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**EFFECT OF DRIFT AND DIFFUSION
PROCESSES IN THE CHANGE OF THE
CURRENT DIRECTION IN A FET TRANSISTOR**

By

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A Dissertation submitted to the program in Electronics, in
partial fulfillment of the requirements for the degree of

**MASTER OF SCIENCE WITH SPECIALTY IN
ELECTRONICS**

At the

National Institute for Astrophysics, Optics and Electronics
(INAOE)

Tonantzintla, Puebla
February, 2014

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DEDICATION

There are several people which I would like to dedicate this work. First of all, to my parents, Margarita González Pantoja and Vicente Huerta Escudero for the love and support they have given me. They are my role models because of the hard work and sacrifices they have made so that my brothers and me could set high goals and achieve them. To my brothers Edgard de Jesus and Jairo Arturo, we have shared so many things, and helped each other on our short lives. I would also like to thank Lizbeth Robles, one special person in my life, thanks for continuously supporting and encouraging me to give my best.

And thanks to every member of my family and friends for their support. They have contributed to who I am now.

ACKNOWLEDGEMENTS

I would like to thank the National Institute for Astrophysics, Optics and Electronics (INAOE) for all the facilities that contributed to my successful graduate studies.

To Consejo Nacional de Ciencia y Tecnologia (CONACYT) for the economic support.

To Dr. Edmundo A. Gutierrez D., for having accepted me in his research team and to the supervision of this thesis.

Also I would like to thank IBM-Fishkill for supplying the samples.

And to all my teachers and classmates, their support and collaboration was especially important during graduation school.

RESUMEN

Típicamente cuando se forma el canal de inversión en un transistor nMOSFET y se barre el voltaje de drenaje, la corriente de canal es positiva, y esto significa que los electrones fluyen de fuente a drenaje. Esto se observa clásicamente en transistores cuyas dimensiones del canal no son menores a 80 nm.

Un conjunto de resultados experimentales mostraron un efecto de inversión de corriente de canal en un transistor de 34nm. Este efecto se traduce en que los electrones sufren un cambio en la dirección de la corriente, fluyendo ahora de drenaje a fuente. Usando modelos numéricos se encontró que el efecto se explica con la incorporación del modelo de Gradiente de Densidad (Density Gradient), el cual es un modelo mejorado de las ecuaciones de difusión-arrastre. La mejora proviene con la incorporación de algunos efectos de naturaleza cuántica que son despreciados en la escala micrométrica (transistores con longitudes de canal mayor a 80 nm),

El fenómeno se explica por un cambio en el signo del gradiente del "potencial cuántico generalizado" en todo el canal. El efecto solo se observa a bajos valores de voltaje aplicado al drenaje, donde un pequeño desbalance inicial en la conductancia del canal provoca que la corriente cambie de dirección cuando el voltaje de compuerta se barre de un valor bajo a uno alto.

ABSTRACT

Typically, when the inversion channel has formed in a nMOSFET and the drain voltage is swept, the channel current is positive, meaning a source-to-drain electron flow. This can be observed in transistors with channel lengths not longer than 80 nm.

A set of experimental results showing a reversible channel current effect in a 34 nm nMOSFET is introduced. This effect means that the electrons suffer a change in the direction, now flowing from drain-to-source. By numerical modeling it was found that the reversible channel current effect is understood by incorporating the Density Gradient (DG) theory, which is considered an enhanced drift-diffusion model. The enhancement comes from considering quantum nature effects that are negligible when working on the micrometer scale (transistors with channel lengths longer than 80 nm).

The phenomenon is explained by a change of sign in the gradient of the generalized quantum potential along the channel. The effect is only observable at low drain voltages, where a slight initial internal channel conductance (at no bias) unbalance causes the channel current to reverse when the gate voltage sweeps from low to high values.

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CHAPTER 1

1.1 INTRODUCTION

One of the most important things in the information era is the capability of processing information; the more efficient a device is, the better. To improve process capability, a larger number of computing units are required in smaller dimensions, but when reducing dimensions of the basic component of a computing unit (the transistor, in this case the Metal-Oxide-Semiconductor Field Effect Transistor, MOSFET), the known models that predict certain behavior fail as unseen effects arise. The case here is one of those unpredicted behaviors.

In Chapter I the classic drift-diffusion transport model is studied. It is important to consider the validity of the model since it fails to describe the observed effect, and maybe some considerations may not be ignored anymore in certain circumstances so it is very important to comprehend the physics in which this model is based. The two main transport mechanisms are studied, the drift and diffusion transport phenomena.

In Chapter II the limits of the DD model are shown. This model does not predict the effects coming up as the downscaling of the devices dimensions, and as it fails, other transport models are studied. Some of them incorporate quantum effects so that they can increase their accuracy in reduced devices, but not losing their macroscopic foundations. This allows them to perform very accurately in a wide dimension range. The end of this chapter focuses on the Density Gradient model, which can be considered as an enhanced Drift-Diffusion model. The purpose of this thesis is to lean on the DG model to

explain the specific observed phenomenon.

Chapter III is dedicated completely to the unpredicted phenomenon that appeared in a 34 nm n-channel MOSFET. The effect arose when operating in the moderate and strong inversion regime. It is supposed that when the inversion layer has formed by a potential applied on the gate of the transistor, there would be a positive drain current increasing as the potential applied between source and drain increases too. However, under these circumstances, the measured current experiences a change of sign from positive to negative when increasing the potential on the gate, the only difference is that this occurs when the V_{ds} is in the range of μV , and the effect slowly disappears as increasing V_{ds} . A possible explanation is developed.

Finally, in Chapter IV the final thoughts are reflected. The steps of the presented analysis are summarized and some other considerations are mentioned. Future work is suggested.

The validity of the study of this effect is that some other phenomena can be studied by the understanding of it, and even more, it could predict what effects are coming on the nanometer scale devices.

1.2 CLASSIC DRIFT-DIFFUSION TRANSPORT MODELING

To understand, design, and optimize electronic devices and circuits it is essential to have a qualitative and quantitative description of the way electrons move in semiconductors and how they interact with connections and isolators. There is a whole world of models trying to describe all these

observed phenomena, and more than one is suitable to the subject of study.

All of these phenomena can be studied according to the scale of the phenomenon. If the size of the device is in the range of micrometers then the electrons behave as particles, and macroscopic descriptions are used. On the other hand, if the size is comparable to a quantity of atoms, the atomistic models are being used to describe the phenomena. The properties of such nanostructures cannot be modeled in terms of classical macroscopic concepts like mobility or diffusion, and that is why the microscopic viewpoint is the needed one.

The difference between macroscopic and microscopic approaches of the electron transport relies on the primitive elements that the theory works on. Microscopic approaches deal with individual particles, electron wave functions, density matrix, etc., and macroscopic theories works on electron populations that have enough electrons with significant average properties.

One of these microscopic descriptions is the fundamental equation of semiclassical transport, the well-known Boltzmann Transport Equation, but working with this model requires a lot of computational effort. The validity of the macroscopic approach of the Boltzmann Transport Equation relies on these assumptions:

- Scattering processes are local
- The scattering is instantaneous in time
- The scattering is very weak
- Only events that are slow compared to the mean free time between collisions are of interest.

Most of these considerations are valid when working in the macroscopic approach. As device dimensions are reduced, those assumptions introduce errors when adjusting the model's parameters of the structure.

The macroscopic Drift-Diffusion classical model is the original and most common continuum theory of electron transport in semiconductors. It can be derived from this BTE model and it is much simpler to work with. It is known that the net flow of electrons and holes in a semiconductor device will generate currents, and the two basic transport mechanisms are drift – electric fields move the charge, and diffusion – charge gradients generate current.

The existence of an electric field in a semiconductor will produce a force on both carriers so that they will show a net movement as long as there are available energy states in the conduction and valence bands. This net movement phenomenon is called drift, and the drift of charges origins a drift current. The drift current density (eq. 1.1) is given by the product of a charge density ρ moving at an average velocity v_d .

$$J_d = \rho v_d \quad (1.1)$$

Equation 1.1 is applied to both electrons and holes, by placing the adequate electron or hole charge density and average velocity. This average velocity is taken from the fact that a charged particle is involved in collisions or scattering events, and these follow the same assumptions as the Boltzmann Transport Equation. If the electric field is constant, it is expected that the velocity increases with time as the charged particle gains energy, but the scattering events alter the velocity characteristics of the carrier. When the particle is scattered it loses most of its energy, but it will accelerate again until

it suffers another scattering event. The average drift velocity is directly proportional to the electric field (eq. 1.2)

$$v_d = -\mu E \quad (1.2)$$

The quantity μ is the carrier mobility. The negative sign for the current density due to electrons shows that the net motion of the electrons is in the opposite direction of the electric field, v_d is positive for holes. Replacing eq. 1.2 into 1.1 and giving the charge density $-qn$ for electrons shows the drift current density for electrons (Eq. 1.3), and to get the respective current density for holes the appropriate quantities must be substituted (Eq. 1.4)

$$J_{dn} = qn\mu_n E \quad (1.3)$$

$$J_{dp} = qp\mu_p E \quad (1.4)$$

The second mechanism that induces current in a semiconductor is the diffusion phenomenon, which is a process where particles flow from a region of high concentration to a region of low concentration and if the particles are electrically charged, which is the case here, the net flow of charge results in a diffusion current. To calculate the current (eq. 1.6), the net flow of electrons per unit time per unit area crossing a plane F_n (eq. 1.5) is determined.

$$F_n = -v_{th} l \frac{dn}{dx} \quad (1.5)$$

$$J_{diff-n} = -qF_n = +qv_{th} l \frac{dn}{dx} = +qD_n \frac{dn}{dx} \quad (1.6)$$

In the absence of an electric field carriers move with thermal velocity v_{th} and

travel a distance equal to the mean free path l , which is the distance between collisions. The quantity D_n is called the electron diffusion coefficient. While the direction of the electron flux is negative, the direction of the electron diffusion current density is positive due to the negative electric charge of the electrons. In the case of holes, the flux and the diffusion current density have both positive directions because of the positive electric charge of holes (eq. 1.7)

$$J_{diff-p} = qF_p = -qv_{th}l \frac{dp}{dx} = -qD_p \frac{dp}{dx} \quad (1.7)$$

