards a pragmatic sensor. In the Figure 7.1 the words in bold elements represent the heart of each chapter and they correspond to individual checkpoints validated in this thesis. While the proof of concept of “in-liquid” sensing was established, there are still important steps for the global project to achieve the final goal of a commercial sensor.
Chapter 7: General conclusion and perspectives

Figure 7.1: The road towards a practical (bio)-chemical sensor based on the out-of-equilibrium potential reading.

A practical sensor should yield fast reading which combines in an excellent way with the dynamic character of the out-of-equilibrium body potential. To explore $V_B$ in dynamic conditions the device was driven from inversion to accumulation (and vice versa) with linear ramps applied to the gate of the pseudo-MOSFET configuration. The implementation of such measurements was described in chapter 2. A part of an electronic circuit was developed with the integration of a voltage follower, necessary for the transient monitoring set-up, to compensate for the large impedance values of the device in the depletion regime, where $V_B$ occurs. The transient character of $V_B$ was examined with various gate voltage signal frequencies, showing the expected enhancement as the $V_G$ scanning rate increases. That result is very promising for practical applications since it has the double benefit of strong signal and faster reading. However, the experiments revealed also a radical increase in the gate current with frequency. The increased gate current originates from the large size of the die and as a result can be engineered to meet the future application specifications.

No matter the signal enhancement of $V_B$ in dynamic conditions, the design of a sensor based on this phenomenon requires its full theoretical understanding. Until now, the major lead on $V_B$ was its association with the displacement current $I_G$ necessary for the BOX capacitance charge. To really explore the mechanisms behind the out-of-equilibrium response we proceed to TCAD simulations in chapter 3. The main challenge with the simulations for the pseudo-MOSFET is that the pressure-controlled probes cannot be captured by the models of the simulator. To surpass this problem a novel simulation architecture with a sequence of $P^+$ and $N^+$ doped regions for each contact was employed. The benchmark with the experiments
confirmed that the structure recreates well not only the drain current but also the body potential and gate current for the full $V_G$ scan (accumulation, depletion, inversion). However, two complementary structures with different sequences of the doped regions are required for the complete $V_B$ simulation for both scanning directions. The main outcome of the TCAD simulations is that the origin of the $V_B$ is an electrostatic barrier that blocks the instantaneous injection of carriers in the silicon film. This electrostatic barrier is caused by the space charge region which is created under one of the highly doped regions of the source contact. Additionally, the TCAD simulations permitted the analysis of the parameters of the structure and illustrated their impact on the out-of-equilibrium body potential. All results confirm that the body potential response increases as the $V_G$ control over the space charge under the source contact region weakens.

Until this point, all the experiments and simulations were done in the pseudo-MOSFET configuration with the pressure-controlled probes. In order to actually move towards the commercial sensor, new integrated devices that exhibit the out-of-equilibrium body potential response must be designed and fabricated. The obvious solution was the replacement of the pressure controlled probes by deposited metal contacts, as discussed in chapter 4. In the pseudo-MOSFET the contacts are repeatedly reported as ohmic [2], while metal/silicon interfaces usually form Schottky contacts [3]. The selection of the deposited metal was to test weather theoretically Schottky (Cr) or ohmic (Au) contacts, deposited on low doped Si film, induce/affect the potential response. The Cr contact devices show an out-of-equilibrium response, while with gold ones the phenomenon is fully supressed. Also, the $I_D$ measurements performed indicate a purely ohmic behaviour for Au contacts while for Cr the type of the contact depends on the applied gate voltage, showing for low $V_G$ that the carrier deficit (associated with the $V_B$ response) is provoked by the Schottky contacts. Interestingly, lower quality contacts seem to favour the out-of-equilibrium; unlike ohmic contacts that usually require an expensive implantation step, for $V_B$ metal contacts are perfectly adapted. Some tested layout options revealed also that $V_B$ can be influenced by the contacts shape, leaving freedom for future design suitable for specific applications.

The origin of the out-of-equilibrium body potential in the SOI devices with metal contacts is finally provided in chapter 5. Starting from the Poisson and continuity equations adapted for undoped silicon films, the phenomenon was simply recreated numerically with a partial differential equation solver (FlexPDE). A Schottky barrier added to the source allowed obtaining simulated curves in excellent agreement with both the experiments in chapter 4 and
TCAD simulations from chapter 3. The origin of the effect is the potential distribution which is distorted in the silicon at the boundary between the region under the source contact and the rest of the SOI. This lead to the idea of modeling our device with an equivalent circuit made of a Schottky diode (corresponding to the region under the contact) in series with a MOS capacitor (corresponding to the rest of the silicon film). The description of the diode was made by the classic Schottky diode equation [4], while the charge of the MOS capacitor was calculated based on the Lambert W function [5], as for FD-SOI transistors. \( V_B \) clearly occurs when the Schottky diode (controlled by \( V_G \)) does not provide the necessary carriers for the inversion charge needed in the MOS, as imposed by \( V_G \). The model describes accurately the phenomenon for all the parameters included into the equations used. Lastly, the model provides also an insight concerning the operation mechanisms of the SOI even in the pseudo-MOSFET configuration, proving that the contact appears as ohmic for \( V_G > V_T \) because the source is providing the necessary carriers in the Si film instantaneously.

