Towards electrostatic doping approaches in ultra-thin body semiconductor materials and devices

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TOWARDS ELECTROSTATIC DOPING APPROACHES IN ULTRA-THIN BODY SEMICONDUCTOR MATERIALS AND DEVICES

DISSERTATION

to obtain
the degree of doctor at the University of Twente,
on the authority of the rector magnificus,
prof. dr. T.T.M. Palstra,
on account of the decision of the doctorate board
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In the loving memory of my father and to the three beautiful
ladies in my life: my mother, wife and sister.

ABSTRACT

In the last seven decades there has been a revolution in the field of microelectronics which started with the invention of the bipolar transistor in 1948 and led to present day advanced computers and handheld devices such as smart phones. Continuous advancements in silicon (Si) based semiconductor devices (such as diodes, bipolar and field effect transistors) with their ever shrinking dimensions have fueled this technology revolution so far. The ability to dope Si with chemical impurities such as arsenic (As) or phosphorous (P) to control its conductivity played a key role in the remarkable success of the Si technology platform till date.

However, with the continuous downscaling of Si device dimensions to the nanometer regime and evolution of complex device architectures such as nanowires, nanofins and fully-depleted silicon-on-insulator (FD-SOI), it is increasingly difficult to match the device requirements by employing conventional chemical doping technologies. In addition, doping is even more challenging in emerging materials such as graphene, carbon nanotubes, 2-D materials, gallium nitride (GaN) and other wide band gap semiconductors. These materials are increasingly being sought for new application areas such as internet of things (IoT), artificial intelligence (AI) and wearable electronics. Among these materials, GaN is particularly interesting for both electronic and optical device applications. However, not only its doping is challenging, its production is also expensive which currently limits its widespread commercial applications. Monolithic integration of functional GaN based devices on a state-of-the-art Si CMOS platform could open up new applications in the area of high-power devices, RF electronics, lighting, sensing and display technologies and that with a reduced cost.

This thesis broadly deals with two aspects. Firstly, it describes possible alternatives to chemical doping in dimensionally scaled semiconductor devices based on alternative emerging materials and investigates the so-called "electrostatic doping (ED)" approach as a possible solution. In this work, various reported ED approaches have been reviewed and new device concepts have been proposed and investigated via TCAD simulations along with electrical and optical measurements of experimentally realized devices. The conditions for ED, *i.e.* inducing localized n-type or p-type regions in semiconductor using suitable metal work functions and gate biases, have been established. Among various possible ED based devices, the thesis particularly focuses on exploring the prospects of utilizing high-barrier Schottky contacts for devices such as LEDs, bipolar-transistors without adding any chemical doping. The thesis also explores the use of extreme work function contacts such as molybdenum oxide (MoO_x) for realizing

high-barrier diodes with bipolar conduction capabilities.

Secondly, this thesis investigates the possibility of utilizing atomic layer deposition (ALD) grown polycrystalline (poly-)GaN thin-films for device applications as a potential solution to low-cost GaN-on-Si technology platform. In this direction, various electrical and optical properties of ALD poly-GaN thin-films have been studied and their potential applications are discussed. The thesis also examines the applicability of various ED ideas developed in this work for ultimately realizing the functional ED-based devices in poly-GaN thin films.

SAMENVATTING

In de afgelopen zeventig jaar heeft er op het gebied van de micro-elektronica een revolutie plaatsgevonden, die geïnitieerd was door de uitvinding van de bipolaire transistor in 1948 en geleid heeft naar de geavanceerde computers en mobiele toepassingen. De aanhoudende vooruitgang in de realisatie van silicium (Si) gebaseerde halfgeleider componenten (zoals diodes, bipolaire en veldeffect transistoren), die gepaard ging met de constante afname van de afmetingen daarvan, was tot dusver de drijvende kracht voor deze technologische revolutie. De mogelijkheid om Si te doperen met chemische verontreinigingen zoals arsenicum (As) of fosfor (P) om de geleidbaarheid te controleren, heeft ook een sleutelrol gespeeld in het opmerkelijke succes van de huidige Si technologie.

Echter, met de aanhoudende afname van de transistorafmetingen naar de nanometer regime en de toename van de complexiteit van transistorarchitecturen, zoals gerealiseerd in nanodraden, nanovinnen en volledig gedepleteerde silicium-op-isolatie (FD-SOI), wordt het steeds moeilijker om de traditionele chemische doteringstechnieken toe te passen. Bovendien is het doperen zelfs een grotere uitdaging in alternatieve materialen zoals grafeen, carbon nanobuisjes, 2-D materialen, gallium nitride (GaN) en andere brede "band gap" (verboden band) halfgeleiders. Deze materialen worden met toenemende mate ontwikkeld en onderzocht voor nieuwe toepassingen zoals internet van dingen (IoT), kunstmatige intelligentie en draagbare elektronica. Met name GaN is interessant, voor zowel elektronische als optische toepassingen. Het doperen van GaN is echter niet het enige probleem. De productie van GaN is relatief duur wat uiteindelijk het succes daarvan zou kunnen beperken. Daarom wordt er meer gekeken naar de mogelijkheden van monolitische integratie van functionele GaN gebaseerde componenten in een geavanceerd CMOS proces. Mocht dit succesvol zijn, dan zou dit kunnen leiden tot nieuwe toepassingen op het gebied van hoogvermogenscomponenten, RF elektronica, verlichting, sensoren en beeldschermtechnologieën, en dat met relatief lage kosten.

Dit proefschrift gaat in brede zin in op twee aspecten. Allereerst beschrijft het mogelijke oplossingen ter vervanging van chemische dotering in agressief geschaalde halfgeleider componenten die gerealiseerd zijn in alternatieve materialen, en onderzoekt het de zogeheten "elektrostatische dotering (ED)" methode als één van die mogelijke oplossingen. In dit onderzoekswerk is een recensie geschreven van verscheidende ED methodes die beschreven staan in de literatuur. Daarnaast zijn er nieuwe concepten van componenten bedacht die onderzocht zijn door middel van TCAD simulaties, en enkele componenten daarvan die gerealiseerd zijn, elek-

trisch en optisch doorgemeten. De randvoorwaarden voor ED, d.i. het induceren van lokale n-type en p-type gebieden in een halfgeleider door middel van een geschikte uittreearbeid van metalen en gate instelspanningen, zijn vastgelegd. Tussen verscheidende mogelijke ED gebaseerde componenten, focuseert dit proefschrift zich vooral op het toepassen van hoge barrière Schottky contacten voor componenten zoals LEDs en bipolaire transistoren zonder daarbij chemische dotering toe te voegen. Het proefschrift bestudeert ook het gebruik van extreme uittreearbeid contacten zoals molybdeen oxide (MoO_x) voor het realiseren van hoge barrière diodes met bipolaire geleidingsmogelijkheden.

Ten tweede, onderzoekt dit proefschrift de mogelijkheden om polykristallijne (poly-)GaN dunne films, die gegroeid zijn door middel van atomaire laag depositie (ALD), toe te passen in componenten als een potentiële oplossing voor goedkope GaN-op-Si technologie. Met dit uitgangspunt zijn er diverse elektrische en optische eigenschappen van ALD gegroeide poly-GaN dunne films bestudeerd en de potentiële toepassingen daarvan bediscussieerd. Dit proefschrift onderzoekt ook de toepasbaarheid van verscheidende ED ideeën die in dit werk bedacht zijn om uiteindelijk functionele ED-gebaseerde componenten in poly-GaN dunne films te realiseren.

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CHAPTER 1

INTRODUCTION

Abstract

In this chapter, the main motivation and objectives of this research are presented. The chapter starts with outlining the limitations of conventional chemical doping approaches in ultra-thin body semiconductor devices and alternative emerging materials other than silicon (Si). Then, a brief introduction to the potentially interesting polycrystalline gallium nitride (GaN) material is given and possible device concepts based on this material are discussed, followed by the challenges involved in realizing such devices. Next the electrostatic doping approach is proposed as one potential solution to overcome the doping challenge in devices based on ultra-thin body semiconductors in general and polycrystalline GaN in particular. Finally, the outline of this thesis is presented.

1.1 Doping in semiconductor devices

Doping semiconductor materials by incorporating chemical impurities has been key to the development of today's cutting edge device technologies [1]. However with device dimensions of only a few nanometers, the conventional impurity doping faces challenges even in silicon (Si). The formation of junctions with extremely high doping gradients (a few nm/decade) is practically difficult [2, 3]. At nanometer scale, a dopant concentration above its solid solubility limit would be required to achieve sufficiently low channel and contact resistances. In addition, random doping fluctuations and the resulting variability has been the key concern for manufacturing nano-scale devices and circuits with high yield [4–6].

The accurate control of doping type, level and spatial distribution in nanostructures such as a nanowire is also challenging because of their complex growth dynamics and geometrical constraints [7, 8]. For any nano-scale device, the requirement of a high carrier density along with unintentional and undesired ionized dopants in the active region points towards impurity-free doping solutions.

In case of alternative emerging material systems such as wide bandgap semiconductors (e.g. GaN, SiC and ZnO), it is still difficult to obtain either p-type or n-type regions via impurity doping. This is mainly because of deep donor or acceptor levels or dopant passivation via complex formation [9–12]. The chemical doping route is also not straightforward for many other semiconductor materials such as carbon nanotubes (CNTs) and emerging two-dimensional (2-D) materials (graphene, phosphorene, silicene and transition metal dichalcogenides (TMDs)) [13, 14]. For example, tunneling-field-effect-transistors (TFETs) based on ultra-thin channels and 2-D materials are potential contenders for beyond-CMOS (Complementary metal oxide semiconductor) technology as they promise sub-60 mV/decade sub-threshold slope [15]. However, their full potential has still not been realized experimentally. The reason for their limited performance lies in the difficulty in realizing highly doped junctions with a steep profile and low defect density, which is critical for an efficient tunneling process [14, 16].

Consequently, various approaches have been proposed in recent years to influence the electron and hole concentrations by means other than chemical doping. In many of these approaches, electrostatic interaction between the semiconductor and a different material at the interface governs the carrier density. These approaches are therefore referred to as "electrostatic doping (ED)"¹ which will be discussed in more detail in the next chapter.

Among many alternative semiconductors discussed above, GaN, more specifically its thin-film polycrystalline counterpart grown on Si, is potentially attractive technology platform for both electronic and optical

¹The term "electrostatic doping" was originally introduced by Antonov and Johnson [17] in 1999 in relation to their CNT diode.

applications and can benefit from ED approaches. Therefore a brief introduction to polycrystalline GaN is given below. A more detailed discussion on polycrystalline GaN will follow in the subsequent chapters of this thesis.