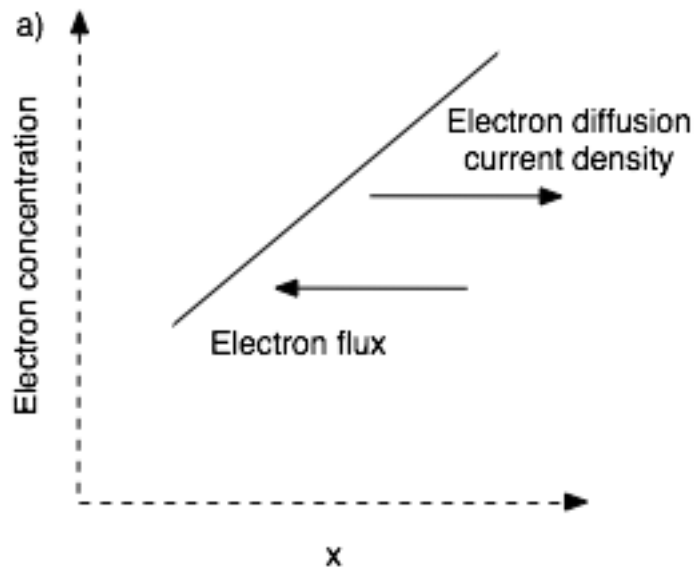


Fig. 1.1 Diffusion of electrons due to density gradient

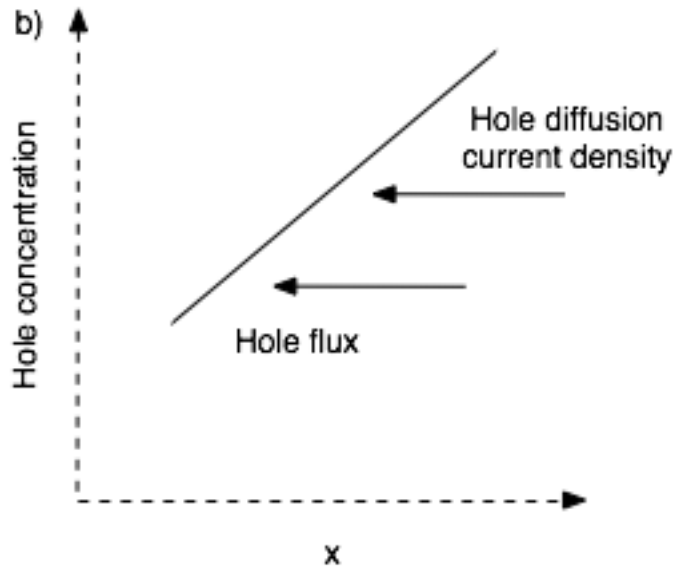


Fig. 1.2 Diffusion of holes due to density gradient

The diffusion-drift description of electrons and holes in a semiconductor is frequently used to obtain a detailed understanding of the physics and engineering of semiconductor devices with technologies above 80 nm [15]. The DD model uses the previous transport mechanisms plus the following basic equations [5]. These are the Poisson equation and the continuity equations for electrons and holes:

$$\text{div} (\varepsilon \cdot \text{grad } \psi) = q \cdot (n - p - C) \quad (1.8)$$

$$\text{div } \mathbf{J}_n = q \cdot \left(R + \frac{\partial n}{\partial t} \right) \quad (1.9)$$

$$\text{div } \mathbf{J}_p = -q \cdot \left(R + \frac{\partial p}{\partial t} \right) \quad (1.10)$$

Where ψ , the electrostatic potential, n and p , the electron and hole concentrations, are the unknown quantities. C is the net concentration of

ionized dopants and R is the net recombination rate. This leads to the generalized DD equation for electrons and holes:

$$J_n = q \cdot \mu_n \cdot n \cdot E + q \cdot D_n \cdot \text{grad}(n) \quad (1.11)$$

$$J_p = q \cdot \mu_p \cdot p \cdot E - q \cdot D_p \cdot \text{grad}(p) \quad (1.12)$$

The first term on the right-hand side is the drift component of the current, and the second term is the diffusion component. The total current in the device is the sum of electron and hole density currents.

CHAPTER 2: Transport models

2.1 DOWNSCALING OF DIMENSIONS

Nowadays, the industry of microelectronics is moving toward giga-scale integration (GSI), this means to have more active components in a smaller area. As stated by the Moore's Law, the circuit area density (number of devices per unit area) scales by a factor of 2 each 18 to 24 months. This is possible by the downscaling of device dimensions, which involves the improving of fabrication technologies. However, this method will not always be the chosen one, at some point these devices will meet technological and physical limitations. Structures and devices can be built with dimensions that are too small so new physical processes become important in the overall transport. Metal-Oxide-Semiconductor Field Effect Transistors (MOSFETs) are the most essential structures in the industry, as they are the basic components for many electronic devices.

Effects such as oxide breakdown, source–drain punch-through, impact ionization in the MOSFET channel, DC gate current, and so on are major candidates for processes to limit downscaling [15]. Because the traditional scaling pathway reducing oxide thickness and channel length to improve device performance could no longer be followed, an alternative option emerged recently in which MOSFETS have different fabrication materials and geometries.

The widely used SiO_x as a dielectric material is being replaced with high K dielectrics, such as hafnium oxide, this allows fabrication technology not to reduce the oxide thickness, leading to a much larger control of the charge in

the substrate; channel strain was introduced to improve carrier mobility, double/tri gate nanostructures are being studied to improve the MOSFET efficiency, and some other nanostructures have arisen, like nanowires [15]. There's still a long way for traditional MOSFET structures though, there are effects emerging continuously that can be exploited by the industry.

The fast downscaling of device technology towards sizes of some nanometers makes the community think of the physical understanding of the classical structures operations, and whether they can be extrapolated down to these new device dimensions without changing the basic macroscopic transport physics. This is where the third intermediate length scale shows up, what is now referred to the mesoscopic regime, in which electron exhibits particle-wave behavior.

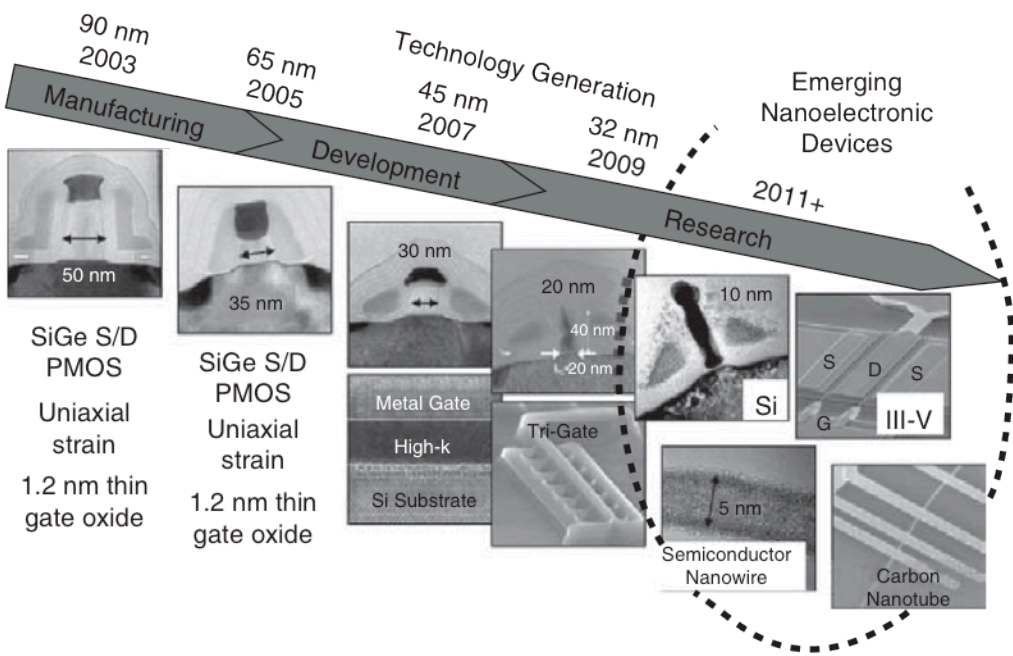
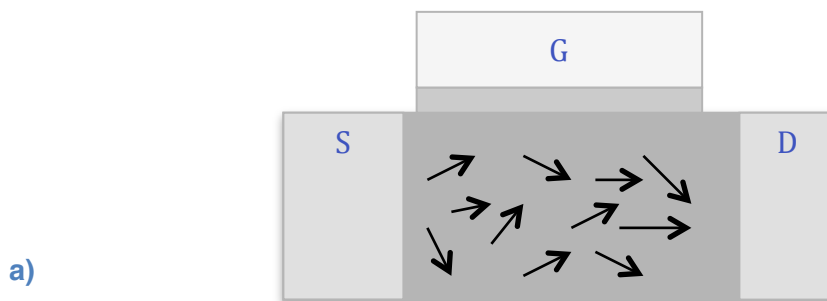


Fig. 2.1 MOSFET tendency for the next generations [15]

The devices in this scale introduce emphasized parameter variations from one device to another in the same fabrication process, which are determinant in the study of phenomena appearing in these structures. These effects are classified in the world of mesoscopic devices.