After establishing the technological and theoretical foundations for the SOI devices with deposited metal contacts, we presented in chapter 6 the proof-of-concept of \( V_B \) sensing in liquid environment. An adapted contact layout liberated sufficient space in the center of the silicon die for the placement of a PDMS chamber to restrain the liquid samples with various pH values. The potential of the liquid was kept constant thanks to an Ag/AgCl pseudo-reference electrode, as suggested in the literature [6]. Devices functionalized with APTES are responsive to the tested pH solutions with repeatable results both with \( V_B \) and \( I_D \). The estimated sensitivity gave a super-Nernstian response of 134mV/pH for the drain current measurements and 117mV/pH for the body potential for the reference device. This amplification is the result of the back-gate sensing with a BOX thicker than the top oxide. While this outcome suggests that the classic drain current reading might be superior in sensitivity, the body potential still has some optimization pathways to be explored.

This thesis proved that the transient body potential can be used as a detection method in liquid conditions. The major advantages of the technique are the possibly lower power needed for sensing with respect to \( I_D \)-based methods since \( V_B \) occurs at low \( V_G \), where the device is strongly resistive. Additionally, a fast reading scheme can also be an asset for applications. Moreover, this thesis also proved that the out-of-equilibrium body potential is highly tunable by optimising the \( V_G \) scan frequency, SOI geometry and metal workfunction, making it easy to integrate and design according to the specifications of the future applications.
7.2 Perspectives

Clearly, the method has many advantages and seems promising as a new sensing technique for future products. However, as already said, numerous development steps are still needed. The obvious first step is issued from the sensing results in TCAD simulations. The sensing area in the experiments corresponds to a portion of the total device surface, while a more adapted version of the sensor will probably be to completely cover it by the liquid. For such device, TCAD simulations in chapter 6 show the body potential response can be more sensitive than the drain current counterpart and this was attributed to three effects. The first one is the proximity of the solution to the source/silicon boundary under the contact, probably affecting the electrostatic barrier height as in [7]. The second is related to the transient character of the phenomenon; as seen, the sensitivity of reading with the body potential during the drop seems to be improved. Lastly the film is depleted when the body potential occurs and this operation regime is more sensitive to charges [8].

As part of practical development of the sensor, the device should be integrated and adapted, ensuring a full coverage of the sensing layer by the liquid and thus be in a configuration similar to TCAD. Of course, one should anticipate in this case any short circuits due to the liquid and provide the necessary isolation. At this stage, one might consider also the evaluation and development of the circuit for the final system. This provides the opportunity to test the effect of the surrounding electronics on the detection. The implementation of an integrated reference electrode might also be employed for liquid sensing. A method to do this was shown in [9] where the reference electrode is fabricated next to the sensing layer of the device. However this is a major development step in which various parameters should be considered such as, the reliability of the electrode, its durability compared to the device and any interactions with the solution necessary for cleaning (or resetting the device) between tests.

The above tests require the implementation of (micro)-fluidic parts so that the quantity of the tested solutions will be accurately controlled. Additionally, this will enable real-time monitoring, which is crucial for some applications. Finally, at this stage the power consumption of the complete system (sensor, electronics, etc...) along with its portability should be evaluated.

All these perspectives are interesting topics to be explored by the next generation of students.
Chapter 7: General conclusion and perspectives

References


Appendices

Table of content of the appendices

Appendix A: Data treatment of the transient $V_B$ measurements ........................................ 198
Appendix B: Characterization of the contact through $I_D$-$V_D$ simulations .......................... 200
Appendix C: Does the resist used affect the $V_B$ response? .................................................. 203
Appendix D: $V_B$ TCAD simulations with Schottky contacts .................................................. 206
Appendix E: Details on the W Lambert function ................................................................. 208
Appendix F: DOS calculation for pH simulation ................................................................. 209
Appendices

Appendix A: Data treatment of the transient $V_B$ measurements

The voltage follower used in the experimental set-up (Figure 2.17) was created on a circuit board without any optimisation. As a result, the connections were realised with thick long wires creating opens loops and introducing noise to the measurement. Since the goal here was the proof of concept and not the optimisation of the electronics, a post-measurement data treatment was used to reduce noise.

The method was based on removing the very high and very low frequencies with a fast Fourier transform filtering. Figures A1, A2, A3 illustrate the selection of frequencies for this treatment for low ($T=24s$), medium ($T=2s$) and high ($T=0.05s$) $V_G$ signal frequencies. In the presented spectra, one can notice the 50Hz harmonic. For the low frequency measurement, blocking the band between 25Hz and 75Hz was sufficient to isolate the parasitic signal and result in a clean $V_B$ signal in the depletion regime. In a second step, the higher frequencies were also removed for a very clean $V_B$ signal in the whole $V_G$ range.

While a similar procedure was successfully followed for the very high SS, for the medium one, the harmonic of 50Hz is very close to the frequency of the measurement leading to an insufficient isolation of the 50Hz, distorting the signal response, even after data treatment. While this does was not a blocking point at this development stage of the project, a full circuit should be developed for a proper $V_B$ measurement.

*Figure A1: a) FFT magnitude of the potential signal versus the signal frequency. b) Measured transient $V_B$ over time. The treated signal is placed over the raw data (black line) for $T=24s$.***
Appendices

Figure A2: a) FFT magnitude of the potential signal versus the signal frequency. b) Transient $V_B$ versus time, raw measurement and filtered curve. The treated signal is traced over the raw data (black line) for $T=2s$.