1.2 Polycrystalline GaN: material and devices

Mono-crystalline gallium nitride (GaN) is currently a widely investigated compound semiconductor material for its interesting properties such as wide and direct bandgap, large breakdown field, suitability for high temperature and high frequency operation [18–20]. It is the material of choice for high (rf-) power transistors as well as optoelectronic devices such as LEDs. Despite this, its expensive production technology currently hinders its widespread commercial adaptability. Monocrystalline GaN is commonly deposited using epitaxial growth methods such as metal organic chemical vapor deposition (MOCVD) and molecular beam epitaxy (MBE) on sapphire substrate at temperatures ranging from 750⁰C to 1200⁰C. The high production costs of GaN based devices can be brought down by employing inexpensive substrates such as silicon (Si). Other than the cost benefit, GaN-on-Si technology is also favorable for monolithic integration of GaN devices with state-of-the-art Si technology [21–23]. However, the requirement of a several-micrometer thick buffer layer [21, 24] for growing monocrystalline GaN on Si makes the idea of monolithic integration somewhat difficult and complex. In addition, the high temperature growth of monocrystalline GaN also limits its compatibility with several processes and applications where a low thermal budget is required.

In this regard, thin-film polycrystalline (poly-) GaN, which has been largely unexploited so far, is an interesting alternative to its thick-film heteroepitaxial mono-crystalline counterpart for its advantages such as lower fabrication cost, choice of large area and flexible substrates and a lower thermal budget. In addition, the fact that GaN-based devices are exceptionally lucrative for many applications, particularly light emission, despite having comparatively high defect densities also raised the curiosity of some research groups to experiment with polycrystalline and even amorphous GaN films. Interestingly, Stumm and Drabold [25] in their early paper entitled "*Can Amorphous GaN Serve as a Useful Electronic Material?*" theoretically predicted that amorphous GaN is promising as a electronic material for device applications.

Poly-GaN thin-films deposited using reactive rf sputtering were reported as early as in 1972 [26, 27] by researchers at IBM corporation. Poly-GaN thin-films have also been explored before for applications such as transparent TFTs [28, 29] ("transparent electronics"), LEDs [30] and field electron-emission [31–33] as illustrated in Fig. 1.1.

Figure 1.1: Examples of various poly-GaN based devices reported till date.

1.3 ALD-grown poly-GaN thin films

Among several other reported techniques to deposit poly-GaN films such as rf-sputtering [26, 28], plasma-assisted molecular beam epitaxy (MBE) [32, 34] and pulse laser deposition (PLD) [35], atomic layer deposition (ALD) is an attractive solution [36, 37]. ALD features excellent wafer-level uniformity, conformal deposition and, most importantly, critical film thickness control. In addition, ALD offers the possibility to grow films at relatively low temperatures ($<500^{\circ}\text{C}$) [38, 39]. Several research groups have recently demonstrated devices such as poly-GaN thin-film transistors realized using ALD [39–41] with reasonable performance considering their polycrystalline nature.

1.4 Challenges in poly-GaN device technology

Generally, polycrystalline semiconductor devices do not perform up to par with their crystalline counterparts. For device applications in polycrystalline material several challenges should be taken into consideration [28, 35, 42], such as obtaining large grain size and reducing the amount of grain boundaries and their role in charge transport, good device stability and reliability, obtaining low defect densities and improving the carrier mobility and lifetime, and good interface control with metals and dielectrics.

Both from technology and device functionality viewpoint, doping is also one important aspect that needs to be addressed for both electronic

and optoelectronic device applications. Doping remains to be challenging in polycrystalline materials mainly because of the requirement of high temperature for dopant activation which forbids its use in films or processes where low temperature processing is important. Moreover, in-situ dopants mixing is not straightforward for certain deposition techniques such as ALD. The situation is even more complex in case of GaN where doping is anyways challenging in crystalline GaN particularly getting p-type material is difficult [9, 10]. For ultra-thin poly-GaN films as deposited by ALD, forming a high device quality p – n junction and their metal contacts becomes even more challenging. Even the polarization doping approach [43, 44], which is normally used in III-nitrides heterostructures to realize two-dimensional electron or hole gases (2DEGs, 2DHGs) is not an attractive solution for poly-GaN material due to their possibly small strain-induced piezoelectric polarization.

1.5 Role of electrostatic doping (ED)

One potential solution to doping problem in thin-film poly-GaN films for device applications could be the electrostatic doping (ED) [17, 45–48] approach where charge carriers are induced in the ultra-thin body semiconductor by using a suitable metal work function or by applying a gate bias. ED has already been demonstrated in various material systems and device geometries where conventional doping is otherwise challenging, as discussed in the next chapter. Moreover, the performance of ED-based devices are found to be at par with their chemically-doped counterparts.

Previously, the use of Schottky barrier (SB) contacts which is one possible type of ED was demonstrated to realize SB GaInN/GaN solar cell devices without any p-doped region [49], [50]. GaN based n-channel SB-MOSFET has also been reported before [51]. Other possible forms of ED such as work function induced doping has also been utilized before to propose an n-type GaN MOSFET using TCAD simulations [52]. Even bias-induced p-type ED has been reported for a wide band gap material such as ZnO [53] though the source of holes is not clear from the report.

The formation of the inversion layer using high-barrier Schottky contacts [54–56] is also interesting for creating local n-type or p-type inverted regions. Such contacts could impart bipolar characteristics to the device which is attractive for applications such as light emission or could even be utilized to realize low-resistance ohmic contacts to the device. Therefore such ED approaches hold a lot of promise as a potential doping solution in ultra-thin poly-GaN devices and are the topic of discussion in this thesis.

1.6 Thesis outline

This thesis broadly deals with the subject of electrostatic doping as a potential solution to circumvent doping issues in ultra-thin body devices and

wide bandgap materials such as GaN where conventional doping is otherwise challenging. In this work, various reported ED approaches have been investigated and new device concepts have been proposed via a theoretical study, TCAD simulations, device physics modeling as well as via electrical and optical measurements of experimentally realized devices. A significant part of this thesis focuses on the physics of high-barrier Schottky diodes in Si and its applicability and adaptability in ultra-thin body devices. The use of extreme work function contacts such as MoO_x has also been explored experimentally to realize work function induced ED. The other part of the thesis is dedicated to the study of electrical and optical properties of ALD-grown poly-GaN thin films and their potential applications. Most of the ED ideas explored in this thesis are initially conceptualized and experimented on Si while the properties of grown poly-GaN films have been investigated in parallel for their suitability for (ED-based) device applications. Specific research questions that this thesis will attempt to answer can be summarized as follows:

- What are the various possible ED approaches and for which materials and device configurations are they most suited for?
- Is it possible to create local n-type or p-type layers in the semiconductors using extreme metal work functions or applied gate biasing? Can such approaches be utilized for innovative device applications such as light emitters or switches?
- Can high-barrier Schottky diodes be interesting for bipolar device applications? What are potential electrode materials with extreme work functions that can be used for realizing high-barrier diodes?
- What are the electrical properties of ALD-grown poly-GaN thin films and for what applications are they suitable?
- How feasible are the envisaged ED solutions in wide-band gap semiconductors, specifically poly-GaN? What are the challenges and limitations?

Below the outline for the subsequent chapters in this thesis is presented.

- **Chapter 2:** Electrostatic doping in semiconductor devices, based on work published in the IEEE Transactions on Electron Devices, 2017 [46]. This chapter reviews various reported ED approaches in Si and emerging semiconductor materials including their applicability to future CMOS devices.
- **Chapter 3:** High-barrier Si Schottky diodes, based on work published in the IEEE Transactions on Electron Devices, 2018 [56]. This chapter deals with the physics of high-barrier Schottky diodes via TCAD simulations and experimental investigation on Si substrates.

- **Chapter 4:** Bipolar characteristics of high-barrier Pd/MoO_x/n-Si diodes. This chapter investigates the bipolar effects in high-barrier Pd/MoO_x/n-Si diodes via electrical and optical measurements.
- **Chapter 5:** The electron-hole bilayer LED, based on work published in Solid-State Electronics, 2020 [57]. This chapter describes a novel light emitting device concept based on the ED approach in an ultra-thin-body semiconductor configuration using TCAD simulations.
- **Chapter 6:** The polycrystalline GaN/p-Si heterojunction diode, based on work published in the Journal of Applied Physics, 2018 [42]. This chapter investigates the charge carrier transport and electroluminescence properties of plasma-enhanced ALD deposited poly-GaN/p-Si diodes.
- **Chapter 7:** Electrical properties of ALD-grown poly-GaN thin films. This chapters describes and compares the electrical and optical properties of ultra-thin poly-GaN layers grown using plasma-enhanced ALD and thermal ALD processes.
- **Chapter 8:** Conclusions and Recommendations. This chapter summarizes the general conclusions of the aforementioned chapters and also provides recommendations and suggestions for future work in this direction. Lastly, a list of original key contributions of this thesis is provided.

ELECTROSTATIC DOPING IN SEMICONDUCTOR DEVICES

Abstract

To overcome the limitations of chemical doping in nanometer-scale semiconductor devices, electrostatic doping (ED) is emerging as a broadly investigated alternative to provide regions with a high electron or hole density in a semiconductor device. In this chapter, various reported ED approaches and related device architectures in different material systems are reviewed. The role of metal and semiconductor work functions, energy bandgap and applied electric field and the interplay between them for the induced ED is highlighted. The effect of interface traps on the induced charge is also addressed. In addition, the merits of electrostatically doped devices are underlined and the major roadblocks of these approaches for potential future CMOS technology are addressed.

2.1 Introduction

The limitations of conventional chemical doping approaches in ultra-thin body (UTB) devices and emerging semiconductor materials other than Si has been highlighted before in chapter 1. In this direction, various electrostatic doping (ED) approaches has been reported in recent years where charge carriers are induced in UTB semiconductors using a suitable metal work function or applied local gate bias. These approaches include devices such as Schottky barrier (SB) metal-oxide-semiconductor field-effect transistors (MOSFETs) [58, 59], charge plasma based ultra-thin body (UTB) devices [60–63], reconfigurable FETs based on silicon (Si) nanowires [64–66], fully-depleted silicon-on-insulator (FD-SOI) devices [48, 67–69], FETs based on graphene [70–73], CNT [74–76] and 2-D materials [77, 78], electron-hole bilayer based TFETs [79–81] and light-emitting devices [82]. ED potentially offers ultra-sharp junctions with a well controlled carrier concentration profile and a reduced defect density. These features make ED an attractive alternative to conventional chemical doping for a broad range of electron devices.

This chapter presents an overview of various reported ED concepts, and is organized as follows. In section 2.2 the ED concept is first defined. Thereafter various reported ED concepts are reviewed under three proposed categories based on the nature of the underlying electrostatics. Here the focus will be on the electrostatics for different types of metal-semiconductor systems. Further, in section 2.3, the major challenges and possible drawbacks of the ED techniques are addressed. Section 2.4 summarizes our findings. For more detailed overview on ED based innovative FD-SOI devices, please refer to [48]. Further, for a more technology focused review on ED based TFETs and reconfigurable FETs refer to [47].