2.2 OTHER TRANSPORT MODELS

Since the 1960s and 1970s, researchers have observed effects of quantum confinement of carriers at surfaces and interfaces, and these were still studied by semiclassical approaches. However, working on tens of nanometers makes classical models very inaccurate, and not appropriate yet to fit quantum mechanical behavior. That is why currently more complex models are being used to solve these mesoscopic phenomena, and this becomes more important in each technology generation. For example, a physical effect that is affected with the downscaling of devices is the appearing of ballistic transport, meaning carriers suffer few or no scattering as they flow through the channel (Fig. 2.2). Quantum effects are expected to play a major role if this happens.



b)

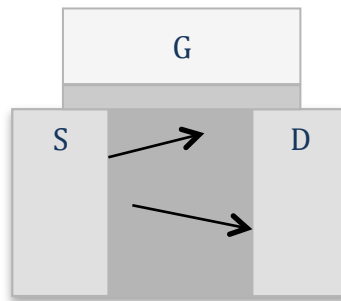


Fig. 2.2 Scattering mechanisms in a MOSFET structure. a) Diffusive motion of carriers, there are several scattering events. In b) there is ballistic transport as there are few scattering events

The case in this work is another example of these unexpected behaviors, a current is measured in a MOSFET device that is not predicted by the classical models used so far. The DD equation is used to replicate the phenomenon in a simulation tool, but this wasn't successfully achieved. It wasn't until a quantum corrected model was used that the phenomenon was qualitatively reproduced, and a physical explanation is needed. The relevance of studying the observed phenomena is that the cause of this may be an important insight into effects that may well be expected to occur in future smaller devices.

The reason the diffusion-drift description fails is not that its equilibrium laws mentioned before are violated but rather that its constitutive theory is inadequate. For example, as shown later, the electrons in the inversion layer no longer act as the simple charge gas assumed by the usual diffusion-drift description.

Since the observation of these unpredicted effects, "new" models are being

used to fit these experimental results, since quantum mechanical theory is not really a practical tool to solve such mysteries as they required a lot of complex numerical work, hence, a great computational labor to reduce time solving the equations.

The models are not really new, they start from the classical macroscopic approach and they are modified to include corrections, of quantum nature in general, to get a final physical model that predicts certain mesoscopic behavior. It is done this way due to the general validity of macroscopic behavior, whereas microscopic theories are always subject to discussion. Just some quantum behaviors are taken into account when adding to macroscopic models [9]:

- a) Quantum compressibility – There is an electronic repulsion (via the Pauli principle) that makes electron gases in solids harder to compress.
- b) Electron evanescence – The wave nature of electrons shows evanescence, and it arises when electron waves encounter a “barrier” region incapable of sustaining their propagation. It is seen macroscopically as quantum confinement and quantum tunneling.
- c) Electron diffraction – The interference and diffraction effects are manifested when dealing with electron waves.

One or more of these quantum behaviors are added to macroscopic models. For example, the quantum corrected equation used in this work to replicate the phenomena adds electron evanescence to the DD macroscopic model. Some of these macroscopic and mesoscopic approaches, other than the DD mentioned previously, are listed below [4, 5, 13].

Classical hydrodynamic model (HD)

This model treats the propagation of electrons and/or holes in a semiconductor device as the flow of a charged compressible fluid. The hydrodynamic should be valid for devices with active regions greater than $0.05 \mu\text{m}$ [13]. In this model carrier temperatures are allowed to be different from the lattice temperature. The model exhibits hot carrier effects missing in the standard drift-diffusion model.

Energy transport model (ET)

The model involves the temperature of the mobile species as a variable of the problem in addition to the density. The temperature changes according to an energy balance equation where the energy fluxes are defined by a similar constitutive relation as the mass flux. There are energy balance equations, which determine the carrier temperatures, added to the basic equations 1.8 to 1.10. These can be set in terms of the carrier temperatures T_n and T_p :

$$\text{div } \mathbf{S}_n = \text{grad} \left(\frac{\varepsilon_c}{q} - \psi \right) \cdot \mathbf{J}_n - \frac{3 \cdot k_b}{2} \cdot \left(\frac{\partial(n \cdot T_n)}{\partial t} + R \cdot T_n + n \cdot \frac{T_n - T_L}{\tau_{\varepsilon,n}} \right) \quad (2.1)$$

$$\text{div } \mathbf{S}_p = \text{grad} \left(\frac{\varepsilon_v}{q} - \psi \right) \cdot \mathbf{J}_p - \frac{3 \cdot k_b}{2} \cdot \left(\frac{\partial(p \cdot T_p)}{\partial t} + R \cdot T_p + p \cdot \frac{T_p - T_L}{\tau_{\varepsilon,p}} \right) \quad (2.2)$$

Where \mathbf{S}_n and \mathbf{S}_p are the energy fluxes. $\tau_{\varepsilon,n}$ and $\tau_{\varepsilon,p}$ denote the energy relaxation times.

Quantum hydrodynamic model (QHD)

The goal of this model is to rigorously handle discontinuities in the potential energy which occur at heterojunction barriers, in quantum semiconductor devices; the hydrodynamic equations get mathematically complex because of these discontinuities. The model is derived from a moment expansion of the Wigner-Boltzmann equation. This process involves taking averages of the kinetic equation to obtain transport equations for charge carrier, momentum and energy densities.

Quantum Drif-Diffusion (QDD) or Density gradient (DG) model

In order to improve the accuracy of the Drift-Diffusion equations (DD) on complex device structures some quantum corrections are not being ignored anymore. The DG model can be seen, in its simplest form, as a direct enhancement of the DD theory. By generalizing the equation of state of the electron gas to include density-gradient dependences, the standard description can be extended to describe much of the quantum-mechanical behavior exhibited by strong inversion layers.

The DG model was developed by observing how the gradient of density in the electron gas, in addition to its density, impacts on its energy. It is assumed that the inversion layer follows the electron gas behavior, and, as such, it changes its properties very rapidly on the vicinity of an interface. It has been demonstrated that this model is very efficient for solving devices with gate lengths ranging from 30 nm to 6 nm [3, 13].

Of course there is some work done on finding computationally efficient methods to include quantum mechanical effects, this is done in order to have

a more practical Computer Aided Design software. Those are based on working on the non-equilibrium Green's function and/or the Wigner's function [13]. But as mentioned before, they cost a lot of computational time and effort. In [19] there are a number of computational methods that solve the Wigner's equation, the computational time is given by the number of iterations, but they could go from 30 to 90 minutes with only 15-20 iterations, pointing out that this depends on the computer capabilities.

CHAPTER 3: Experimental and simulation results, explanation.

3.1 EXPERIMENTAL RESULTS

A Metal-Oxide-Semiconductor Field Effect Transistor (FET) with technology of 34 nm, and high-k metal-gate was used. The company IBM provided the device, and because of this the information on the device parameters is just partial. The original purpose of the experiment was to confirm the classical voltage-current characteristics of the device, but when applying the following experimental conditions something happened:

- V_{gs} swept from 0 V to 1.2 V, with .05 V increments.
- V_{ds} swept from $75\mu\text{V}$ to $275\mu\text{V}$, with $25\mu\text{V}$ increments.
- Body and source terminals were grounded.

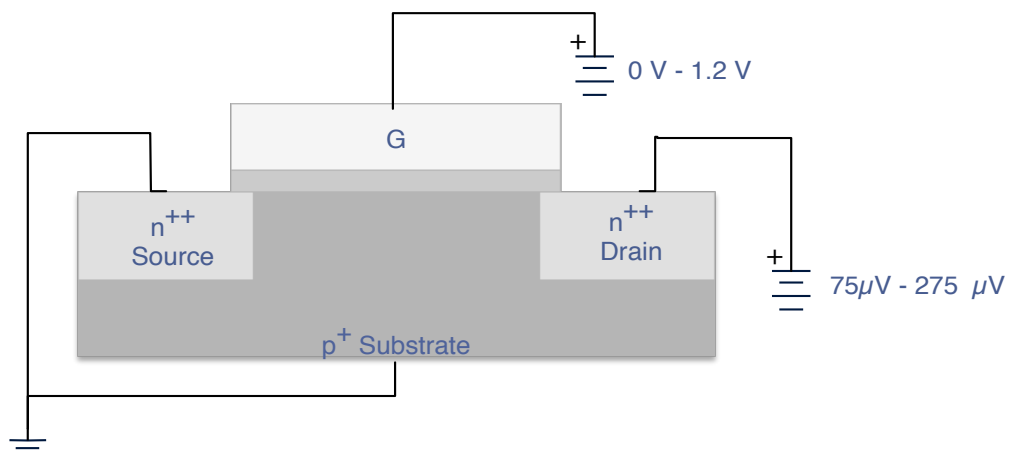


Fig. 3.1 Experimental conditions

A peculiar phenomenon was observed inside the transistor. Classical charge

transport theory says that when applying certain potential on the gate, a depletion region is created in the bulk, and this will eventually turn into the inversion channel, in which carriers will move from source to drain, at a V_{th} value, which is around 0.4 V. In this case, the device is a n-channel MOSFET, and the inversion layer will be formed by electrons.

There are two driving forces capable of transporting carriers, an external source and an internal one. The external one is by applying an electric field between source and drain, this electric field induces a force on electrons so that they will experience a net movement, the drift force. The other force is the one caused by an internal equilibrium of charges along the channel, where the flow of charges moving from a high concentration region to a low concentration region causes an electric current, the diffusion current. So, even if the inversion layer has already formed, if there's very low potential between source and drain there is a small electric field between these two terminals to transport carriers in the channel, and this should cause the current to be positive. In addition, classically it is considered a homogenous inverted channel when V_g is greater than V_t , and small V_{ds} values (the case here shows those conditions since $V_t \sim 0.4$ V), so there should be no concentration gradients, and no diffusion component should be added. Those predictions weren't observed in the experimental results (Fig. 3.2).