Figure A3: a) FFT magnitude of the potential signal versus the signal frequency. b) Transient $V_B$ versus time, raw measurement and filtered curve. The treated signal (red line) is traced over the raw data for $T=0.05s$. 
Appendix B: Characterization of the contact through $I_D$-$V_D$ simulations

As described in chapter 2, the $I_D$-$V_D$ curves in the pseudo-MOSFET configuration depend also on the applied $V_G$ voltage. To verify whether or not, this experimental behaviour is also reproduced with the novel simulation architecture with the PN contacts, we have simulated the $I_D$-$V_D$ curves. Since the alternating contacts (PN-PN and NP-NP) showed a better agreement with the experimental $I_D$-$V_G$, only these configurations were considered in the following simulations. Figure B.1, illustrates the simulated $I_D$-$V_D$ curves for structures with NP-NP contacts and various applied back gate voltages. For $V_G$ between -5V and 5V, the contacts show a rectifying behaviour for negative $V_D$, while for the rest of the applied voltages the contacts show an ohmic behaviour, especially for low $V_D$ values. Similar results were reported in the experiments of Figure 2.6. Note that, the threshold voltage (see Figure 3.13) seems to be close to 5V and the flat-band one close to -5V.

The simulation of the second structure with PN-PN contacts is depicted in Figure B.2. A similar effect is observed in the graphs. However, the contacts now have a rectifying behaviour for positive $V_D$ instead of negative in the complementary structure. This is in agreement with Figure 3.7, in which NP-NP structure favours the body potential occurrence for the forward and PN-PN in the reverse scanning direction. This is a consequence of the contact emulation with highly doped P and N regions and add another adjustment parameter: the contact length.

![Figure B.1: Drain current versus drain voltage characteristics of a simulated structures with NPNP contacts for a) positive and b) negative applied gate voltages.](image)
Figure B.2: Drain current versus drain voltage characteristics of a simulated structure with PN-PN contacts for a) positive and b) negative applied gate voltages.

The simulated $I_D-V_D$ curves corresponding to an electron channel was made for $V_G$=5V and a hole current for $V_G$=-5V and plotted in Figure B.3. $V_G$ was chosen close to the $V_T$ value of the structures. The graph compares the simulated curves calculated with a structure with NP-NP contacts and for three contact lengths: $L_C$=0.1μm, $L_C$=0.3μm and $L_C$=0.5μm. The complementary simulation structure (PN-PN) is used for tracing the curves of Figure B.4. For the selected $V_G$, the shortest contact always exhibits an ohmic behaviour. Once more, one can anticipate such a response from the $I_D-V_G$ curves of Figure 3.13. However, when the contact size increases, the linearity seems to decline rapidly leading to more “Schottky-like” behaviour. One can explain the origin of this effect based on the ratio of the contacts length relative to the length of the device in the simulation. Remember that, the extension of the Si part “outside” the contacts does not affect strongly the body potential compared to the contacts. So, considering the results from the rest of the simulations in this chapter, the explanation should be found elsewhere. Also, another argument could be the 2D TCAD simulation compared to the 3D experimental structure. Although, a 3D structure would affect the distribution of the current lines in the film [1], a 3D simulation is more complex and time consuming. We preferred to keep the 2D with this contact architecture that was fully capable of reproducing the experimental results and provided an insight on the mechanisms involved.
Figure B.3: Drain current versus drain voltage curves simulated with NP-NP sequence for contacts for \( V_G=5\text{V} \) and \( V_G=-5\text{V} \) and three contact lengths.

Figure B.4: Drain current versus gate voltage curves simulated with PN-PN sequence for contacts for \( V_G=5\text{V} \) and \( V_G=-5\text{V} \) and three contact lengths.
Appendix C: Does the resist used affect the $V_B$ response?

In chapter 4, the electrical response of the fabricated devices was presented. The fabrication process started with classic process steps and followed by some trials and errors until the desirable to achieve a strong potential response. The main focus of the thesis was not the optimization of the process but rather to obtain devices reproducible enough for the proof of concept and the study of $V_B$ in SOI with deposited metal contacts. Under this framework, this appendix provides additional details on the influence of the fabrication process on the $V_B$.

During the lift-off process, the prepared samples with the deposited resist are heated in the deposition chamber at 120°C for 5 hours prior to metal deposition. According to the manual [2] of the resists used (AZ1505 and AZ1518) for the process, the softening point of the resists is around 100-110°C. Thus a viscosity reduction of the resist is expected beyond this temperature. Following the material restrictions and capabilities of the fabrication room, the use of a different resist (e.g. the family of AZ nLoF 2020 resists show stability until 250°C) is not possible. Thus, the two available resists are tested in research for the optimum solution.