2.2 Electrostatic Doping Concept

Electrostatic doping (ED) is a technique in which charge carriers (electrons or holes) are induced in an ultra-thin semiconductor material as a result of its band alignment near its interface with another (semi)conducting material. In the ED approach, the relative separation between the Fermi level and the semiconductor energy bands, that governs the active doping concentration, is controlled by the potential and the work function of the electrode adjacent to the semiconductor body rather than by the chemical impurities as in conventional doping. The electrostatic condition at the metal-semiconductor (MS) interface¹, which influences the band alignment, is a strong function of the metal work function (ϕ_m), the semiconductor's energy bandgap (E_g), electron affinity (χ_s) and work function (ϕ_s). In

¹For simplicity sake, in this thesis ideal interfaces are considered unless stated otherwise. Parasitic charge, such as interface or a fixed charge, will also affect the electrostatics at interfaces.

Figure 2.1: Schematic energy band diagrams for: (a) traditional n-type Schottky contact. A depletion layer is formed at the MS interface. (b) n-type Schottky contact with a large MS work function difference. The excessive band-bending near the interface results in inversion (p-type) charge in an n-type semiconductor. A similar situation can be obtained with Schottky contacts on a p-type semiconductor.

addition, the applied electric field, if any, also influences the electrostatic properties near the interface. Note that in this chapter, the focus is only on metal (or metallic compound) induced ED; other heterostructure based doping like polarization doping e.g. in III-nitrides [43] is beyond the scope of this work.

The ED approaches are subdivided into three categories: (1) Schottky barrier based devices, (2) work function induced ED, and (3) bias-induced ED. In the upcoming subsections, these ED techniques as applied to different devices and material systems will be reviewed.

2.2.1 Schottky Barrier Based Devices

Schottky barrier (SB) based devices are devices in which the current is limited by one or more Schottky contacts. The physics of a Schottky barrier formed at the metal-semiconductor (MS) interface has been well described earlier [83].

An SB with height $q\phi_b$ is formed when $\phi_m > \phi_s$ for an n-type semiconductor (Fig. 2.1(a)) and $\phi_m < \phi_s$ for a p-type semiconductor, where q is the elementary charge. The Schottky barrier height (SBH) $q\phi_b$ is $(\phi_m - \chi_s)$ for an n-type and $(E_g - \phi_m + \chi_s)$ for a p-type semiconductor. The presence of this potential barrier ϕ_b at the MS interface results in the fundamental difference in the operation of SB devices from p-n junction devices. For the former, the MS interface, hence ϕ_b , fully controls the majority unipolar current [83]. The electron or hole emission in SB devices is governed by thermionic (-field) emission over (through) the barrier in contrast to p-n junction based devices, where processes such as drift-diffusion and

band-to-band tunneling (BTBT) of both electrons and holes control the current.

However, for an ideal unipolar Schottky type operation, it is essential to limit the band bending such that for an n-type semiconductor, at the interface, the intrinsic Fermi-level E_{FI} falls below the Fermi level E_F which implies that $\phi_b \leq u_T \cdot \ln(N_c/n_i)$ where N_c is the conduction band effective density of states, n_i is the intrinsic carrier concentration, and u_T is the thermal voltage ($= kT/q$, where k is the Boltzmann constant and T is the temperature). Therefore, the limiting conditions at the MS interface ($x=0$) for a unipolar Schottky type operation can be expressed as:

$$(E_c - E_F)|_{x=0} = q\phi_b \leq kT \cdot \ln\left(\frac{N_c}{n_i}\right) \quad (2.1)$$

for an n-type semiconductor, and

$$(E_F - E_v)|_{x=0} = q\phi_b \leq kT \cdot \ln\left(\frac{N_v}{n_i}\right) \quad (2.2)$$

for a p-type semiconductor. E_c and E_v represent the conduction band edge and valence band edge respectively and N_v is the valence band density of states. The terms $kT \cdot \ln(N_c/n_i)$ and $kT \cdot \ln(N_v/n_i)$ are approximately equal to $E_g/2$ for most semiconductors. Excessive band-bending at the MS interface may result in a bipolar type operation as discussed in the Section 2.2.2 and later investigated in more detail in chapter 3-4 of this thesis.

Next, some specific examples of SB devices which could be interesting for future CMOS, but also for electro-optical devices, are discussed.

Schottky Barrier (SB) MOSFETs

The idea to replace doped source/drains (S/Ds) in conventional MOSFETs with metal was first proposed by Nishi [84] in 1966. In 1968, Lepselter and Sze reported the first Si p-type MOSFET (PMOS) device where S/Ds were replaced by PtSi [58]. Thereafter a series of developments resulted in the metal S/Ds SB-MOSFET (Fig. 2.2(a)) technology which basically replaces impurity doped S/Ds in conventional MOSFETs with metal, typically silicide.

In this transistor the charge carriers are injected from the metal into the semiconductor channel via thermionic (-field) emission as in a Schottky diode. However, in the SB-MOSFET, the gate field further influences the effective barrier height and width as illustrated in Figs. 2.3 (a) and (b). The SB-MOSFET technology is claimed to offer several benefits for sub-30-nm scaling such as a low parasitic S/D resistance, sharp junctions, better control over the off-state leakage current, elimination of parasitic bipolar action, and low thermal budget processing [59]. Further, the use of mid-gap silicides allows the realization of SB-PMOS and SB-NMOS devices, as required for CMOS technology. Recently [86], the SB-FINFET was realized featuring a 6 mV/dec subthreshold swing at room temperature.

Figure 2.2: Schematic cross section of an (a) Si based SB-MOSFET [59], (b) Si nanowire based SB-MOSFET with single backgate design [85], Si nanowire based reconfigurable SB-MOSFET, (c) with front and back dual gate design [66], (d) with dual gate-all-around design [64].

Figure 2.3: Schematic energy band diagram: Si based SB-MOSFET [59] (Fig 2.2(a)) for (a) n-type operation ($V_{GS} > 0$ V), (b) p-type operation ($V_{GS} < 0$ V). Si nanowire based reconfigurable SB-MOSFET [66] (Fig 2.2(c)) for (c) n-type operation ($V_{PGS} > 0$ V), (d) p-type operation ($V_{PGS} < 0$ V). V_{PGS} and V_{CGS} denotes the polarity gate and control gate bias respectively. An electron (hole) channel is formed for a positive (negative) $V_{(P)GS}$. The V_{CGS} controls the current in the channel.

The concept of SB-MOSFETs has also been adopted in CNTs [75, 76, 87]. For a thorough review on SB-MOSFET technology refer to [59].

Reconfigurable SB-MOSFETs

The idea of using SB contacts for ED has also been embraced by the research community for applications other than traditional CMOS. The Si nanowire FET [85] with a SB source and drain were shown to exhibit ambipolar

Figure 2.4: CNT SB light emitting FET, schematic (a) device cross section (b) energy band diagram. Electrons are injected in the CNT channel at the source electrode while holes are injected from the drain electrode into the channel [89].

characteristics (Fig. 2.2(b)). The ambipolarity in this device was successfully suppressed by the introduction of an additional terminal, *i.e.* polarity gate (Figs. 2.2(c) and (d)). This terminal offers a new degree of freedom in the device: the polarity of conduction can be controlled which was utilized in [64–66, 88] to demonstrate a reconfigurable FET operation. In these reconfigurable (or polarity controlled) devices, one gate electrode (control gate) controls the conduction through the channel while the other gate electrode (polarity gate) controls the polarity of conduction (see Figs. 2.3 (c) and (d)).

SB electro-optical devices

Misewich *et al.* [89] demonstrated polarized infrared light emission from a CNT SB-MOSFET structure (see Fig. 2.4(a)). The simultaneous injection of electrons and holes at the source and drain Schottky barrier junctions resulted in radiative recombination and thus light emission. The gate electrode was biased such that $V_{GS} > 0$ but $V_{GS} < V_{DS}$. In this way band bending was formed in the opposite direction at source and drain electrodes which facilitated simultaneous injection of electrons and holes from those electrodes via narrow tunneling barriers, as shown in Fig. 2.4(b).

SB contacts have also been utilized to collect photo-generated carriers in solar cells [90]. SB based solar cells are interesting as they can be realized using only a single type (n or p type) of chemical doping unlike conventional p-i-n type cells which require both a p-type and n-type region to function. Other than in conventional Si-based material, the SB based solar cell has also been demonstrated in CNTs [91], cadmium sulphide (CdS) [92] and molybdenum disulfide (MoS₂) [93]. In addition, an SB based solar cell has been demonstrated in the GaInN/GaN material system without any p-type doped region [49], [50].

The choice of the electrode metal in these devices determines the resultant SBHs for electrons (ϕ_{bn}) and for holes (ϕ_{bp}) at the junction. Unipolar operation ($\phi_{bn} \neq \phi_{bp}$) is desirable for conventional SB-FETs while ambipolar operation ($\phi_{bn} \approx \phi_{bp}$) is interesting for polarity controlled SB-MOSFETs

and light emitting devices [89]. Importantly, the current in the devices described so far is limited by the SBH.

2.2.2 Work function induced ED

Brattain and Bardeen [45] first reported an experimental observation that could be explained as metal induced doping. In their report, a thin layer of p-type conductivity is believed to be induced near the surface of the n-type bulk Ge via a Schottky point-contact which resulted in the bipolar-like amplification. Although noticed by only a few readers or authors, later on many reports actually followed this "scaled point-contact transistor" idea as discussed further in this section.

In this section the general analytical understanding of work function induced ED in one dimensional (1-D) Schottky contacts is first developed. Thereafter the case of two dimensional (2-D) gated Schottky contacts is discussed which is important for future CMOS devices such as ED-TFETs.

1-D Schottky based devices

Excessive band bending near the MS interface may result in charge carrier inversion (similar to gate-induced inversion in MOSFETs) as illustrated in Fig. 2.1(b). This will induce a bipolar type behavior in an otherwise unipolar 1-D Schottky diode which could be of interest to BTBT devices. As in a MOS capacitor [1], the onset of strong inversion near the interface is defined when the inversion charge carrier density is equal to the background doping concentration (N_d for n-type, N_a for p-type) of the semiconductor. Next the conditions for the occurrence of strong inversion are derived.

For an n-type semiconductor, as shown in Fig. 2.1(b), the condition of strong inversion at the interface would result in E_F to lie below the E_{FI} with an energy difference $q\psi_{BI} \geq q\psi_B$, where $q\psi_B = kT \cdot \ln(N_d/n_i)$. The latter represents the relative position of E_F from E_{FI} in the bulk region as defined by the background doping. This leads to the condition that at the interface $\phi_b \geq u_T \cdot \ln(N_c/n_i) + \psi_B$. Therefore for strong inversion and thus bipolar pn junction like behavior, the following conditions hold.