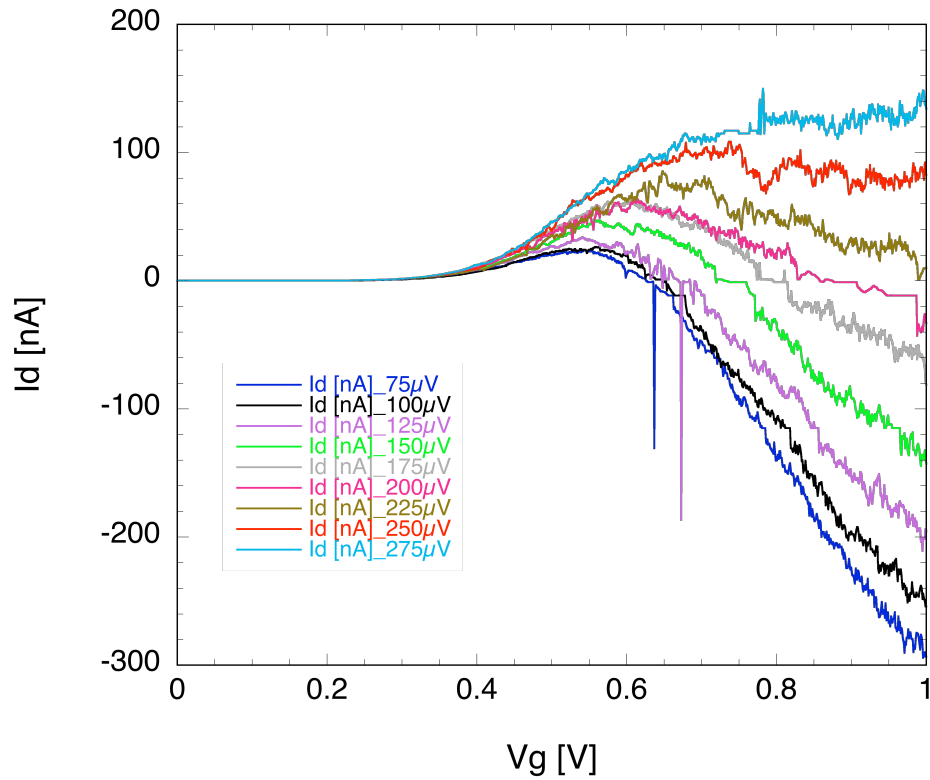


Fig. 3.2 Experimental results for $V_d = 75 \mu\text{V}, 100 \mu\text{V}, \dots, 275 \mu\text{V}$. $(W/L) = (1\mu\text{m}/34\text{nm})$, $T = 300 \text{ K}$.

3.2 EXPLANATION THROUGH ANALYSIS AND SIMULATION

At the presence of a positive electric field, even if its magnitude is too small, carriers should flow from source to drain, not in the opposite way. As can be seen, for small values of V_d s, the I_d current begins as positive, meaning that the current flows from drain to source, and then the current reverses its sign as V_g is increased, which means that the current flows now from source to drain. As V_d s is increased the reversal of the sign is less emphasized until it follows the regular expected behavior. A physical explanation is needed on why does the current reverses its sign, and the reason this effect slowly disappears on increasing V_d s.

It is first thought that this phenomenon must be related to diffusion of charges since the low electric field between source and drain predicts a positive current. There should be a gradient somewhere inside the device that causes a key diffusion component, being responsible of the direction of the current over the drift component. A second thought is to prove this by making use of a TCAD tool that includes the drift-diffusion model to prove the origin of the current is found on a charge gradient. What if this tool could reproduce this phenomenon? The result could throw some answers.

TCAD (Technology Computer-Aided Design) solutions refer to the use of computer simulations to develop and optimize semiconductor processing technologies and devices. Nowadays, simulation tools are very helpful in order to understand certain phenomena. They are generally used to prove whether some theoretical analysis can replicate experimental results; however, in this case, if the simulated result could be compared with the experimental one, the purpose would be to find the theoretical explanation through the simulation analysis.

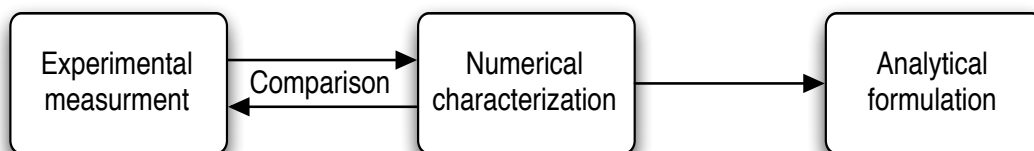


Fig. 3.3 Suggested analysis process

The MINIMOS-NT simulation tool was used. It is part of the GTS Framework 2013, a state-of-the-art framework developed by the company Global TCAD

Solutions in collaboration with the Institute for Microelectronics, TU Wien, Austria. This is a semiconductor device simulator for commercial purpose in which the transient and small signal analysis will be very useful. This tool facilitates simulation of several device structures by solving carrier transport equations iteratively and it allows simulating the device by only giving the specific known characteristics (Table 3.1).

Table 3.1: Known device parameters

Parameter	Value	Units
Substrate impurity concentration	1×10^{17}	cm^{-3}
Source/Drain impurity concentration	2×10^{18}	cm^{-3}
Effective gate oxide thickness	~ 2	nm
K (HfO_2)	25	-

The gate oxide thickness is considered as the effective one because of the way it is formed, the oxide is constituted by a hafnium oxide layer between two silicon oxide layers.

The first simulation was implemented with the previous parameters, and the bias conditions are the same as the experimental ones:

- V_g swept from 0 V to 1.2 V, with .05 V increments.
- V_{ds} swept from 0 V to 500 μV , with 25 μV increments.
- Body and source terminals were grounded.

The device is represented in the simulation tool as in Fig. 3.4, and the classical DD model was implemented.

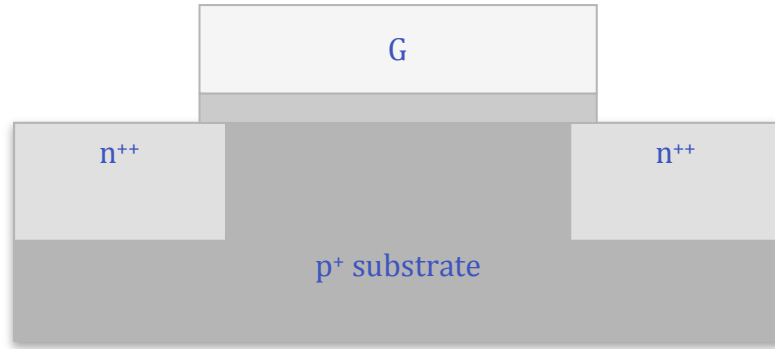


Fig. 3.4 The MOSFET in the simulation tool

This model solves the following equations to find the electron and hole current densities [5].

$$J_n = q \cdot \mu_n \cdot n \cdot \left(\text{grad} \left(\frac{\varepsilon_c}{q} - \psi \right) + \frac{k_B \cdot T}{q} \cdot \frac{N_{C,0}}{n} \cdot \text{grad} \left(\frac{n}{N_{C,0}} \right) \right) \quad (3.1)$$

$$J_p = q \cdot \mu_p \cdot p \cdot \left(\text{grad} \left(\frac{\varepsilon_V}{q} - \psi \right) - \frac{k_B \cdot T}{q} \cdot \frac{N_{V,0}}{p} \cdot \text{grad} \left(\frac{p}{N_{V,0}} \right) \right) \quad (3.2)$$

being μ_n and μ_p the electron and hole mobility, n and p the electron and hole concentrations and ψ is the electrostatic potential. The band edge energies, ε_c and ε_V , are position-dependent, same as the effective masses, which are included in the effective density of states, $N_{C,0}$ and $N_{V,0}$. The index '0' shows these quantities are evaluated at an arbitrary reference temperature T_0 . [5]

The solution using this model is the expected theoretical classical analysis result, a positive current was measured, meaning current flows from source to drain as in Fig. 3.5.

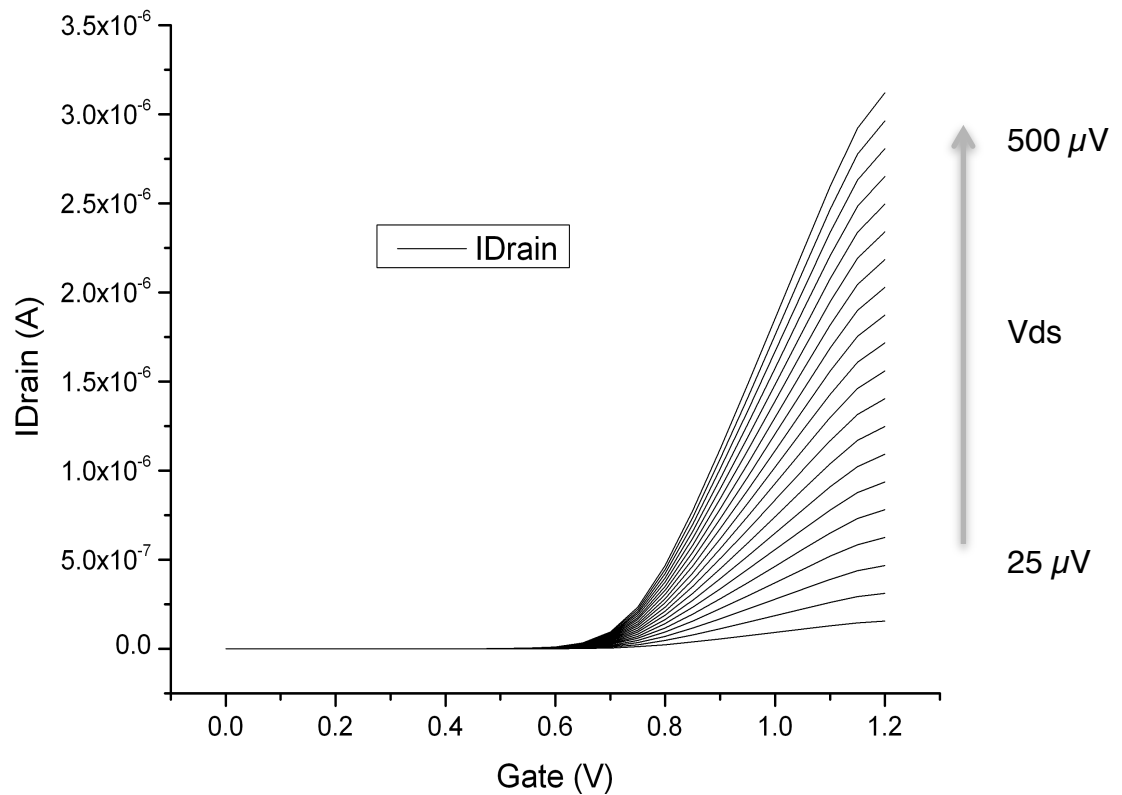


Fig. 3.5 Simulation results using the DD model. Expected increasing positive current is found.