To test which resist produces well defined metal patterns on the Si mesa an AFM topography of the two samples is illustrated in Figure C.1 along with the indicated height profiles along the cutlines are. Samples fabricated with the thin (AZ1505) resist show a more abrupt transition between the metal contacts and the SiO$_2$ regions. Along the edge of the metal contact, an increase in the high is observed. This was expected and stems from Cr deposited to the sides of the resists along the patterns. The height of the extra Cr is around 150nm. However, the contact definition is not smooth. Along the edge of the metal a fluctuation in the order of magnitude of 100nm is observed on the edges of the pattern. Thicker resist (AZ1518) in Figure C.1c, on the other hand, show a more complex pattern. Around the desired metal pattern a secondary Cr zone is formed. The height of Cr linearly decreases as we move towards the SiO$_2$ region. This indicates that the resist was deformed around the edges due to the long exposure in high temperatures when placed in the deposition chamber. Note that, in any case the deposited Cr was around 350nm, as expected from the deposition time. Although, the AFM experiment reveal that the thin resist should be a better candidate for the devices, the final process selection depends also on the measured $V_B$ signal from the fabricated devices.
Figure C.1: AFM topography of sample prepared with AZ1505 resist (a) and height profile in the three indicated cutlines (b). AFM topography of sample prepared with AZ1518 resist (c) and height profile in the three indicated cutlines (d).

The measured body potential from devices with contacts close to the corners of the mesas is presented in Figure C.2. For all the above samples the body potential manifests itself in a $V_G$ range between roughly -1V and 1V. The maximum potential values exceed the 1V, mostly for the sample prepared with the thin resist. The body potential of the reverse scan reached the value of 1.5V in both samples. Let us focus on the shape of traces. In Figure C.2a the majority of the measurements present a very clear linear increase, which starts roughly at the same $V_G$ and a sharp drop, similar to the simulated one (chapter 3). $V_B$ measured in devices fabricated with the thick resist presents high variability between the traces (Figure C.2b). More specifically, $V_B$ presents double peaks and the starting point of the increase is not always the same. Additionally, the drop appears to happen in two parts, indicating two different conditions for carrier injection. The last assumption is supported by the poorly defined edges of the contact between the metal contact and the rest of the device. It is possible that metal is deposited over parts of SiO$_2$ layer, possibly affecting the barriers formed by the contact. The experimental curves shows that the contact provokes the carrier barrier that induces $V_B$. If the boundary between the contact and the rest of the device is not well defined then, the properties of the contacts are not homogenous and the injection of the carrier appears at different $V_G$ values.
This leads to an unpredictable shape of the body potential, which is not ideal for applications. However, the traces produced from the sample with the thin resist (AZ1505) show (Figure C.2a) that an optimised process can lead to the desired $V_B$ signal. As a result, the thin resist was chosen for the development of the sensor. As the device approaches the application this process will need to be optimised to gain reliable, well-defined and reproducible $V_B$ signal.

Figure C.2: Body potential versus gate voltages of various sensing layouts as in Figure 4.23 for samples prepared with a) AZ1505 (thin) resist and b) AZ1508 (thick) resist. A total of 15 measurements was performed for each sample.
Appendix D: $V_B$ TCAD simulations with Schottky contacts

Given the findings from FlexPDE numerical solutions (chapter 5), we revisited the TCAD simulations. The goal is not to fine tune $V_B$ with metal contacts but rather to verify why the simulation of the transient $V_B$ failed in our first attempt. The first issue was related to the dimensions. The TCAD simulation structure is a planar 2D device, very small with respect to the experimental 3D device. A 3D equivalent simulation would be time-consuming. To compensate for the small size, we increase the scanning speed to 200V/s, strengthening the $I_{inv}$ component of the response. We also reduce the electron mobility to 10cm$^2$/V/s. The idea is to slow down the carriers and increase the dynamics that will allow the occurrence of the out-of-equilibrium conditions. Then we define a simulation structure with Schottky contacts on the SOI and dimensions similar to the ones used in chapter 3 as in, Figure D.1: Schematic of the TCAD structure with Schottky contacts and low electron mobility.

![Figure D.1: Schematic of the TCAD structure with Schottky contacts and low electron mobility.](image)

The workfunction values ($\phi_M$) of the source and body contacts were varied from 4.1eV to 4.6eV and the simulated body potential and gate current were plotted in Figure D.2. The body potential manifests itself under these conditions. It also seems to be enhanced by the increase of the workfunction. The highest response is obtained for a workfunction of 4.4eV. After that, it seems to lose the regular shape. In this simulation the properties of holes were not altered. Since the behaviour depends on both types of carriers (chapter 3 sub-section 3.6.1) any abnormalities can also be attributed to this element. This caused a suspension of the effect or maybe it is expressed for a very limited combinations of parameters with small values and thus it was difficult to identify by our simulations.
Figure D.2: Simulated body potential (a) and gate current (b) versus gate voltage curves obtained with TCAD simulation of a structure with metal contacts.
Appendix E: Details on the W Lambert function

For an FD-SOI transistor with undoped body and relatively long channel (neglect quantum effects), the inversion charge has been modelled in [3]. The idea was the development of the model that describes well the device response in a wide range of regions and including the subthreshold one. The calculated drain current for a double-gate FD-SOI [3] reads:

$$I_D = \mu_0 \frac{2W}{L} \frac{4\varepsilon_{Si} \cdot kT}{q \cdot t_{Si}} \int_0^V q_i(V) dV$$  \hspace{1cm} (E.1)

where $\mu_0$ is the low field electron mobility, W the width and L the length of the channel and $V_D$ the applied drain voltage. V is the quasi-Fermi level potential, $Q_i$ is the sheet carrier density and $q_i=Q_i/(4\varepsilon_{Si}kT/q \cdot t_{Si})$ is the normalised sheet carrier density. The calculation of $q_i$ is explained in [4] and for approximations valid in the inversion regime yields [3]:

$$q_i = \frac{C_{ox}}{2C_{Si}} \frac{LambertW}{\varepsilon_{ox}} \left[ \frac{n_i \cdot \varepsilon_{Si}}{2kT \cdot N_A} \exp \left( q \left( V_G + \Delta V + V_{FB} - V \right) \right) \right]$$  \hspace{1cm} (E.2)

where $C_{ox}$ and $C_{Si}$ are the oxide and Si capacitances respectively, $N_A$ the acceptor concentration and $\Delta V_T$ is the modulation of the device threshold voltage due to short channel effects (for long devices, $\Delta V_T=0$) and $V_{FB}$ is the flat-band voltage. Equation (E.1) captures accurately the FD-SOI response [3]. Later, the device drain current was also based in Equation (E.2) according to the following formula [5]:

$$I_D = \frac{W}{L} \frac{\mu_0}{1 + \theta_1 \frac{q_i}{C_{ox}} + \theta_2 \left( \frac{q_i}{C_{ox}} \right)^2} \cdot q_i \cdot V_D$$  \hspace{1cm} (E.3)

where $\theta_1$ and $\theta_2$ are the first and second order attenuation factors and $\mu_0$ the low field mobility. Equation (5.8) fully describes the drain current response of FD-SOI MOSFET from low to strong inversion and was proven successful for parameter extraction [5]. Later, the inversion charge calculated based on the Lambert W function was used also for modeling of the inversion charge in split-CV measurements and calculation of the interface trap densities in SOI wafers in [6].

The inversion charge calculated based on the Lambert W function described superbly the mobile charge in SOI films. This is true for devices used in this thesis, as shown in chapter 2. We used this appendix for $Q_{inv}$ calculation in chapter 2, 5 and 6.
Appendix F: DOS calculation for pH simulation

For the TCAD pH simulation we need to give the equivalent electrical properties to a material included in the simulator. The purpose of this appendix is to explain how the values used in the Sentaurus TCAD simulation tool were calculated.

In a semiconductor, according to the Boltzmann law, the carrier concentration for electrons (n) and holes (p) are described by:

\[ n = N_C e^{\frac{(E_c - E_f)}{kT}} \quad \text{and} \quad p = N_V e^{\frac{(E_V - E_f)}{kT}} \]  

(F.1)

where \( E_f \) is the Fermi level, \( E_V \) and \( E_c \) is the valance and conduction bands energy levels, and \( N_C \) and \( N_V \) the effective densities of states (DOS) the conduction and valance bands accordingly. Note that, in a semiconductor, DOS is a function of the effective mass of the carriers and the temperature. At equilibrium \( p_n = N_C N_V e^{-E_g/2kT} n_i^2 \), with \( n_i \) the intrinsic carrier concentration.

Considering that the equation \( \text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{HO}^- \) describes water, its ionic product should be \( K_w = [\text{H}^+] [\text{HO}^-] \), where \([\text{H}^+]\) the concentration of protons in the solution. At 25°C and at chemical equilibrium \( K_w = 10^{-14} \). The pH value of water is defined as \( \text{pH} = -\log[\text{H}^+] \), considering the species activity equal to 1. For a neutral solution (pH=7), \([\text{H}^+] = 10^{-7} \text{ mol/L}\). In semiconductor physics, concentration is expressed in \( \text{cm}^{-3} \). To transform the units we multiply with the Avogadro number (\( N_A = 6.022 \cdot 10^{23} \text{ atoms/mol} \)) and change the L to \( \text{cm}^{-3} \), so \([\text{H}^+] = 10^{-7} \text{ mol/L} = 10^{-7} \cdot 6.022 \cdot 10^{23} \text{ atoms /1000cm}^3 = 6.022 \cdot 10^{13} \text{ions/cm}^3 \). Considering the ions charges and an intrinsic-like behaviour, the assumption of Passeri et al [7] mandates, \([\text{H}^+] = p \) and \([\text{HO}^-] = n \). For \( E_g = 1.5 \text{eV} \), \( kT = 0.0257 \text{eV} \) and \( p = 6.022 \cdot 10^{13} \text{ions/cm}^3 \) equation (1) yields:

\[ p = N_V e^{\frac{(E_c - E_f)}{kT}} \rightarrow N_V(pH_7) = p e^{\frac{E_g}{2kT}} = 6.022 \cdot 10^{13} \cdot 4.72 \cdot 10^{12} = 2.84 \cdot 10^{26} \text{cm}^{-3} \]

And since in a neutral solution \([\text{H}^+] = [\text{OH}^-] \), \( N_C = 2.84 \cdot 10^{26} \text{cm}^{-3} \).

This methodology was published also in [8] and summarized the above calculations in a set of equations:

\[ N_C = 10^{-14 + pH} N_A \cdot 10^{-3} e^{E_g/2kT} \]  

(F.2)

\[ N_V = 10^{-pH} N_A \cdot 10^{-3} e^{E_g/2kT} \]  

(F.3)
The rest of the values are calculated based on the equations F.2 and F.3 and they are summarised in the Error! Not a valid bookmark self-reference. below.