For an n-type semiconductor:

$$\phi_b = (\phi_m - \chi_s) / q \geq u_T \cdot \ln\left(\frac{N_d}{n_i}\right) + u_T \cdot \ln\left(\frac{N_c}{n_i}\right), \quad (2.3)$$

and for a p-type semiconductor:

$$\phi_b = (E_g - \phi_m + \chi_s) / q \geq u_T \cdot \ln\left(\frac{N_a}{n_i}\right) + u_T \cdot \ln\left(\frac{N_v}{n_i}\right). \quad (2.4)$$

Using Boltzmann's approximation ($n \ll N_c$ or $p \ll N_v$), the hole (electron) concentration in n-type (p-type) semiconductors can be expressed as:

$$p = n_i \cdot \exp\left(-\frac{\psi_{BI}}{u_T}\right) = n_i \cdot \exp\left(\frac{\phi_b - E_g/2q}{u_T}\right) \sqrt{\frac{N_v}{N_c}}. \quad (2.5)$$

$$n = n_i \cdot \exp\left(\frac{\psi_{BI}}{u_T}\right) = n_i \cdot \exp\left(\frac{\phi_b - E_g/2q}{u_T}\right) \sqrt{\frac{N_c}{N_v}}. \quad (2.6)$$

The above equations indicate that for a suitable ϕ_m , that governs ϕ_b , charge carriers of opposite polarity type from the background doping can be induced near the interface of a 1-D Schottky contact. This creates a very shallow p-n junction near the MS interface where drift-diffusion or possibly even BTBT governs the current, which is different from conventional SB based devices where ϕ_b at the interface solely controls the emission of charge carriers.

In case of an intrinsic semiconductor where $\psi_B=0$, Eqs. (2.3)-(2.4) can be transformed into the following equations for p-type doping:

$$\phi_m \geq \chi_s + \frac{E_g}{2}, \quad (2.7)$$

and n-type doping:

$$\phi_m \leq \chi_s + \frac{E_g}{2}. \quad (2.8)$$

By using metals with different work functions, it is possible to make an intrinsic semiconductor p-type or n-type locally via the ED approach. The term $\chi_s + (E_g/2)$ is essentially the position of Fermi level in the intrinsic semiconductor, *i.e.* its work function ϕ_s .

Experimentally, inversion layer effects in high-barrier Schottky diodes have been reported before in [55, 94]. Recently, such 1-D Schottky based p-n junctions have also been reported using TCAD simulations for a vertical bipolar junction transistor (BJT) structure [95] and for a GaAs tunnel diode [96]. For the tunnel diode however Fermi-Dirac statistics should be applied and consequently Eqs. (2.5)-(2.6) do not hold. Nonetheless, a suitable ϕ_m is still required for a p-n junction formation. The physics of such high-barrier diodes will be discussed in more detail in chapter 3-4 of this thesis.

Gated Schottky based UTB devices

In this section, the ED concept is discussed in devices in which a dielectric layer is placed between the metal and semiconductor body. In addition, the semiconductor device makes use of a fully depleted (FD) UTB devoid of any depletion charge [97]. Fig. 2.5 shows a schematic cross-section of the system under discussion which is similar to an FD 2-D MOS system.

The potential drop across the device perpendicular to the gate electrode is given by the following equation:

$$V_{GB} = V_{ox} + \psi_s + \phi_m/q - \chi_s/q - (E_c - E_{FI})/q \quad (2.9)$$

where V_{GB} is the applied gate potential difference between gate and semiconductor body, V_{ox} is the potential drop across the oxide and ψ_s is the surface potential *i.e.* shift in the Fermi-level from its intrinsic position. For

Figure 2.5: Schematic cross-section of a UTB device with 2-D gated Schottky contact for work function or bias-induced ED (left). Schematic energy band diagram for a p-type formed region perpendicular to the gate along the red dashed line (right).

not too high carrier concentrations ($n, p \ll N_c, N_v$), $V_{ox} \approx 0$ for an FD UTB with ideal interfaces, and $V_{GB}=0$ for a purely work function induced ED case.

Then it can be obtained that

$$\psi_s = (E_{FI} - E_F)/q = \chi_s/q - \phi_m/q - u_T \cdot \ln \left(\frac{n_i}{N_c} \right). \quad (2.10)$$

Eq. (2.10) is the condition for ED in a UTB gated Schottky system which is equivalent to Eq. (2.7) for p-type doping ($\psi_s < 0$) and to Eq. (2.8) for n-type doping ($\psi_s > 0$). Analogous to the p-n junction formation in a 1-D Schottky contact, the concentration of the induced charge can be expressed as:

$$p = n_i \exp \left(-\frac{\psi_s}{u_T} \right), \quad (2.11)$$

$$n = n_i \exp \left(\frac{\psi_s}{u_T} \right). \quad (2.12)$$

Fig. 2.6(a) shows the induced hole density against the oxide thickness for an Si/SiO₂ gated Schottky structure (Fig. 2.5) with $\phi_m = 5.1$ eV. Eq. (2.10) indicates that the induced charge carrier density is independent of insulator and semiconductor thicknesses for UTB devices as $V_{ox} \approx 0$ in our simplified model. However TCAD [98]² produces somewhat different results. This is attributed to the presence of a high amount of mobile charge resulting in a finite V_{ox} (~ 30 mV at $t_{ox}=6$ nm and $t_s=10$ nm). Still, the model is useful for studying trends. For more accurate results, a numerical model can be derived [99], which is beyond the scope of this chapter.

²TCAD simulations wherever referred throughout this thesis are performed with Sentaurus device simulator software [98] unless stated otherwise.

Figure 2.6: Induced hole concentration for an Si/SiO₂ gated Schottky structure (see Fig. 2.5) with $\phi_m = 5.1 \text{ eV}$ for (a) varying oxide thicknesses with ideal interfaces and (b) varying interface trap densities. In the TCAD simulations, a uniform distribution of both donor and acceptor traps across the bandgap [1] has been assumed. The carrier density was extracted at a lateral distance of $0.5 \mu\text{m}$ from the Schottky side contact.

Now taking into account the effect of the interface trap charge (Q_{it}), Eq. (2.10) can be modified as:

$$\psi_s = \chi_s/q - \phi_m/q - u_T \cdot \ln\left(\frac{n_i}{N_c}\right) + \left(\frac{Q_{\text{it}}}{C_{\text{ox}}}\right), \quad (2.13)$$

with $Q_{\text{it}} = -C_{\text{it}}\psi_s$ (assuming a uniform interface trap density) where $C_{\text{ox}} = \epsilon_{\text{ox}}/t_{\text{ox}}$ and $C_{\text{it}} = q^2 D_{\text{it}}$ are the oxide and interface trap capacitance per unit area respectively, and D_{it} is the interface trap density [1]. Rearranging the terms in Eq. (2.13) gives the following condition for the work function induced ED including the effect of interface states:

$$\psi_s = \frac{\left(\chi_s/q - \phi_m/q - u_T \cdot \ln\left(\frac{n_i}{N_c}\right)\right) \cdot C_{\text{ox}}}{(C_{\text{it}} + C_{\text{ox}})}. \quad (2.14)$$

Eq. (2.14) along with Eqs. (2.11)-(2.12) expresses the essential condition for induced ED in a gated Schottky device with interface trap charge. It shows that the ED reduces with an increase in interface trap density. From Fig 2.6(b), where the induced charge concentration is plotted against the interface trap density using Eq. (2.14), it can be seen that the effect of interface traps is more pronounced for a larger oxide thickness. The charge concentration is reduced by a maximum of two orders in magnitude when the trap density is increased to $10^{12}/\text{cm}^2$ for an oxide thickness of 6 nm.

The physics of gated Schottky contacts discussed above lays the foundation for the charge plasma concept as applied to FD UTB devices such as the TFET. This is discussed in the next paragraph.

Charge Plasma Devices

Hueting *et al.* [60, 61] proposed to adopt two different work function metals to induce different polarity of charge carriers in the semiconductor. The

Figure 2.7: Schematic cross section of the CP p-n diode (left) and its simulated energy band diagram along the dotted red line at equilibrium (right). $\phi_{mC} = 4.17$ eV and $\phi_{mA} = 5.1$ eV are cathode and anode metal work functions respectively. L_c and L_a denote cathode and anode gate lengths respectively. L_i denotes the length of the intrinsic region i.e. the gap between the two electrodes. The thickness of UTB Si (t_{Si}) is 20 nm and gate oxide thickness (t_{ox}) is 5 nm. [60].

schematic cross section of the so-called charge plasma (CP) p-n junction diode is shown in Fig. 2.7. The CP diode comprises a gated anode and a gated cathode with metals of different ϕ_m . From Eqs. (2.10)-(2.12) it can be concluded that for the anode region a high ϕ_m is required, while the opposite holds for the cathode region.

Fig. 2.7 also shows the energy band diagram of a CP diode along the lateral direction as obtained from 2-D TCAD simulations indicating that a p-n junction has formed. The band diagram is similar to a typical chemically doped p-n junction with some key differences which were also highlighted in [74]. The quasi-neutral regions of this diode are formed by the ED gates. A typical feature of the lateral ED configuration is that the potential distribution is linear in the intrinsic gap region because of the absence of impurities, unlike a conventional p-n junction which has a parabolic potential profile in the depletion region. The built-in electric field in an impurity doped p-n junction is formed by fixed donor or acceptor ions near the junction to balance drift and diffusion components at equilibrium. This built-in field also exists in the CP p-n diode but is primarily formed by the work function difference at the edges of the gated regions. Further, the band bending near the electrodes is attributed to the 2-D fringe field effect. Analytical drift-diffusion models for the $I - V$ curves in the CP p-n diode [100] also showed good agreement with TCAD simulations.

In the first experimental realization [61], Pd was employed for the anode contact and Er for the cathode. The fabricated device showed good rectifying behavior with a low constant leakage current of 1 fA/ μm and an on/off-current ratio of around 10^7 at $V_D = 1$ V forward bias and room temperature. Fig. 2.8(a) shows measured³ $I - V$ characteristics of various fabricated CP diodes with different combinations of anode and cathode metals. The experimental results indicate that both the hole and electron current are important for the CP diode. The current increases as the anode

³The CP diode fabrication and measurements were performed by B. Rajasekharan [61].

Figure 2.8: (a) $I_c - V_{ca}$ characteristics for various valence and conduction level metal combinations Pt–Er, Pd–Er, Co–Er and Pd–TiW on either side of silicon. $L_a = L_c = 0.9 \mu\text{m}$, $L_i = 3 \mu\text{m}$ (see Fig.2.7). The substrate potential (V_{ga}) was kept at 0 V. (b) Top view of a realized CP diode showing the effect of placing a wafer with high work function (Pd) and low work function (TiW) metal islands in a chemical etching solution. The combination of the metals with the solution formed an electrolyte cell which resulted in the corrosion of highest work function (Pd) metal [61]. Image courtesy: B. Rajasekharan.

work function is reduced by replacing Pt with Pd or Co, or conversely, by increasing the cathode work function by replacing Er with TiW. By using the same metal for anode and cathode contact and the substrate as back gate, MOSFET characteristics were obtained [61].