But this model considers the channel to be homogenous, and therefore the model cannot prove that the reversal of the current is caused by a gradient of charges. Working on this range of sizes introduces random fluctuations of dopant atoms; the incorporation of strain, halo doping, trenches, and different oxide and gate materials in the device must affect the channel and make it non-homogenous along it.

Then, the simulation may be forced to introduce a non-uniform density of charges in the channel, and this is done by placing a reduced region in the channel with a local dopant concentration that is different from the substrate, replicating a non-homogenous channel once it's inverted (Fig. 3.6) and

therefore, when simulating the device a diffusion current would appear.

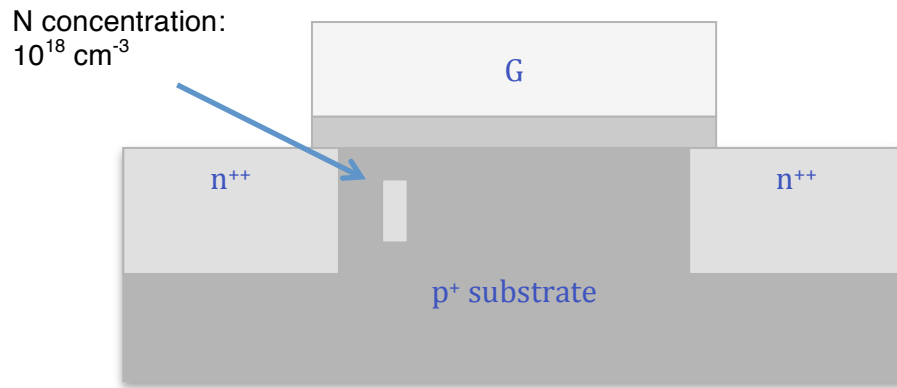


Fig. 3.6 Transistor schematic representation with the inclusion of a doped area.

However, such a negative current didn't show up. The same results as in Fig. 3.5 were observed, but with an almost negligible increase in magnitude of the current. This leads to the thought that some of the conditions assumed by the drift-diffusion classical analysis cannot be applied to this device, and quantum corrections must be incorporated in the analysis to get a more accurate result.

There is one obligated quantum mechanical effect that needs to be incorporated. In transistors with very thin oxides and large substrate doping, which is the case here, the electric field magnitude and the band bending near the surface are larger than typical MOS structures; the potential well determined by the oxide interface and the conduction band of the semiconductor, in which charges of the inversion layer are located, becomes very narrow, and these charges follow the quantum physics of confined particles [18].

This quantum phenomenon causes the second-order effect known as inversion layer centroid, where the inversion layer peak concentration is not found immediately next to the semiconductor-oxide interface but away from it by a short distance corresponding to the minimum point of conduction band edge E_c (Fig. 3.7). The effect of the inversion layer centroid must be included in the simulation tool in order to describe the transport properties more accurately.

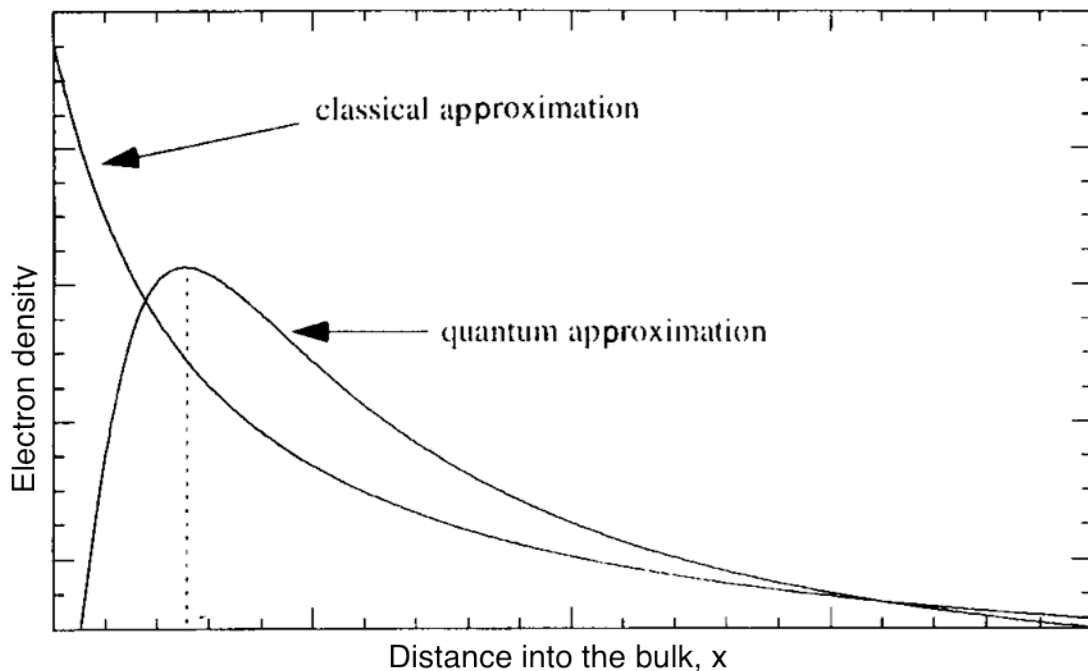


Fig. 3.7 Representation of the electron density in an inverted surface as function of the x-position for classical and quantum mechanical approaches [18]

López-Villanueva, et. al. [6] developed a semi-empirical inversion layer centroid model capable of locating the charge centroid at a distance Z_i for a wide range of electrical and technological variables and it shows the dependence of the inversion layer centroid location with the inversion charge

density (Eq. 3.3). According to this model, the more the inversion layer is inverted the closer is the charge centroid to the semiconductor-oxide interface.

$$Z_i = Z_{i0} \cdot \sqrt{\frac{1 \times 10^6 \text{ V}}{\text{cm}}} \cdot \left[\sqrt{\frac{Q_D}{\epsilon_{si}} \left(\frac{Q_D}{\epsilon_{si}} + \frac{1}{2} \frac{Q_I}{\epsilon_{si}} \right)} \right]^{-1/3} \quad (3.3)$$

Z_{i0} is fitting parameter based on several numerical simulations, and 1.2 nm provides a good agreement with numerical results; the work that establishes that value is found in [8]. The depletion and inversion charges Q_D and Q_I are calculated with the following expressions:

$$Q_D = \sqrt{2 \epsilon_{si} q N_B \left(\varphi_{dep} - \frac{kT}{q} \right)} \quad (3.4)$$

$$\varphi_{dep} = \left(\psi_s - \frac{1}{\epsilon_{si}} Z_i Q_i \right) \quad (3.5)$$

$$Q_i = C_{ox}' \left(V_{GS} - V_{FB} - \varphi_{dep} - \frac{Q_D}{C_{ox}'} \right) \quad (3.6)$$

$$C_{ox}' = \frac{\epsilon_{ox}}{T_{ox} + \frac{\epsilon_{ox}}{\epsilon_{si}} \cdot Z_i} \quad (3.7)$$

where φ_{dep} is the potential associated with the depletion layer band bending and ψ_s is the surface potential. The region in the substrate between the charge centroid and the semiconductor-oxide interface can be taken as an extension of the dielectric material, which is equivalent to having a thicker gate oxide and this is taken into account for certain analysis. In this case, C_{ox}'

is the effective capacitance measurement that includes the oxide capacitance and a centroid capacitance.

As mentioned before, the relevance of this is that it predicts that the inversion layer density, related to the potential, determines the position of the charge centroid [6, 8], and this is related to the subject of this work since V_g controls the inversion region in the substrate and therefore, the location of the inversion layer centroid in the substrate [Fig. 3.8]. However, the parameters included in the model are all said to be non-changing along the channel given it is homogenous from source to drain when working at very low V_{ds} values, which means that the location of the charge centroid, given in terms of distance from the semiconductor-oxide interface, is the same along the channel.

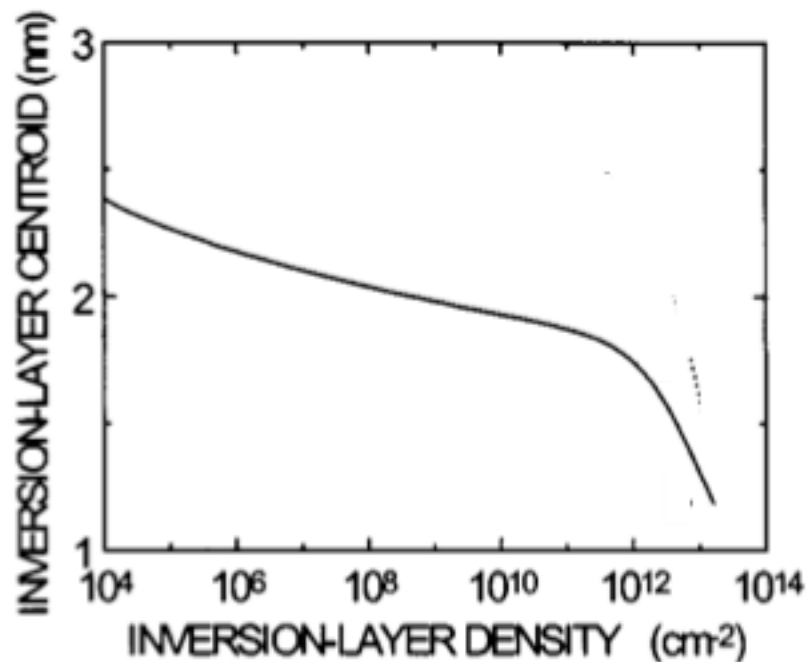


Fig. 3.8 Charge centroid location variation with the Inversion layer density

It was stated before that these non-varying assumptions are no longer valid. This means that there should be a fluctuation of the charge centroid position along the channel, given that the random dopant fluctuation affects the distribution of the electric field and therefore the carrier concentration, even in the inversion layer [18, 20]. Even more, this variation is emphasized near the drain-to-bulk and source-to-bulk interfaces due to the strong potential variation because of the gate and drain voltage modulation [18].