**Table F.1: Calculated densities of states for the emulation of the pH solution in the TCAD simulations**

<table>
<thead>
<tr>
<th>pH</th>
<th>( N_C (cm^{-3}) )</th>
<th>( N_V (cm^{-3}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( 2.84 \times 10^{20} )</td>
<td>( 2.84 \times 10^{32} )</td>
</tr>
<tr>
<td>3</td>
<td>( 2.84 \times 10^{22} )</td>
<td>( 2.84 \times 10^{30} )</td>
</tr>
<tr>
<td>5</td>
<td>( 2.84 \times 10^{24} )</td>
<td>( 2.84 \times 10^{28} )</td>
</tr>
<tr>
<td>7</td>
<td>( 2.84 \times 10^{26} )</td>
<td>( 2.84 \times 10^{26} )</td>
</tr>
<tr>
<td>9</td>
<td>( 2.84 \times 10^{28} )</td>
<td>( 2.84 \times 10^{24} )</td>
</tr>
<tr>
<td>11</td>
<td>( 2.84 \times 10^{30} )</td>
<td>( 2.84 \times 10^{22} )</td>
</tr>
<tr>
<td>13</td>
<td>( 2.84 \times 10^{32} )</td>
<td>( 2.84 \times 10^{20} )</td>
</tr>
</tbody>
</table>
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Dispositifs de silicium-sur-isolant avec contacts métalliques pour détection de pH basée sur le potentiel hors-équilibre
(résumé en français)

1. Introduction et etat de l’art


   Pour améliorer les propriétés de détecteurs de type ISFET, les chercheurs ont proposé des autres architectures comme les nano-fils de silicium [3] ou des ISFET avec un membrane de détection prolongée [4]. De tous les composants dérivés, le ISFET avec double grille fabriquée sur un substrat silicium-sur-isolant (Silicon-On-Insulator, SOI) a une capacité unique: si le composant opère par la grille arrière et la détection est faite avec la grille supérieure, la sensitivité du capteur est augmentée et elle dépasse la limite de Nernst (>60m/pH) [5]. Cet avantage bien apprécié [5]–[7], est toujours exploitée en mesurant le courant de drain.

   Dans cette thèse, un composant avec double grille fabriquée sur SOI est utilisé mais contrairement à la détection grâce au courant de drain de la littérature, le potentiel hors équilibre est choisi comme mode de lecture [8].

   Le potentiel hors équilibre est un phénomène transitoire observé dans les MOSFETs sur SOI et normalement il est considéré comme parasite [9]–[11]. Le même effet se manifeste dans la configuration de mesure pseudo-MOSFET, qui a servi comme base pour conception de notre capteur. Pour le pseudo-MOSFET, deux pointes métalliques sont possées directement sur la
fine couche de silicium et elles agissent comme source et drain. L’oxyde enterré sert de diélectrique et le substrat (bulk) est utilisé comme grille (V_G) en formant une structure MOSFET inversée. Dans cette configuration, lorsque V_G est balayé de l’inversion à l’accumulation et parce que les points sont métalliques, les porteurs ne sont pas injectés instantanément. Par conséquence, le «body» (couche de silicium supérieur) rentre dans un état hors d’équilibre et son potentiel (V_B), suit la variation du signal appliqué sur la grille. Quand la tension de la grille est suffisamment élevée et les porteurs pour la création du canal sont injectées par les pointes, la valeur du potentiel chute brusquement et le dispositif rentre dans un état d’équilibre [8].

Pour exploiter cette phénomène comme technique de détection, trois éléments expérimentaux d’amélioration technologiques ont été étudiés et implémentés pédant cette thèse : 1) au niveau du composant, 2) de type de mesure et 3) du milieu de détection. Un schéma avec des points de départ et les objectifs est illustré dans la Figure 1. Pour soutenir et valider les résultats expérimentaux, deux autres axes théoriques ont été étudiés. En premier lieu, les simulations TCAD de la structure 2D ont contribué à la compréhension du phénomène et en deuxième lieu, la modélisation du potentiel hors équilibre a permis d’établir l’origine du comportement. Les cinq éléments mentionnés ci-dessus correspondent aux 5 principaux chapitres de cette thèse, que nous résumerons pour la suite.

![Figure 1: Schéma du point de départ [12] de la thèse accompagné de la définition des principaux objectifs expérimentaux.](image)

2. Mesures transitoires dans la configuration pseudo-MOSFET

Le deuxième chapitre de cette thèse est focalisé sur les conditions de mesure pour la détection du potentiel hors équilibre. D’un point de vue pratique, un capteur devrait donner une lecture rapide, ce qui se combine de manière excellente avec le caractère dynamique du
potentiel hors d'équilibre. Pour explorer $V_B$ dans des conditions dynamiques, le composant a été conduit de l'inversion à l'accumulation (et l'inverse) avec des rampes linéaires (Figure 2a) appliquées sur la grille arrière de la configuration pseudo-MOSFET. Un circuit électronique a avec l'intégration d'un suiveur de tension (voltage follower) a été nécessaire pour la lecture de $V_B$ en conditions transitoires, pour compenser les fortes valeurs d'impédance de le composant en régime de déplétion, où la potentiel hors équilibre apparaît (Figure 2b). Le caractère transitoire de $V_B$ a été examiné avec plusieurs fréquences de signal pour la tension de grille, montrant une amélioration sur la valeur maximal de $V_B$ quand la vitesse de balayage $V_G$ augmente. Ce résultat est très prometteur pour des applications pratiques puisqu'il présente le double avantage d'un signal fort et d'une lecture plus rapide (Figure 2c). Toutefois, les expériences ont également révélé une augmentation radicale du courant de grille avec la fréquence. L'augmentation du courant de grille est due à la grande taille du dispositif et, par conséquent, peut être optimisée ultérieurement pour répondre aux futures spécifications des applications.