The CP based ED concept has been extended to various other devices. Kumar and Nadda [62] proposed and investigated the CP based lateral BJT by replacing the doped emitter, base and collector regions of a conventional bipolar device with ED regions using metals with different work functions as shown in Fig. 2.9(a). The authors proposed Hf ($\phi_{mE} = 3.9 \text{ eV}$) for the emitter, Pt ($\phi_{mB} = 5.65 \text{ eV}$) for the base, and Al ($\phi_{mC} = 4.28 \text{ eV}$) for the collector electrode, thereby achieving an $n^+ - p - n$ configuration. The results obtained from 2-D TCAD simulations show similar device characteristics but a higher current gain compared to the conventional impurity doped counterpart with the same dimensions.

Another device based on the CP concept is the doping-less TFET, proposed by Kumar and Janardhanan [63], shown in Fig. 2.9(b). Similar to the CP-BJT, again the impurity doped regions of the conventional TFET were replaced with ED regions by employing metals with a different work function: Hf for the n-type drain and Pt for the p-type source. The performance of the CP based doping-less TFET was found to be similar to the conventionally doped TFET with the same device geometry.

Other proposed CP-devices are summarized in Table 2.1. So far most of these architectures have not been experimentally realized. Similar ideas for graphene doping via metal contacts have also been reported [70–73, 101–103].

Figure 2.9: Schematic cross section of the CP based (a) Lateral BJT [62], (b) TFET [63]. The "n" and "p" indicate electrostatically doped regions.

2.2.3 Bias-induced ED

The applied electric field at the MS interface also plays a decisive role in governing the electrostatics and thereby charge induction in the UTB semiconductor. It can be argued whether the principle of bias-induced ED is not simply based on the conventional field-effect. However, in conventional FETs, the charge carriers originate from doped semiconductor regions in close vicinity (like doped S/D regions), whereas in the ED concept the charge carriers originate from a metal electrode which is in direct contact with the semiconductor body⁴. Hereby, Fig. 2.5 is again referred. A similar expression as derived previously for the work function induced ED (Eq. (2.10)), however with an additional term to account for non-zero V_{GB} , is obtained for bias-induced ED case:

$$\psi_s = V_{GB} + \chi_s/q - \phi_m/q - u_T \cdot \ln \left(\frac{n_i}{N_c} \right). \quad (2.15)$$

For a bulk or partially depleted channel, similar relations can be obtained using a non-zero V_{ox} term in Eq. (2.9). The term $(\chi_s/q - \phi_m/q - u_T \cdot \ln(n_i/N_c))$ is actually the work function difference $(\phi_m - \phi_s)/q$, which is zero in case of a purely bias-induced ED. In this case it is easy to understand that a positive V_{GB} will induce n-doping while a negative V_{GB} will induce p-doping. Further, the effect of interface traps can be accounted for as

$$\psi_s = V_{GB} + \chi_s/q - \phi_m/q - u_T \cdot \ln \left(\frac{n_i}{N_c} \right) + \left(\frac{Q_{it} + Q_{inv}}{C_{ox}} \right), \quad (2.16)$$

with Q_{inv} is the mobile inversion charge. Note that earlier modeling work on I-V curves of asymmetric dual-gate (DG) devices [99] could be used to derive a model for bias-induced ED including traps.

The simultaneous induction of p-type and n-type charged regions in a semiconductor body via an applied field can be realized using a dual (or multiple) gate structure [48]. By biasing two gates with opposite polarities, electrons and holes can be simultaneously induced in a semiconductor

⁴In the absence of any direct metal contact with a suitable work function, the supply of charge carriers is limited by thermal generation rate (refer to chapter 5). Alternatively, doped regions can be employed for carrier supply [48].

Figure 2.10: Schematic cross section of the CNT p-n diode [74]. The split gate configuration was used to electrostatically induce a lateral p-n junction. Biasing $V_{GS1} < 0$ would give a p-type region in the adjacent CNT channel and $V_{GS2} > 0$ would result in an n-type region.

body as analytically explained by Eqs. (2.15) and (2.16). Depending on the relative position of such gates, electrostatically induced local bipolar regions have been reported both in lateral [74] and in vertical structures [79] as discussed in the next paragraph.

Lateral p-n Junction

Bias-induced ED was first experimentally demonstrated in a CNT system [74] where a lateral p-n junction diode was formed adopting a split gate configuration as shown in Fig. 2.10. Biasing a first gate electrode with a positive voltage with respect to the CNT body resulted in an n-type doping of a CNT channel region adjacent to it. Similarly a negative voltage with respect to the CNT body at a second gate resulted in p-type doping. This led to the formation of a lateral p-n junction diode in the CNT channel. The experimentally fabricated device showed rectifying characteristics of a p-n junction diode with an ideality factor close to one. In addition, the same polarity biases at both gate electrodes resulted in an n-channel or p-channel FET. BTBT was also observed in CNTs [104] demonstrating an ED p-n junction which could be interesting for the TFET.

Recently, the concept of bias-induced ED was also experimentally applied in an advanced and mature FD-SOI process to demonstrate the reconfigurable device [68] which can be configured into nine types of devices with different functionalities such as virtual diodes, TFETs, p-i-n diodes and band-modulation FETs. For more detailed overview on this and related work, please refer to [48].

Vertical p-n Junction: Electron-Hole Bilayer (EHB)

An opposite polarity gate bias configuration in the vertical direction can be utilized to form a bias-induced electron-hole bilayer (EHB) as illustrated in Fig. 2.11. This was demonstrated in [105, 106] using a dual-gate $\text{SiO}_2/\text{Si}/\text{SiO}_2$ system.

In case of a relatively thick semiconductor with a partially depleted channel, the two metal gates do not have any electrostatic coupling and

Figure 2.11: Schematic cross-section of the electron-hole bilayer concept (left). Schematic energy band diagram perpendicular to the gates along the red dashed line (right). By enforcing an opposite polarity bias between the top and bottom gate a tunnel junction can be formed. The wavefunction curves represent the electron (left) and hole (right) distribution in the EHB structure for illustration purposes.

therefore the bias-induced charge near each gate can be independently described using Eq. (2.15) (for $n, p \ll N_c, N_v$). In case of a dual asymmetric gate structure with an FD UTB channel however, the electrostatic interaction between the two gates needs to be taken into account. Analogous to the previous work of Lim and Fossum [107] and assuming a not too high charge carrier concentration, the following equation is derived for the vertical electric field in the semiconductor body for the EHB concept in the coupled dual gate system (see appendix A):

$$E_s = \frac{(V_{GT} - V_{GB}) - (\phi_{mT} - \phi_{mB})}{\frac{\epsilon_s}{\epsilon_{ox}}(t_{oxT} + t_{oxB}) + t_s}, \quad (2.17)$$

where the subscripts T and B refer to the top and bottom of the structure, respectively. Fig. 2.12(a) plots E_s against the semiconductor body thickness t_s for an $\text{HfO}_2/\text{Si}/\text{HfO}_2$ EHB structure. The figure shows that TCAD simulations are in good agreement with Eq. (2.17). Semi-classically, there will be an induced electron density near the top gate electrode if $\psi_{sT} > 0$ (refer to Eq. (A.6)) with an electron density at the interface $n = n_i \exp(\psi_{sT}/u_T)$. Similarly if $\psi_{sB} < 0$ (refer to Eq. (A.7)) there will be an induced hole density near the bottom gate electrode at the interface $p = n_i \exp(-\psi_{sB}/u_T)$. Obtaining closed form solutions for ψ_{sT} and ψ_{sB} is however rather difficult. Moreover, quantum effects can change this picture [108] as qualitatively shown in Fig. 2.12(b) using TCAD simulation. The effect of fixed or interface charge can also be accounted for as described by Eq. (A.9) (see appendix A) by assuming non-zero Q_{fT} and Q_{fB} .

Lattanzio *et al.* [79, 80] have applied the EHB concept to a DG-TFET geometry. This transistor was conventionally symmetrically biased for better electrostatic control over the channel. Under asymmetric bias, a bias-induced EHB forms in the channel. For a certain top-bottom bias difference

Figure 2.12: (a) The vertical electric field in the $\text{HfO}_2/\text{Si}/\text{HfO}_2$ EHB structure (refer to Fig. 2.11) for various semiconductor body thicknesses. Quantum Mechanical (QM) effects have not been taken into account both in the model (Eq. (2.17)) and TCAD simulation [98]. (b) TCAD simulation of charge carrier distribution and electric field profile in the vertical direction along the red dashed line of Fig. 2.11 with $t_s = 10$ nm and $V_{GT} = 0.2$ V and $V_{GB} = -0.2$ V shown using both semi-classical and QM (Density-gradient model [109]) approaches. The detailed quantitative calibration of the QM model in TCAD is not the focus of this work.

(~ 0.1 - 0.5 V), BTBT of charge carriers in the EHB p-n junction occurs which results in an increase in the drain current [108]. In this case the direction of tunneling is parallel to the gate field. This results in more on-state tunneling current compared to e.g. the doping-less TFET [63] because of the large tunneling surface area and a stronger electrostatic control over both n-type and p-type regions in the subthreshold region. However, there has been some debate on the effectiveness of the EHB formation [81, 110]. In [81] experimentally realized EHB-TFET structures were reported and it was argued that conditions to meet efficient BTBT and the formation of the EHB cannot simultaneously be satisfied: there is a trade-off between the induced field and quantum-confinement.

The use of EHB concept for undoped light-emitting device application [57, 82] will be discussed in chapter 5.

2.3 Electrostatic Doping Approaches: Discussion

Table 2.1 provides a summary and classification of the various ED device concepts. From the literature, it can be deduced that a high carrier density of both p and n-type (10^{18} - 10^{20} cm $^{-3}$) can be electrostatically induced in UTB devices, particularly for narrow bandgap semiconductors. Fig 2.13 shows the calculated induced charge carrier concentration using Eq. (2.10)-(2.12) for gated Schottky regions of the UTB CP device shown in Fig. 2.7.

For electrons, ED is mainly governed by the electron affinity of the semiconductor and the metal work function, ϕ_m . Therefore, obtaining a high electron density is relatively easy by adopting a suitable elemental metal with low ϕ_m such that Eq. (2.8) is satisfied. The ϕ_m of available

Table 2.1: Summary of various reported electrostatically doped materials and device concepts till date. The notation (*exp.*) denotes experimentally demonstrated concept while others have been investigated via modeling and TCAD simulation only.