The next step is to include the quantization of the inversion layer in the simulation tool. It will help to reinforce the theory of a varying charge centroid location and its impact on the transistor current. The MINIMOS-NT integrates the Density Gradient model (DG), which is one model that enhances the DD classical model with quantum corrections, such as particle confinement. This would be the way to add the inversion layer centroid.

This model can be seen as a mathematical description with two different approaches, as a phenomenology or as a theory. In the first approach, the model is obtained through a rigorous mathematical description in which the equations may not be grounded on physical principles, but it parts from a well founded theory [9]. On the other hand, in the theoretical approach, the involved equations have their foundations on physical phenomena and, thus, can be predictive. The Density-Gradient model incorporated in the MINIMOS-NT simulation tool makes use of the phenomenology method, which is the most common approach in quantum mechanical analysis.

This model solves Eq. 3.8 and 3.9:

$$J_n = q \cdot \mu_n \cdot n \cdot \left(\text{grad} \left(\frac{\varepsilon_C}{q} - \psi - \gamma_n \right) + \frac{k_B \cdot T}{q} \cdot \frac{N_{C,0}}{n} \cdot \text{grad} \left(\frac{n}{N_{C,0}} \right) \right) \quad (3.8)$$

$$J_p = q \cdot \mu_p \cdot p \cdot \left(\text{grad} \left(\frac{\varepsilon_V}{q} - \psi - \gamma_p \right) - \frac{k_B \cdot T}{q} \cdot \frac{N_{V,0}}{p} \cdot \text{grad} \left(\frac{p}{N_{V,0}} \right) \right) \quad (3.9)$$

The quantities γ_p and γ_n are defined as the quantum corrected potentials, and this quantities are the summary of a more complex quantum analysis, which, according to a microscopic theory, involves solving the Wigner's distribution equation by the method of moments [1, 5]. Later on this work a much simpler valid analysis is presented, the macroscopic theoretical approach.

The simulation result showed that, when the model is changed to Density-Gradient, the current turns out to be negative, and a qualitative comparison with the experimental results can be made (Fig. 3.9). On the other hand, the result shows that the phenomenon must be related to a charge distribution issue since the introduction of the inversion layer centroid causes the current to be negative, as not predicted by the theoretical classical DD analysis. The comparison shows that there's a negative I_d current in the device in both cases that decreases as incrementing V_{ds} for the same applied V_g . Now that there's a qualitative replica of the experimental results, the analysis can be done over the simulation data to find why the current suffers a change on its direction from a positive to a negative value from the physical point of view.

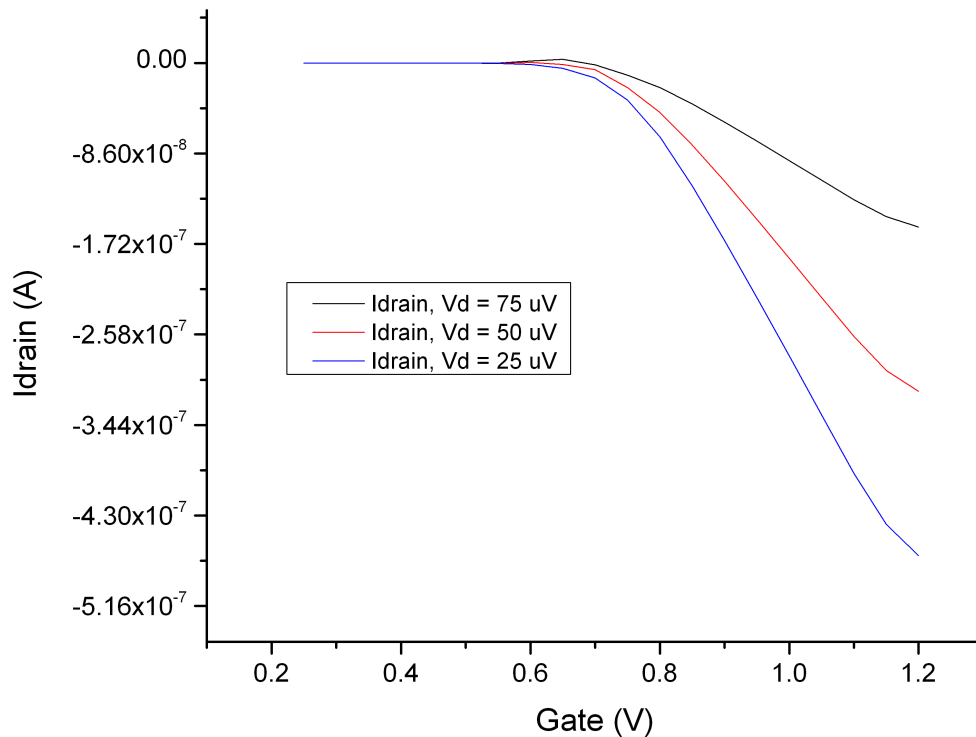


Fig. 3.9 Simulation result using the DG model

Fig. 3.9 shows a qualitative comparison with the experimental results. The following step was to implement a better adjustment of the parameters until a better simulation result could be found. The parameters to adjust were basically related to doping concentrations and boundary conditions. Fig. 10 shows the better qualitative comparison between the experimental and the simulation results. It is also shown the I_d gate current, and it can be seen that its magnitude is at least two orders of magnitude smaller compared to the I_d current. This is just to rule out that the I_g gate current could contribute to the reversible current effect.

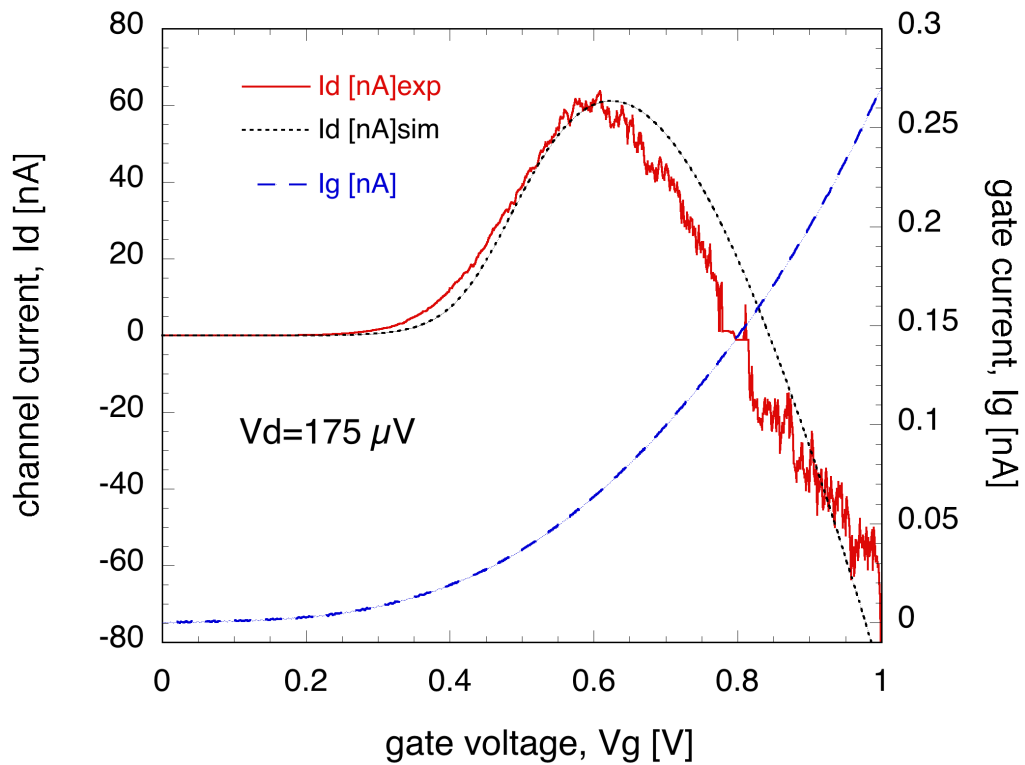


Fig. 3.10 A better parameter adjustment shows a better comparison.

In summary, when the DD model was used to simulate the transistor, the result is the expected behavior, positive current is flowing between drain and source. However, when the DG model was chosen and a non-homogenous channel was implemented in the simulation tool, the result showed a qualitative similitude with the experimental results. It is inferred that the explanation should be the difference between one model and the other, taking into account the concentration gradient introduced to simulate a non-homogenous channel.

Fig. 11 and fig. 12 show graphically the change in the direction of the current density vector in the simulation tool for $V_g=0.4$ V and $V_g=1$ V, respectively.