Figure 2:a) Rampes de signal triangulaires appliquées à la grille pour les expériences transitoires. b) Configuration expérimentale pour la lecture de $V_B$ en conditions transitoires. c) $V_B$ en conditions transitoires mesuré avec le nouveaux montage expérimental illustré en b.
3. Simulations TCAD du potentiel hors équilibre avec une structure innovante

Même si le nouveau montage dynamique garanti la lecture du potentiel hors équilibre en conditions transitoires, la conception d'un capteur basé sur ce phénomène nécessite sa compréhension théorique complète. Jusqu'à présent, la piste majeure sur l’origine du $V_B$ était sa corrélation avec le courant de déplacement $I_G$ nécessaire au chargement de la capacité de l’oxyde enterrée (BOX) [8]. Pour vraiment explorer les mécanismes responsables de la réponse hors équilibre, nous procédons aux simulations TCAD (Sentaurus) dans le chapitre 3. Le principal défi avec les simulations pour le pseudo-MOSFET est que les pointes de pression contrôlée ne peuvent pas modéliser dans le simulateur. Pour pallier ce problème, une nouvelle architecture de simulation avec une séquence alternative des régions dopées $P^+$ et $N^+$ pour chaque contact a été utilisée, comme illustrée dans la Figure 2a. La comparaison avec les expériences a confirmé que la structure crée bien, non seulement le courant de drain, mais aussi le potentiel du «body» (Figure 2b) et le courant de grille pour le balayage $V_G$ complet (accumulation, déplétion, inversion). Cependant, deux structures complémentaires avec des alternances différentes des régions dopées sont nécessaires pour la simulation $V_B$ pour les deux directions de balayage. Le résultat principal des simulations TCAD est que l’apparition du $V_B$ est due à la barrière électrostatique qui bloque l’injection instantanée de porteurs des contacts vers la couche de silicium. Cette barrière électrostatique est imposée par la zone de jonction qui se crée sous l'une des régions fortement dopées du contact source, dans la couche de silicium faiblement dopé. De plus, les simulations TCAD ont permis d’analyser les paramètres de la structure et d'illustrer leur impact sur le potentiel hors d'équilibre. Tous les résultats indiquent que la réponse en $V_B$ du «body » s’affaiblit quand le contrôle par $V_G$ de la zone de la jonction diminue.
Figure 3: a) Schéma de la configuration expérimentale du pseudo-MOSFET et la nouvelle structure de simulation TCAD, avec source et drain dopés, avec des 2 types de dopage placés en alternance. b) Simulation du potentiel du body en fonction de la tension de grille, pour différentes vitesses de balayage.

4. Dispositifs de SOI avec contacts métalliques déposés

Jusqu'à présent, toutes les expériences et simulations ont été réalisées dans la configuration pseudo-MOSFET avec les pointes de pression contrôlée. Afin d'évoluer vers un capteur plus réaliste, des nouveaux composants qui gardent la réponse en potentiel du «body» hors d'équilibre doivent être fabriqués. La solution évidente était le remplacement des pointes de pression contrôlée par des contacts métalliques déposés, comme présentée dans le chapitre 4. Pour le pseudo-MOSFET, les contacts sont signalés plusieurs fois comme ohmiques [13] dans la littérature, alors que généralement les interfaces métal/silicium forment des contacts Schottky [14]. Pour un couche de silicium faiblement dopé, il y a deux options pour la sélection du métal pour les contacts: les contacts théoriquement Schottky (la chrome Cr a été choisi pendant la thèse) ou ohmiques (l’or Au a été choisi pour cette thèse). La Figure 3a montre une coupe transversale et une vue de dessus des composants fabriqués avec des contacts métalliques. Les dispositifs avec contacts en Cr montrent une réponse similaire avec le pseudo-MOSFET, comme indiquée dans les Figures 3b et 3c. Pour les dispositifs avec les contacts en
Or, les caractéristiques $I_D-V_G$ ressemblent plus le comportement de n-MOS transistor, comme illustré en Figure 3b, et le potentiel hors équilibre est complètement effacé. De plus, les mesures du courant de drain effectuées indiquent un comportement purement ohmique pour les contacts en Or. Au contraire, pour les contacts en Cr le comportement $I_D-V_D$ dépend de la tension de grille appliquée, montrant que le déficit de porteurs (à l’origine de la réponse en $V_B$) est provoqué par les contacts Schottky. De façon intéressante, les contacts de moindre qualité semblent favoriser le potentiel hors-équilibre, ce qui élevé le besoin des étapes d’implantation normalement mises en place pour obten des contacts ohmiques obligatoires pour les bonnes jonctions des transistors.