Material	SB based devices	Work function induced ED	Bias-induced ED
Si, Si UTB and Si Nanowire	SB-MOSFETs (<i>exp.</i>) [58, 59], FinFET (<i>exp.</i>) [86], Si nanowire based SB-MOSFETs (<i>exp.</i>) [85], reconfigurable FETs (<i>exp.</i>) [64–66]	CP based p-n diode (<i>exp.</i>) [60, 61], BJTs [62, 95, 111, 112], TFET [63], IMOS [113], Junctionless transistor [114], Biristor [115], SiGe-on-insulator MOSFET [116], graded channel MOSFET [117]	EH bi-layer TFET [79, 80], EH bilayer TFET (<i>exp.</i>) [81], virtual diode (<i>exp.</i>) [67], Esaki diode (<i>exp.</i>) [69]
CNT	SB-MOSFETs [75, 76, 87], Light emitting SB-FET (<i>exp.</i>) [89]		p-n diode (<i>exp.</i>) [17, 74], FET (<i>exp.</i>) [104]
Graphene		Graphene ED [72]	Graphene ED [101], Graphene FET (<i>exp.</i>) [70, 71, 73, 102, 103]
III-V materials	GaN n-type SB-MOSFET (<i>exp.</i>) [51]	GaAs Tunnel diode [96], GaN n-MOSFET [52], InAs TFET [118]	GaAs EH Bilayer (<i>exp.</i>) [119], InAs EH bilayer LED [57, 82]
Polycrystalline materials		CP based poly-Si TFT [120], IGZO TFT (<i>exp.</i>) [121]	
2-D materials	n-type, p-type SB-MOSFET (<i>exp.</i>) [122, 123]		2-D transistors [77, 78]

elemental metals varies roughly between 2.14 eV for Cesium (Cs) and 5.65 eV for Platinum (Pt) [1, 125].

On the other hand, obtaining a high hole density is rather difficult, particularly for wide bandgap semiconductors, as large bandgap raises the demand for high ϕ_m metal (see Eq. (2.7)). For example, in case of GaN with $E_g = 3.4$ eV and electron affinity $\chi_s = 4.1$ eV, the condition for the work function induced n-type ED i.e. $\phi_m < (\chi_s + E_g/2)$ can be satisfied

Figure 2.13: Calculated induced carrier concentration using Eq. (2.10)-(2.12) in "n-type" and "p-type" gated Schottky regions of the CP diode structure (refer to Fig. 2.7) with a varying ϕ_m of the gate electrode. The calculation is performed for different semiconductor channel materials (Si ($E_g=1.12$ eV, $\chi_s=4.07$ eV), GaAs ($E_g=1.42$ eV, $\chi_s=4.07$ eV), GaN ($E_g=3.39$ eV, $\chi_s=4.1$ eV), WSe₂ ($E_g=1.56$ eV, $\chi_s=4.03$ eV) [124]) in the UTB device. TCAD simulation (symbols) for Si shows good agreement with the model.

with a lower ϕ_m metal like Al. However similar p-type ED in GaN would require a ϕ_m higher than 5.8 eV (refer to Eq. (2.7)), which is not available from any elemental metal. A possible solution to this problem in wide bandgap semiconductors could be the use of extreme ϕ_m materials other than traditional metal such as MoO_x [123, 126] with reported ϕ_m as high as 6.6 eV. MoO_x based contacts on Si will be the subject of our investigation in chapter 4.

Among various reported ED devices discussed so far, the SB-MOSFET, the reconfigurable FET and the TFET based on FD semiconductors and 2-D materials appear to be the most promising for future CMOS⁵. The performance of ED devices with well-optimized interface electrostatics could be at par with impurity doped devices. However more extensive experimental investigation is required to confirm whether ED could replace conventional doping in mainstream Si-CMOS technology. Nevertheless, ED could be the potential solution for alternative materials systems like Graphene, CNTs, TMDs, nanowires where conventional impurity doping is a big challenge. The ED is also interesting for innovative device concepts such as EHB-TFETs and RFETs which could not be realized using conventional doping.

Although ED based approaches look very promising, there are still some limitations and drawbacks which need to be addressed from a technology perspective.

⁵For detail discussion on performance, technological aspects and merits of various potential ED-based devices for future CMOS, please refer to [46–48].

First, the ED concept is usually designed assuming ideal MS contacts. However, there has been much experimental evidence that the observed SBHs (ϕ_b) and thus "effective" work functions on various MS systems deviate from their bulk values and the linear relationship between ϕ_b and ϕ_m may not hold in certain cases [83]. The assumption of an ideal, abrupt and non-reactive MS interface does not hold in practice. The chemical reactivity between a metal and a semiconductor, interdiffusion and the presence of interface dipoles make the observed ϕ_b to deviate from the ideal Schottky-Mott relation [127] where ϕ_b has a linear relationship with ϕ_m .

Recently, Tung [128] has reported a detailed review on physics and chemistry of Schottky barriers at MS interfaces. The author reviewed various strategies of modifying ϕ_b at the MS interface by an insertion of a thin (≈ 2 nm) interfacial layer. This avoids chemical interdiffusion and also decouples the electron states in the semiconductor from the influence of the metal [83]. ϕ_b obtained from such an metal-insulator-semiconductor (MIS) system with a thin interfacial layer shows a much stronger dependence on the metal work function than an MS interface without any intentionally grown interfacial layer [128, 129]. Such a thin interfacial layer could be a solution for the realization of work function induced ED devices with a better control over ϕ_b [130]. Moreover, the presence of additional dipoles from the interfacial layer opens up the possibility to further tune ϕ_b . Since, most ED devices can be realized via low temperature processing, the metastability of the interfacial layer should also not be a big concern.

More recently van der Waals MS junctions [131] have been demonstrated where atomically flat metal thin film were laminated onto 2-D semiconductors without any direct chemical bonding thereby resulting in the MS interface essentially free from defects and Fermi-level pinning. Such contacts could be a way forward to realize MS junction where the Schottky-Mott limit can be closely followed.

Second, metal work function variation could also be a concern [132, 133], particularly for metal nitride gates like TiN [134] due to their polycrystalline nature. This could have serious implications on the effectiveness and uniformity of work function induced ED and device variability.

Third, implementing several metals in galvanic contact may lead to corrosion during wet processing (see Fig. 2.8(b)). This effect was observed for several combinations of electrode metals [61]. Rather than wet etching, other metal patterning approaches are recommended, such as dry etching, damascene, or lift-off.

Fourth, the scaling approach for ED devices may differs from chemically doped ones as reported in the recent study by Ilatikhameneh *et al.* [77]. The atomistic simulations of such ED 2-D material transistor showed a different behavior from devices with same EOT (equivalent oxide thickness) but with varied physical oxide thicknesses. The authors therefore proposed a new scaling theory and design guidelines for such ED devices

where the actual physical oxide/dielectric thickness is more critical unlike conventional transistors where scaling is regulated by the EOT. The authors proposed to employ ultra-thin wide bandgap oxides as gate dielectric for both optimized ED and suppressed gate leakage.

Fifth, ED in general is more effective, for inducing both electrons and holes, in narrow bandgap semiconductors as discussed before.

Further, in general for any material, the smallest lateral spacing between the gates is desired for optimized performance of ED devices [77] which is largely limited by the lithographic resolution. This becomes more critical in case of wide bandgap materials as the highly resistive intrinsic gap between the two ED regions may lead to a reduced on-current and very high turn-on voltages. Recently, Pan and Chui [118] proposed to overcome this limitation in their new ED-TFET design. Such ideas can be explored for other ED devices as well.

Finally, the presence of interface traps could adversely affect the effectiveness of ED as discussed before. The use of a thin interface layer is a potential solution to minimize the effect of interface traps on induced charge [128, 130].

2.4 Conclusion

In this chapter, various reported ED approaches were reviewed. Using basic 1-D electrostatic relations, the conditions for ED were established and simple expressions for induced charge carrier densities as applied to different ED approaches were derived. The derived expressions highlight the role of metal and semiconductor work functions, energy bandgap, electron affinity and applied electric field, and the interplay between them for the induced ED. From various reported results and the developed analytical understanding, it can be concluded that ED techniques can be utilized to induce high charge concentrations in UTB active devices. In general, ED is more effective for narrow bandgap semiconductors.

ED can be obtained by low temperature processing with a fewer lithography steps. The performance of ED devices is also found competitive with that of conventional counterparts especially for SB-MOSFETs, RFETs and TFETs. However, many of these device architectures, in particular TFETs, have only been studied via TCAD simulations. Experimental realization of such structures will assist in evaluating the true merit of these device ideas for alternative material systems and innovative device concepts for future CMOS.

The effective work function variation, presence of fixed charge, interface traps, processing with multiple metals and applicability to wide bandgap materials are identified as the current major limitations to ED approaches. These need to be extensively addressed for developing future CMOS technology.

CHAPTER 3

HIGH-BARRIER SI-SCHOTTKY DIODES

Abstract

In this chapter, the presence of minority carriers and their role in charge carrier transport in silicon (Si) Schottky diodes with a high potential barrier at a metal-semiconductor (MS) interface is investigated. Using TCAD simulations along with an analytical model, it is shown that in a high-barrier diode with an induced inversion charge, the minority diffusion current becomes comparable (or even higher) than the majority carrier thermionic emission current which imparts bipolar characteristics to otherwise conventionally known unipolar Schottky diode. It is also shown, via TCAD simulations, that the diffusion component and therefore minority carrier injection efficiency becomes more pronounced in case of a reduced substrate Gummel number, downsized Schottky contact area and at elevated temperatures. Further, the role of minority carriers at low injection in a moderately high barrier Al/p-Si Schottky diode has been experimentally verified via a prior-reported 2-diode electrical test method and by measuring infrared electroluminescence. The improved minority carrier injection efficiency in high-barrier Schottky contacts could be utilized for bipolar device application as an alternative to conventional chemically doped counterparts.

3.1 Introduction

Conventional chemical doping of semiconductor devices via impurities has become more challenging for nanometer scale devices with an extremely high doping gradient [2, 3]. Moreover, chemical doping is also not yet technologically matured for emerging material systems other than silicon (Si) such as wide bandgap semiconductors (*e.g.* GaN, SiC and ZnO), carbon nanotubes (CNTs) [9–12] and emerging two-dimensional (2-D) materials (graphene, phosphorene, silicene and transition metal dichalcogenides (TMDs)) [13, 14] which are increasingly relevant for future electronic as well as optoelectronic devices. From this viewpoint, electrostatic doping (ED) as discussed in chapter-2 ([46], and references therein) is being extensively investigated to overcome the challenges of conventional doping approaches in dimensionally-scaled devices.