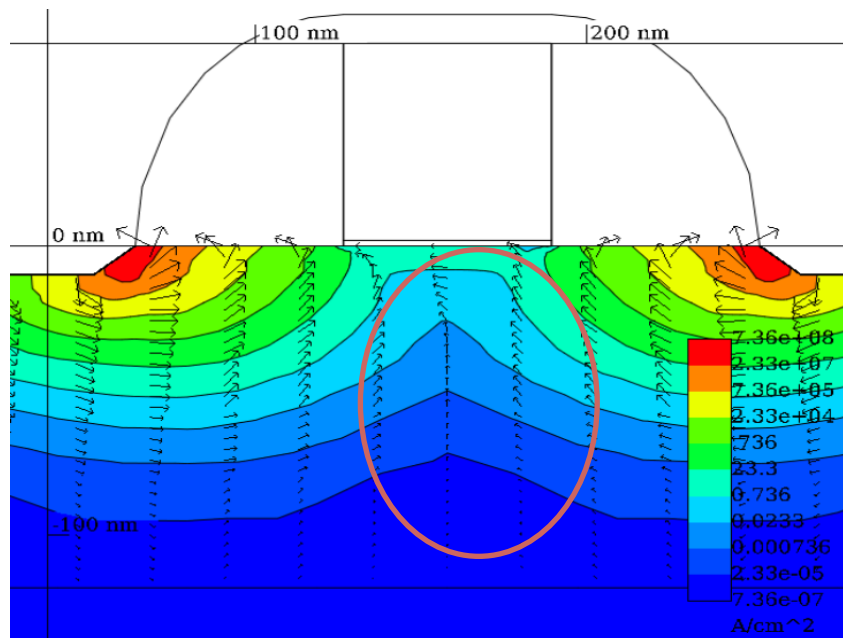


Fig. 3.11 Density current vector at $V_g = 0.4 \text{ V}$

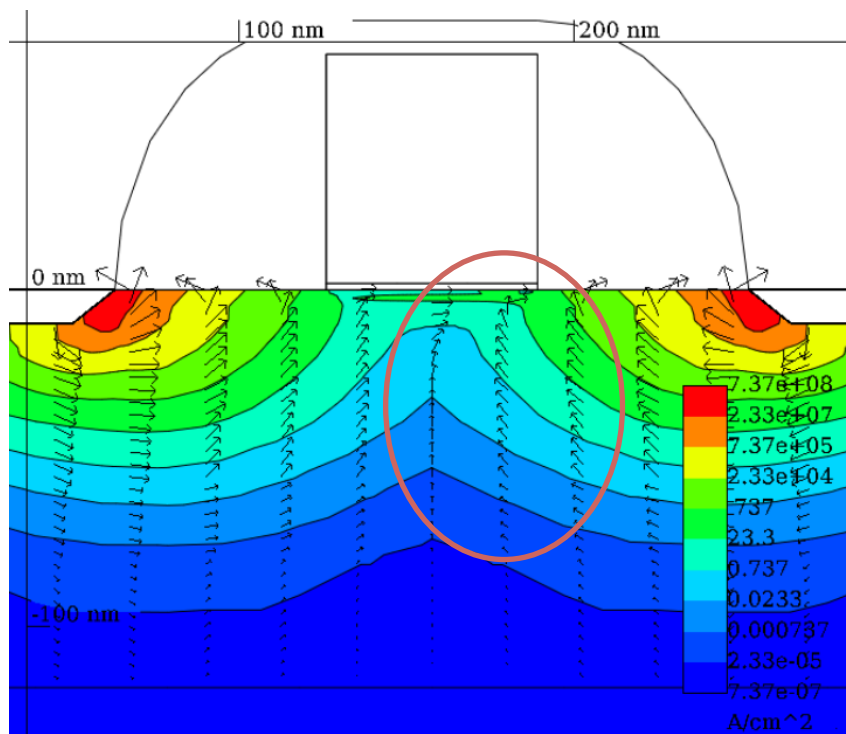


Fig. 3.12 Density current vector at $V_g = 1 \text{ V}$. Comparing with fig. 3.11 there's a change on the direction

A comparison between the set of equations of the DD model (Eq. 3.1 and 3.2) with the DG model equations both implemented in the MINIMOS-NT tool (Eq. 3.8 and 3.9) is done. The only difference is the addition of the quantum corrected potentials γ_p and γ_n (Eq. 3.10 and 3.11), which are the first order approximations derived from the Wigner's equation [5].

$$\gamma_n = \frac{\hbar}{12 \cdot \lambda_n \cdot m_0} \cdot \text{div grad} \frac{\psi + \gamma_n - \varepsilon_c/q}{k_B \cdot T} \quad (3.10)$$

$$\gamma_p = \frac{\hbar}{12 \cdot \lambda_p \cdot m_0} \cdot \text{div grad} \frac{\psi + \gamma_p - \varepsilon_v/q}{k_B \cdot T} \quad (3.11)$$

This is the set of equations solved by the simulation tool, but this is the microscopic approach, a result of the mathematical analysis to get a numerical result. The physical origin of the model must be studied in order to have a better understanding of the difference between the DD and DG equations.

The macroscopic origin of the DG model is found on the work done by M. G. Ancona and G. J. Iafrate [9, 10]. They developed a macroscopic description of transport of electrons in a semiconductor in which the equation of state for the electron gas was generalized to include a dependence on the gradient of the density.

As mentioned in Chapter II, the Density-Gradient model takes the quantum electron evanescence into its macroscopic theory as a prime purpose. The physical principles of the DG theory are classical, they consist of the conservation of charge and momentum, meaning that the conservation of the total electron or hole charge in a volume increases in time only due to entry

through its surface via generation process inside the volume [9], plus the laws of electrostatic; its theory is based on treating the semiconductor as an electron gas, a hole gas, and a rigid lattice continuum, just like the DD theory.

There are some material response functions developed in the model that come from an energy balance analysis, and those are especially important to include electron and hole gas interactions. These equations are incorporated to distinguish between different semiconductors, otherwise the system of equations would dictate that every system is identical. The most important material response functions of the Density-Gradient theory are the equations of state that describe the electron and hole gases. These equations are not simple relationships between pressure and density but general expressions relating stress to density.

The generalization of the equation of state for the electron gas led to a new transport equation expressible as a DD eq., and called the Quantum DD equation, or Density Gradient [13]. Basically, the result is that the set of these equations (Eq. 3.12 and 3.13) are comparable with the DG equations included in the MINIMOS-NT.

$$J_n = -q \cdot \mu_n \cdot n \cdot \nabla(\phi + \phi_{DGn}) + q \cdot D_n \cdot \nabla(n) \quad (3.12)$$

$$J_p = -q \cdot \mu_p \cdot p \cdot \nabla(\phi + \phi_{DGp}) - q \cdot D_p \cdot \nabla(p) \quad (3.13)$$

D_n and D_p are the Diffusivity terms of electrons and holes, respectively, and as mentioned before, they account for position-dependent band edges and effective masses. The quantities ϕ_{qn} and ϕ_{qp} are called the generalized quantum potentials (Eq. 3.14 y 3.15).

$$\phi_{DGn} = 2b_n \left(\frac{\Delta\sqrt{n}}{\sqrt{n}} \right), \quad b_n = \frac{\hbar^2}{12 \cdot q \cdot m_e^*} \quad (3.14)$$

$$\phi_{DGp} = -2b_p \left(\frac{\Delta\sqrt{p}}{\sqrt{p}} \right), \quad b_p = \frac{\hbar^2}{12 \cdot q \cdot m_p^*} \quad (3.15)$$

They are called by that name because of their similitude with the quantum potential introduced by Bohm [4]. As mentioned before, there are some material response functions, and those are the b_n and b_p parameters, they measure the strength of the gradient responses of the gases. The purpose of comparing the set of equations proposed in the simulation tool (eq. 3.8 and 3.9) and the model developed by M. G. Ancona (eq. 3.12 and 3.13) is shown.

The relevance of these models is the way they were obtained. Both have the generalized form of the DD, with quantum corrections included; however, the DG model used by the simulation tool is obtained through the solution of the Wigner equation by the method of moments [1, 5], and it may be seen as the result of some mathematical treatment in order to reduce and save computational effort in order to get a simpler model. On the other hand, the macroscopic model developed by M. G. Ancona [10, 11, 12] has a more physical treatment since it is obtained through the inclusion of density-gradient dependence in the equation of state in the electron gas. That is why the explanation of the change in the direction of the current through the latter is valid.

Eq. 3.12 and 3.13 are the quantum Drift-Diffusion current equations, but these are the result of the inclusion of the quantum potentials ϕ_{qn} and ϕ_{qp} in the two generalized current equations 3.16 and 3.17 [12]:

$$J_n = -q \cdot \mu_n \cdot n \cdot \nabla(\phi) + q \cdot D_n \cdot \nabla(n) - 2q \cdot \mu_n \cdot b_n \cdot n \cdot \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) \quad (3.16)$$

$$J_p = -q \cdot \mu_p \cdot p \cdot \nabla(\phi) - q \cdot D_p \cdot \nabla(p) + 2q \cdot \mu_p \cdot b_p \cdot p \cdot \nabla\left(\frac{\Delta\sqrt{p}}{\sqrt{p}}\right) \quad (3.17)$$

The physical meaning is that this set of equations can be seen as the classical drift and diffusion current equations (the first two terms at the right-hand side) with the addition of a third quantum corrected term. This term arises as result of incorporating gradient effects and observing the electron gas response, and this means that the last term is of the same physical character as the diffusion term, and thereby it can be viewed as quantum diffusion current.

Equations 3.16 and 3.17 are simplified mathematically to get to equations 3.12 and 3.13. The third quantum corrected term is manipulated to be incorporated as a quantum potential in the first term and the latter can be treated as current driven by an effective electric field although it physically has its origin in a concentration gradient. All of this development validates the thought that the cause of the reversal of the direction of the current must be the presence of a concentration gradient caused by quantum confinement on the inversion layer.

As the potentials are of interest, the quasi-Fermi potential can be observed in the simulation tool. As can be seen, there is a particular change on the sign of the slope of the quasi-Fermi potential. The following is to emphasize this.