**Figure 4:** a) Schéma du dispositif sur SOI avec contacts métalliques déposés vue en coupe et vue de dessus. b) Courant de drain et c) potentiel hors équilibre en fonction de tension de grille pour les pointes métalliques du pseudo-MOSFET et des contacts Cr et Au/Ti.
5. Origine du potentiel hors équilibre dans les dispositifs SOI avec contacts métalliques

L'origine du potentiel de body hors d'équilibre dans les dispositifs SOI avec des contacts métalliques est présentée dans le chapitre 5. En commençant par l’équation de Poisson couplé avec l’équation de continuité, le phénomène a été reproduit numériquement en utilisant un solveur d’équations différentielles (FlexPDE). Une barrière Schottky (|V_{Sb}|) a été ajoutée à la source, ce qui a permis d'obtenir des courbes simulées en excellent accord avec les expériences du chapitre 4 et les simulations TCAD du chapitre 3. L'origine de l'effet est la distribution du potentiel qui change rapidement dans le silicium, à la frontière entre la région sous le contact source et le reste du SOI. Sur la base de l'observation précédente, nous avons modélisé notre composant avec un circuit équivalent constitué d'une diode Schottky (correspondant à la région sous le contact), en série avec une capacité MOS (correspondant au reste du film de silicium). Un schéma du circuit équivalent est présenté dans la Figure 5a. La diode a été modélisée avec l'équation classique de la diode Schottky [15] légèrement modifiée pour prendre en compte également la chute du potentiel sur l’oxyde enterré. La charge de la capacité MOS a été calculée sur la base de la fonction Lambert W [16] comme pour les transistors FD-SOI. V_B apparaît parce que la jonction Schottky (contrôlée par V_G) ne fournit pas les porteurs nécessaires pour la création de la charge d'inversion demandé par V_G dans la capacité MOS. La validation du modèle est faite grâce à deux paramètres essentiels pour la manifestation du phénomène, la vitesse de balayage (SS) et la barrière Schottky. Les figures 5b et 5c montrent que le V_B s’améliore quand SS ou |V_{Sb}| augmente, comme le confirment toutes les conclusions des chapitres précédentes. Le modèle décrit correctement l’évolution de V_B avec tous les autres paramètres inclus dans les équations utilisées.
Figure 5: a) Schéma du circuit équivalent avec deux composants. L’interface Si/BOX sous le contact est remplacée par une jonction Schottky. b) Potentiel hors équilibre calculé par rapport à la tension de grille pour SS=5V/s et SS=10V/s. Le barrière $|V_{SB}|$ est fixée à 0.3V. c) Potentiel hors équilibre calculé par rapport à la tension de grille pour $|V_{SB}|=0.3V$ et $|V_{SB}|=0.4V$ dans (c). SS est fixée à 5V/s. La valeur de $V_G$ pour laquelle le composant revient à l’équilibre est représentée par des lignes en pointillé.

6. Détection de pH basée sur le potentiel hors équilibre

Une fois que le potentiel hors équilibre a été démontré avec les composants SOI avec contacts métalliques, nous présentons dans le chapitre 6 la preuve de concept de la détection avec $V_B$ en milieu liquide. En utilisant un positionnement des contacts adapté, nous libérons suffisamment d'espace au centre du film de silicium pour placer une chambre PDMS qui contient les solutions avec différentes valeurs de pH. Le potentiel du liquide a été maintenu constant grâce à une pseudo-électrode de référence Ag/AgCl [17]. Un schéma du composant utilisé avec les mortifications pour la détection en milieu liquide est illustré dans la Figure 6a. Les composants fonctionnalisés avec (3-Aminopropyl)triethoxysilane (APTES) sont sensibles aux solutions de pH testées. En plus, nous avons montré que les résultats étaient reproductibles pour la détection avec la lecture de potentiel hors l’équilibre, $V_B$. La Figure 6b montre un exemple des données brutes de la mesure de $V_B$ et identifie les points de lecture pour la détection. La sensibilité obtenue est super-Nernstienne de 134 mV/pH (Figure 6c) pour les mesures de courant de drain et de 117 mV/pH (Figure 6d) pour le potentiel hors équilibre pour le même composant testé. Cette amplification est le résultat de la détection par la grille arrière.
avec une BOX plus épais que l'oxyde supérieur [5]. Bien que ce résultat montre que la lecture classique par courant de drain était supérieure en sensibilité pour ce dispositif, le potentiel hors équilibre peut encore être optimisé. Nous avons exposé quelques options par le simulations TCAD.

Figure 6: a) Schéma du capteur avec des contacts métalliques dans les coins, la chambre PDMS et l'électrode de référence. b) Caractéristiques potentiel hors équilibre en fonction de la tension de grille pour un dispositif SOI avec la couche de silicium de 70 nm et oxyde entière de 145nm avec des contacts en Cr. Les points identifiés dans les graphiques seront utilisés pour l'analyse de la courbe d'étalonnage. Courbes d'étalonnage de composant pour différentes valeurs de pH basées sur le décalage $V_G$: c) pour $I_D=3\mu A$ et d) pour $V_B=0.4V$.

7. Conclusions

Cette thèse montrée que le potentiel hors équilibre qui se manifeste dans les dispositifs de type ISFET sur SOI peut être utilisé comme méthode de détection dans des conditions liquides. Un des principaux avantages de la technique est la puissance plus faible, nécessaire pour la détection, par $V_B$ car la réponse est forte à fiable $V_G$ ou le courant $I_D$ est également fiable. Par ailleurs, un schéma de lecture rapide peut également être un atout pour les applications. Pedant
Résumé

cette thèse nous avons également prouvé que le potentiel hors équilibre peut être optimisé en ajustant la fréquence de balayage de $V_G$, la géométrie du SOI ou encore le travail de sortie du métal. Toutes ces capacités de cette nouvelle méthode de détection peuvent faciliter la conception et l’intégration d’un composant selon les spécifications des futures applications issues.

Références


- The end -