In this direction, the case of a shallow p-n like junction induced by a large metal-semiconductor (MS) work function difference in a one dimensional (1-D) Schottky diode was previously discussed [46, 95, 96]. In conventional Schottky barrier (SB) based devices, the current is governed by one or more Schottky contacts. The physics of an SB formed at the MS interface has been well described earlier [83]. There is a prevalent perception that at low injection the SB diode is a majority carrier unipolar device in which the current is solely governed by thermionic emission (TE) (*e.g.*, [135]) which can be expressed as:

$$J_{TE} = A^* T^2 \exp\left(-\frac{q\phi_b}{kT}\right) \left[\exp\left(\frac{qV}{kT}\right) - 1\right], \quad (3.1)$$

where J_{TE} is TE current density for majority carriers, A^* is Richardson's constant, ϕ_b is the Schottky barrier height, k is Boltzmann's constant, T is the temperature, q is the elementary charge and V is the applied voltage. The contribution of minority carrier current which is governed by diffusion at low injection is generally considered negligible in conventional Schottky diodes. For p-type Schottky diodes with uniformly doped substrate, the minority (electron) diffusion current density can be expressed as [1]:

$$J_D = \frac{qD_n n_i^2}{L_n N_a} \left[\exp\left(\frac{qV}{kT}\right) - 1\right], \quad (3.2)$$

where D_n and L_n is the diffusion constant and diffusion length of the electron in substrate bulk, N_a is the active acceptor doping concentration of the substrate and n_i is the intrinsic carrier concentration of the semiconductor. For situations where $\phi_b \ll E_g$, where E_g is the semiconductor bandgap, the diffusion current ($\propto \exp(-E_g)$) is generally much lower than the TE current ($\propto \exp(-\phi_b)$) and therefore can be safely ignored as done conventionally.

However, as ϕ_b is raised to higher values, TE is suppressed while the diffusion current remains unaffected. For a sufficiently high ϕ_b , the diffusion current can be comparable (or even higher) to the TE current. In

addition, in a high- ϕ_b diode, excessive band-bending near the MS interface will result in charge carrier inversion. The induced inversion charge will then act as a source of minority carriers for sustaining the diffusion current which otherwise could reach injection limitation in case of a low- ϕ_b diode. These two important phenomena which occur together as a result of a high- ϕ_b at the MS interface *i.e.* suppression of TE current and the sufficient supply of minority carriers transform an otherwise unipolar Schottky device into a (bipolar) p-n junction type device even at low injection.

An analytical model and the conditions for obtaining a sufficiently high- ϕ_b leading to strong inversion (thus possible bipolar behavior) [55] at a 1-D Schottky electrode were derived before in the chapter 2 [46]. The model indicates that for a suitable metal work function (ϕ_m), that governs ϕ_b , a sheet of charge carrier of polarity opposite to that of the substrate doping is induced near the MS interface. For a p-type semiconductor, the inversion layer is induced or its effects becomes important provided that [46, 55],

$$q\phi_{bp} > E_g - kT \ln \frac{N_c}{N_a}, \quad (3.3)$$

where ϕ_{bp} is the barrier height for holes, N_c is conduction band effective density of states and N_a is the acceptor doping density. Eq. (4.1) is equivalent of stating that the induced peak inversion charge (electrons) density ($n_0 = N_c \exp(-q(E_g - \phi_{bp})/kT)$) is more than the background doping density (N_a) of the substrate.

In the past, the two-carrier approach for MS junctions was adopted before by Schwarz and Walsh [136] (refer to appendix B) in connection with their Ge based surface barrier transistor (SBT) device as early as in 1953. The SBT [54] was an interesting demonstration of potential bipolar device technology solely based on MS junctions without any chemical doping. The concept however did not attract much attention after the advent of planar processes and advancement of chemical doping technology¹.

Scharfetter [137] also investigated the minority carrier injection in Schottky diodes. He concluded that under moderate to high forward bias, Schottky diodes show bipolar behavior where the injection ratio, γ (*i.e.* the ratio of minority carrier current to total current) rises linearly with the applied bias. This was attributed to the drift current of minority carriers which becomes important at higher biases. In this work, Scharfetter [137] did not specifically consider the case of a high- ϕ_b diode where the diffusion current could have been important resulting in a high γ even at low biases. Moreover, the contact limitations *i.e.* its ability to supply the required minority carriers was not taken into account in his formulations of current equations which would have otherwise restricted the continuous linear rise of γ with increasing forward bias [55] to some maximum value for a given ϕ_b . Other reports in the literature [138–140] pertaining to minority carrier injection in Schottky diodes have also been more focused on the

¹The SBT will be discussed in more detail in chapter 4.

high injection regime where the minority drift component becomes important, while the diffusion component at low injection was found to be negligible in conventional Schottky diodes.

A more detailed theoretical analysis on the minority carrier injection in Schottky diodes was reported by Green and Shewchun [55] by applying a combined TE-diffusion theory [141] to account for both majority and minority carrier current flows. They predicted that minority carrier effects could be of considerable importance in case of high- ϕ_b diodes even at low injection. Also the effect of high injection and the contact limitations on γ was discussed. The work was further extended by Elfsten and Tove [142].

High- ϕ_b MS contacts with a considerable minority injection, also referred to as bipolar-mode Schottky contacts [143] could be interesting for power devices to balance the trade-off between the forward voltage drop and breakdown voltage in epitaxial Schottky diodes. Recently, TCAD simulation studies on such 1-D Schottky junctions have been reported for a bipolar transistor [95] and a tunnel diode [96]. Such junctions can also be used for realizing light emitting devices without the need for chemically doped p-n junctions [144]. Moreover this approach of electrostatically forming a localized p-type or n-type region could also be relevant for future CMOS ultra-thin body (UTB) devices where conventional doping is a challenge.

In this chapter, the work of Green and Shewchun [55] on minority carrier injection in Schottky diodes at low injection is further extended with the viewpoint of utilizing this effect for bipolar device applications. The extensive TCAD device simulations are reported to better understand the charge transport mechanisms in different ϕ_b Si diodes, taking into account the effect of the device geometry on current spreading and series resistance. In addition, minority carrier effects in moderately high- ϕ_b Al/p-Si Schottky diodes are experimentally investigated and compared with TCAD simulations. The experimental findings on an extremely high- ϕ_b Pd/MoO_x/n-Si diodes will be discussed in the next chapter. Furthermore, the technological applications of high- ϕ_b Schottky junctions are discussed along with some practical considerations before concluding the findings of this chapter.

3.2 Device Physics and TCAD Simulation

3.2.1 Simulation parameters and models

Fig. 3.1(a) shows the test structure that was investigated via TCAD simulations [98]. A p-type Si substrate with thickness t_{Si} of 525 μm and a doping level N_a of 10^{15} cm^{-3} was used. For such doping, a $\phi_m < 4.34 \text{ eV}$ will result in surface inversion as derived in chapter 2 [46] and possibly bipolar type operation, while $\phi_m \geq 4.6 \text{ eV}$ will result in a typical Schottky type operation (*i.e.* unipolar majority carrier transport). Therefore metal work functions

Figure 3.1: (a) Schematic cross-section of the experimental and TCAD simulated device. Optical micrographs (not to the same scale) of fabricated devices: (b) circular electrode with diameter $d = 100 \mu\text{m}$, (c) ring geometry as used for the 2-diode test method and (d) hexagonal openings (side $a = 10 \mu\text{m}$) in the circular electrode ($d = 550 \mu\text{m}$) used for infrared light emission measurements.

between 4.2 eV (bipolar operation) and 4.6 eV (Schottky) were adopted for our simulation study. For computation efficiency, a 2-D Delaunay mesh with triangular elements was used. The minimum mesh spacing near the MS interface in the center of the device was $\sim 7 \mu\text{m}$ in the x -direction and $\sim 7 \text{ nm}$ in the y -direction. Also, for comparing with experiments and taking minority current spreading into account, a cylindrical symmetry was incorporated around the y -axis to solve the Poisson, current and continuity equations. Fermi-Dirac statistics along with the Philips unified mobility model [145] were used. For recombination, doping and temperature dependent Shockley-Read-Hall (SRH: $\tau_{n\text{max}} = 10^{-5} \text{ s}$, $\tau_{p\text{max}} = 3 \times 10^{-6} \text{ s}$) and Auger models [98] were included. Schottky contacts with varying ϕ_m , however with a fixed (default) surface recombination velocity ($S_n = 2.5 \times 10^6 \text{ cm/s}$ and $S_p = 1.9 \times 10^6 \text{ cm/s}$ [98]), were used as a top electrode for all simulations unless otherwise specified. For the bottom electrode, neutral contact, *i.e.* a one having space charge neutrality and thermal equilibrium at the MS interface, was assumed. The effect of boundary conditions at the bottom electrode on the minority carrier injection is discussed separately in the section 3.2.4. Moreover, ideal interfaces (following the Schottky-Mott relation [127]) were assumed initially for the conceptual understanding of the device operation. Then, the effect of interface traps is discussed.

3.2.2 Charge transport mechanisms

Fig 3.2 shows the simulated band diagram and charge carrier profile, both in equilibrium condition, for two different ϕ_m . The use of $\phi_m = 4.6 \text{ eV}$ results in a typical Schottky condition with a depletion region at the interface and ϕ_b of 0.58 V. However $\phi_m = 4.2 \text{ eV}$ results in excessive band-bending at the interface with ϕ_b of 0.98 V. In this case, the Fermi level at the interface is close to the conduction band, implying surface inversion with a peak induced electron concentration, n_0 , of $\sim 10^{17} \text{ cm}^{-3}$.

Fig. 3.3 shows simulated $I - V$ characteristics of such Si p-type Schottky diodes for three different ϕ_b (ϕ_m). The conduction for the low $\phi_b = 0.58$

Figure 3.2: Simulated band-diagrams (left) and charge carrier profiles (right) for a Schottky diode with a metal work function $\phi_m = 4.6 \text{ eV}$ ($\phi_b = 0.58 \text{ V}$) and $\phi_m = 4.2 \text{ eV}$ ($\phi_b = 0.98 \text{ V}$) at thermal equilibrium. The origin of the x-axis (Distance) is located at the bottom of the substrate. V_{bi} is the built-in voltage of the diode.

Figure 3.3: Simulated I – V characteristics of Schottky diodes for different ϕ_b (ϕ_m). γ is calculated at -0.2 V (forward bias). For the TE model, $A^* = 45 \text{ Acm}^{-2}\text{K}^{-2}$ [98] was used for p-type Si.