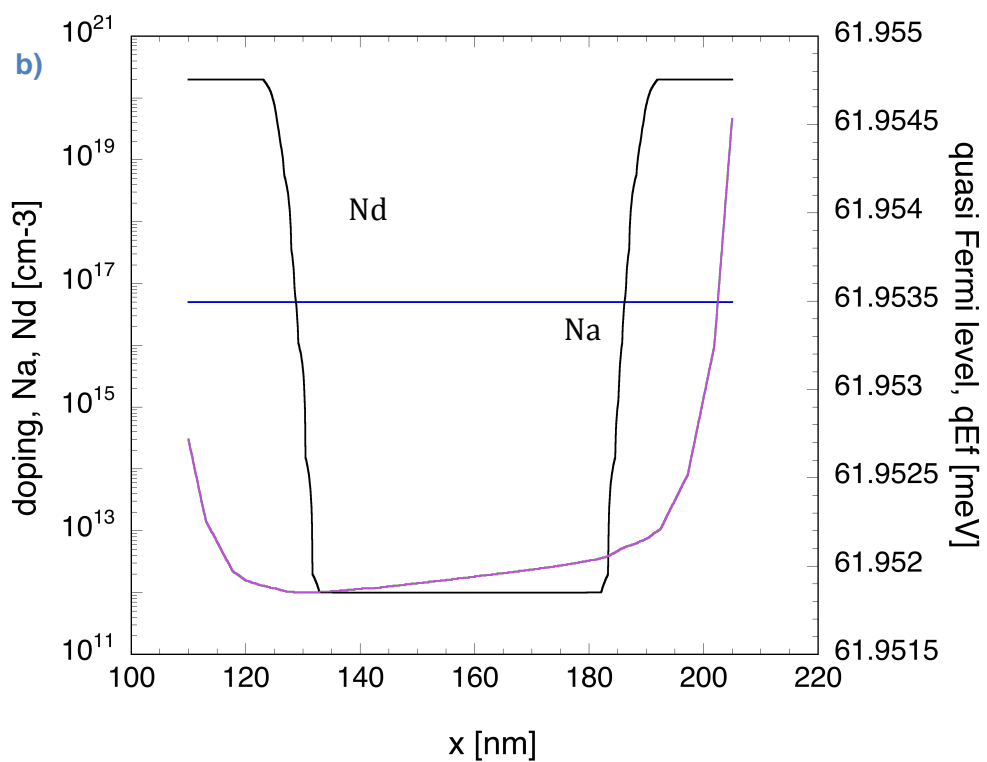
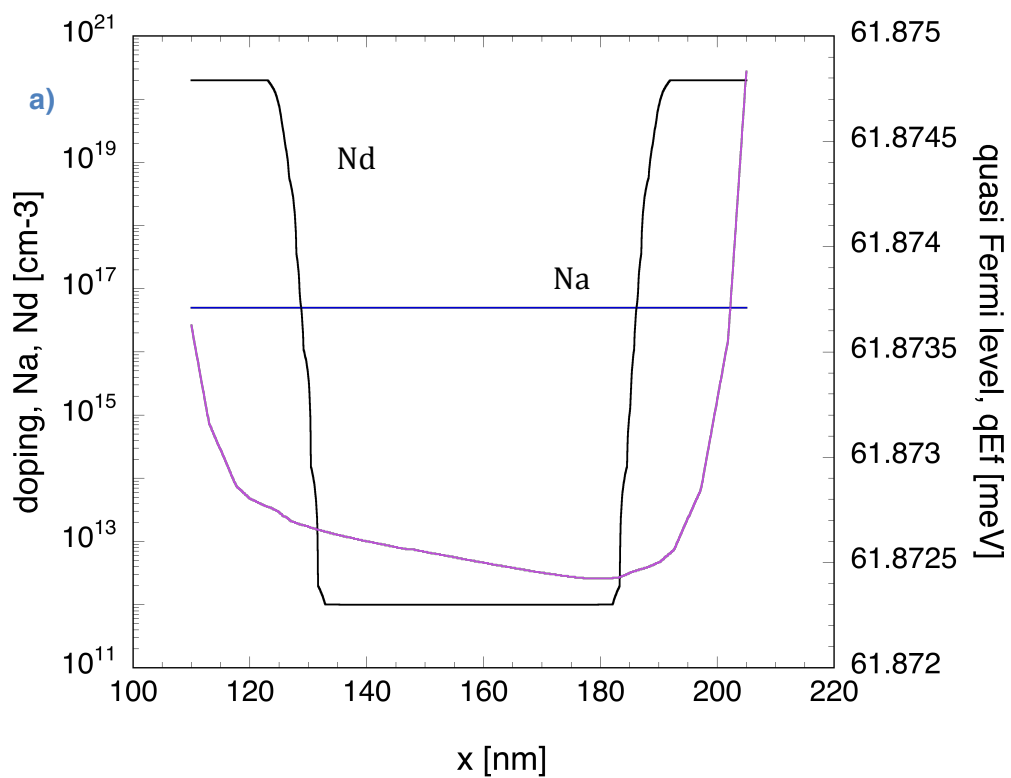


Fig. 3.13 quasi-Fermi potentials for a) $V_g = 0.75$ V, and b) $V_g = 0.95$ V

When working with the DD model it is very common to get the current in terms of the gradient of the quasi-Fermi potential. Some analogous work can be done, in which the Density gradient current equation is manipulated to be seen as the gradient of a quasi-Fermi potential (eq. 3.18 and 3.19).

$$J_n = n \cdot \mu_n \cdot \nabla \Phi_n \quad (3.18)$$

$$J_p = p \cdot \mu_p \cdot \nabla \Phi_p \quad (3.19)$$

This potential is a generalized form though, it includes the traditional electrochemical potential plus a quantum potential arose from the correction (eq. 3.20 and 3.21).

$$\Phi_n = \phi_n^{DD} + \phi_n^{DG} \quad (3.20)$$

$$\Phi_p = \phi_p^{DD} + \phi_p^{DG} \quad (3.21)$$

When the simulation tool used the classical DD model there was no negative current flowing, but when incorporating the DG model this current showed up, so the focus must be on the quantum potential ϕ^{DG} .

What could be stated is that this potential arises from the third term in equation 3.16 and 3.17, the gradient of this quantum potential acts as the driving force of that current, just as the drift and diffusion currents are originated by the quasi-Fermi potentials. The term coming from considering density gradient effects and the carrier responses to them says that its nature must be related to a diffusion physical character. The third term on these equations vanishes as the density gradients go to zero, and this occurs when the quantum physics are negligible compared to the macroscopic physics, in this case, when there's no quantum confinement below the semiconductor-

oxide interface. By vanishing the term, the classical drift-diffusion current equations are obtained.

The quantum confinement of carriers occurs when the channel is inverted. The peak concentration of carriers located away from the semiconductor-oxide interface and modulated by the potential on the gate is what induces this second order effect. Because of this dependency, the stronger the potential applied on the gate the closest is the charge centroid location to the semiconductor-oxide interface, and this means the quantum confinement is higher.

From this point of view, the only way that the current would change its sign is if the gradient of this generalized electrochemical potential Φ_n changes its sign, but the current only changes when considering quantum confinement on the inversion layer, so the most significant contribution of this phenomena is reflected on the quantum potential ϕ_n^{DG} instead of the classical ϕ_n^{DD} . Equation 3.14 tells that this potential is related to the electron concentration, the variation of it modulates the potential, and therefore the gradient of the current, reinforcing the theory that the phenomenon is a diffusive transport mechanism, and this was proven by the simulator by the addition of a local dopant concentration different from the substrate concentration, as in Fig. 3.6. What happens when the channel is also modulated by the V_{ds} potential? The impact of this electric potential impacts on the potential ϕ_n^{DD} . As this electric field gets stronger the current will be driven by the contribution of it, meaning the potential ϕ_n^{DD} is much greater than the quantum potential ϕ_n^{DG} .

CHAPTER 4: Final Thoughts

It has been a while since these quantum correction models were introduced to fit classical models. The Density Gradient model was originally introduced with the idea of simplifying the derivation of equations from the Boltzmann equation, including quantum corrections. [1]. The quantum correction models acquired more relevance since miniaturizing semiconductor devices reached a dimension in which some unpredicted singularities emerge.

The case here presented is just one of these singularities. No model could predict what happened in the device, it is not found in the literature. In spite of the years the Density Gradient has around, it's a very popular quantum correction model, and in this case this model helped understand the quantum behavior involved in the phenomenon.

It was shown that there's a relationship between the inversion layer centroid location and the inversion charge in the channel. This would mean that when V_g is modulated, so is the inversion layer centroid. Even more, the charge centroid is located differently along the channel because of this dependence.

This happens because it is well known that the inversion charge is not uniformly distributed along the channel, instead they are randomly distributed with large fluctuations in the actual concentration on this size scale. However, the lightly major charge concentration is commonly located at the middle of the channel length and then the inversion layer centroid is located closer to the semiconductor-oxide interface in the middle of the channel length, and it would then be moving away from the interface towards the source and drain

regions. All of these fluctuations would cause the quasi-Fermi level to be fluctuating as well, inducing a diffusion current. When V_g is altered, so are the gradients in the channel, and the quasi-Fermi level suffers a change in its magnitude, and this could be a positive or negative unbalance, therefore changing the direction of the current.

This happens at small V_{ds} values, meaning that the driving force which originates the third term in eq. 3.16 is greater than the force induced by the longitudinal electric field. At greater values of V_{ds} , the current is positive and follows the regular behavior because of the greater value of the drift current.

How many unpredicted effects will show up as technology heads to even smaller devices. Will all of these unexpected effects be explained? Although not predicted, will these phenomena be useful? Will they be helpful in any application?

There are a number of things to consider when studying these effects. For example, when there are some discrepancies between simulation and measurements, a decision must be made on whether considering that the simulation may be right, and measurement may be “wrong”, or vice versa. It is often considered that the device simulator unlikely produces incorrect results on correct structures, and maybe on these unpredicted effects this consideration may not be right.

But sometimes the cause of not getting the desired results on the simulations is that the structures are not well represented. For example, the result may depend on:

- The accuracy of the gate oxide thickness

- The doping profiles, the junction depths, uniform or non-uniform concentrations, etc.
- Choosing an inadequate grid on the device.
- The incorrect or incomplete specification of mobility and other physical models.

It can be seen that the user is very important in determining whether the structure is correctly represented.

In this work, replicating the phenomenon by trying to fit a simulation to the experimental results was a very important part of the analysis. However, this was done until a qualitative replica was found. This threw an acceptable physical explanation about the phenomenon, but this could be improved if the simulation result could also be fitted both qualitative and quantitatively. If so, some important parameters could be measured. This would tell how much impact has each parameter on the change of the direction of the current. The first impression is that they do have a big impact, since this phenomenon follows a quantum behavior and the presence or absence of the parameters involved seriously affect quantum physical phenomena.

Based on this, it would be important to have a mathematical model to introduce this effect in other related phenomena.

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