V ($\phi_m = 4.6 \text{ eV}$) is solely governed by TE of majority carriers which is much higher than the minority diffusion current as evident from the excellent agreement of TCAD (both forward and reverse current), with the analytical TE I – V model (Eq. (3.1)) [1]. For moderate $\phi_b = 0.78 \text{ V}$ ($\phi_m = 4.4 \text{ eV}$), the majority hole current via TE is still dominant. However, a clear deviation from the TE theory is observed for the high $\phi_b = 0.98 \text{ V}$ ($\phi_m = 4.2 \text{ eV}$). The TE theory only accounts for the hole current component. The extra current component is attributed to the contribution of electron (minority carrier) diffusion. In this case, with ϕ_b as high as 0.98 V , the TE hole current (I_h) is sufficiently suppressed that it become comparable to the electron diffusion current (I_e). The significant contribution of minority current, I_e , to the total current ($I = I_e + I_h$) can be noted from a high minority carrier injection ratio γ (I_e/I) [1] in Fig. 3.3. The higher reverse leakage current

Figure 3.4: Simulated forward bias (at $V_d = -0.2$ V) band-diagram of the Schottky diode with $\phi_b = 0.98$ V.

than predicted by the TE model in case of the high- ϕ_b diode is attributed to generation current (see also Fig. 3.5(a)). The observed bipolar conduction in the high- ϕ_b diode with a significant γ at low injection is counterintuitive to the prevalent perception where Schottky barrier diodes are considered to be majority carrier unipolar devices [1, 146].

The forward bias band diagram of a Schottky diode (see Fig. 3.4) can further be used to gain more insight into the prevalent charge transport mechanism at low injection. The presence of minority diffusion current in a Schottky diode can be ascertain from the slope of the electron quasi-Fermi level (E_{Fn}) in Fig. 3.4. The hole quasi-Fermi level (E_{Fp}) in turn remains flat across the whole device confirming TE as the dominant transport mechanism for the majority carriers [1]. Further, the peak induced electron concentration, n_0 , which is determined by the position of E_{Fn} with respect to the E_c at the MS Schottky interface, remains fixed to its thermal equilibrium value and doesn't change with the applied bias.

Fig. 3.5(a) shows the electron current (I_e) components of the simulated $I - V$ curves (Fig. 3.3) for varying ϕ_b . The diffusion component I_e , being governed by the Gummel number of the substrate ($G_b = \int_0^{t_{si}} N_a(x) dx$) [147], remains unchanged with varying ϕ_b in the exponential region of the $I - V$ curves. However, γ (see inset Fig. 3.5(a)) varies with ϕ_b because the latter affects I_h . Therefore, I_e can be neglected for a low- ϕ_b (low γ) diode but cannot be ignored for a high- ϕ_b (high γ). It is also commonly known that the series resistance of a Schottky diode is higher than that of a p-n junction diode [146] because of the poor supply of minority carriers, (see Fig. 3.5(b)). For $\phi_b = 0.58$ V and 0.78 V, the minority carrier concentration is still below N_a and therefore doesn't affect the overall series resistance

Figure 3.5: (a) Electron current components (I_e) of the simulated I – V characteristics of Fig. 3.3 at different ϕ_b (inset: I_e and I_h for varying ϕ_b at a fixed forward bias $V_d = -0.2$ V), (b) Simulated electron (minority carrier) profile across the device at $V_d = -1$ V forward bias for different ϕ_b . Note that the peak electron concentration at the MS interface is not affected by the bias. I_e and I_h are probed at the top Schottky electrode.

much. However in case of an extreme $\phi_b = 0.98$ V, the minority carrier concentration is comparable to N_a which lowers the series resistance. The effect of ϕ_b on the series resistance can be observed from the I – V plots in Fig. 3.3 and Fig. 3.5(a) at higher biases ($V_d = -1$ V, forward) where the current increases with ϕ_b .

Interestingly, such high- ϕ_b diodes ($\phi_b = 0.982$ V for IrSi/Si) can be realized experimentally, as reported by Wittmer [148, 149], using silicided contacts on bulk Si. However, contrary to our simulation, the author concluded that the measured current fully obeys a single carrier TE theory in the range 200 K - 300 K and did not consider the possibility of (minority) diffusion. A possible reason for this could have been the use of a Si substrate with relatively higher Gummel number which actually diminishes the contribution of the diffusion component as discussed further in this chapter. Also, measurements beyond 300 K were not reported where diffusion would have become relatively more noticeable. Moreover, a possibly high surface recombination velocity at the Schottky contact could also enhance the TE current and thereby degrading the γ , which otherwise would have been expected to be relatively high for such ϕ_b .

3.2.3 Role of inversion layer: Injection limited regime

The contact limitations upon injecting minority carriers at high injection has been highlighted before by Green and Shewchun [55]. In order to understand the role of inversion layer at the contact in limiting the minority current at moderate to high forward biases, its important to first minimize the effect of series resistance while keeping the minority (electron) current the same. For this purpose, a Si Schottky diode structure with a thin, 5 μm , p-type (10^{15} cm^{-3}) layer on top of a p^+ (10^{19} cm^{-3}) substrate is considered.

Figure 3.6: (a) Minority (electron) current components (I_e) of the simulated $I - V$ characteristics of the pp^+ Schottky diode with the same effective Gummel number as that of bulk p-type substrate in Fig. 3.3 but with a lower series resistance. The dotted horizontal lines indicate the upper limit of the minority current that the Schottky contact with the given ϕ_b can supply.

The thickness of the p^+ substrate was adjusted such that the (effective) Gummel number of this structure is the same as that of the earlier used bulk, 525 μm thick, p-type (10^{15} cm^{-3}) substrate. From hereafter, this type of device will be referred as a pp^+ Schottky diode.

Fig. 3.6 shows the electron current (I_e) against the voltage for varying ϕ_b in case of the pp^+ Schottky diode with a lower series resistance. Clearly, the minority current which is governed by diffusion at lower biases becomes injection limited at higher biases. The upper limit of the minority (electron) current that the contact with given ϕ_b can supply is approximated as $I_e \sim A_E q n_0 v_{\text{sat}}$. Here n_0 refers to the peak induced electron concentration at the MS interface for given ϕ_b , A_E is the area of top electrode and v_{sat} is the saturation velocity for electrons, $\sim 10^7 \text{ cm/s}$. Therefore, it can be concluded that the inversion layer and consequently a high- ϕ_b is important in sustaining a minority diffusion current at moderate to high biases for any bipolar device application.

A similar argument holds true even for majority carriers. For a neutral type back contact, the maximum value of majority current is then limited by the doping density of the substrate and is given by $I_e = A_E q N_a v_{\text{sat}}$. Beyond this limit, the majority current will then become bulk limited and will be no longer governed by TE. In practice, for bulk substrates, such effects are masked by the series resistance effect which comes into play before the injection limited regime for minority carriers or bulk limited regime for majority carriers sets in. However, this could be important for thinner substrates or high mobility semiconductors where the series resistance is lower.

Figure 3.7: Simulated $I - V$ characteristics of a Schottky diode (a) with $t_{Si} = 100$ nm for both high- ϕ_b and low- ϕ_b diodes. γ is calculated at -0.2 V (forward bias) (b) I_e and I_h against the temperature for the high- ϕ_b diode ($V_d = -0.2$ V, $t_{Si} = 525$ μm).

3.2.4 Tuning the minority diffusion component

Substrate thickness reduction

The diffusion current can be further increased by reducing the Gummel number of the substrate. By reducing t_{Si} from 525 μm to 100 nm, γ increases from 0.6 to 0.99 for $\phi_b = 0.98$ V as shown in Fig. 3.7(a). Here a larger deviation from the TE model is observed implying that the current is largely diffusion dominated. However varying t_{Si} doesn't affect the TE majority current and therefore the current for a device with $\phi_b = 0.58$ V is still following the TE model. The pronounced effect of the diffusion current for smaller substrate thicknesses in high- ϕ_b diodes could be relevant for bipolar applications in advanced UTB devices.

Elevated temperatures

Also the temperature dependence of diffusion is larger than that of TE because of the relatively high potential barrier in case of the former [1]. Therefore, for the high- ϕ_b diode, γ increases with the temperature as shown in Fig. 3.7(b). Such a rise in the diffusion current at higher temperatures was also observed experimentally in our Schottky diodes as discussed in section 3.3.3.

Role of bottom contact

For the simulation study performed so far in this chapter, the substrate bottom contact was assumed to be neutral in nature. However, it has been shown before [137, 150] that the boundary conditions at the bottom contact also affect the minority injection at the top contact. The effect of the bottom contact becomes important when the (minority) diffusion length is larger than or comparable to the substrate thickness. In order to illustrate this, TCAD simulations were performed using a thin Si substrate ($t_{Si} = 5$

Figure 3.8: Simulated (a) energy band diagram at thermal equilibrium and (b) minority (electron) current at top Schottky contact (with fixed $\phi_b = 0.98\text{ V}$) for varying boundary conditions at the bottom substrate contact from depleting to accumulating. $t_{\text{Si}} = 5\text{ }\mu\text{m}$ was used for this simulation.

μm) for three different types of bottom contact, *i.e.* depleting, neutral and accumulating. The ϕ_b at the top Schottky contact was fixed to 0.98 V .

Fig. 3.8(a) shows the energy band diagram for the three different conditions at the bottom contact. In case of the depleting contact, downwards band bending at the bottom contact favors the electron extraction and, as a result, the electron current is enhanced at the top contact as can be seen in Fig. 3.8(b). For the neutral contact, the electron current is the same as that of the depleting contact but with a lower series resistance. However, in case of the accumulating contact, the upward band bending act as a barrier for the electrons extraction at the bottom contact and, as a result, the electron current is suppressed at the top contact. The accumulating type of contact, though preferred for their lower resistance, adversely affects the minority injection which could be a concern if a high γ is desired. The majority (hole) current (not shown) at the top contact remains the same for all three cases except for the series resistance part which shows the same trend as depicted in Fig. 3.8(b) at higher bias voltages.

3.2.5 Small-size Schottky contacts

Other than tuning the minority diffusion component alone by varying the substrate Gummel number, the injection ratio γ can be increased further by suppressing the majority current component. One approach of achieving this is by reducing the area of the Schottky contact to which the majority carriers TE current is directly proportional. The minority current on the other hand spreads away from the contact into the substrate (discussed further in section 3.3.3) and therefore depends both on area as well as the perimeter of the contact. For a very small-size contact (sub 100 nm) with a large minority current spreading, a high γ is therefore expected.

To study this effect, the area of the top Schottky contact was greatly reduced by decreasing its radius (r) from $50\text{ }\mu\text{m}$ to 50 nm and the relative

Figure 3.9: Simulated electron (I_e) and hole (I_h) current components for two different radii (r) of the top Schottky contact with (a) $\phi_b=0.78$ V and (b) $\phi_b=0.98$ V. The dotted horizontal lines indicate the upper limit of the minority current that the Schottky contact with a given ϕ_b can supply.

magnitudes of I_e and I_h were then compared in both cases. Note that for this simulation, in order to minimize the series resistance effect, the pp^+ Schottky diode structure was used as introduced before with the same Gummel number as that of the bulk substrate.

For $\phi_b=0.78$ V, see Fig. 3.9(a), the γ in the low bias region is significantly higher for the 50 nm contact as compared to that of 50 μm where it is negligible. For $\phi_b=0.98$ V, γ which is already high even for the 50 μm contact, is further improved when the contact radius is reduced to 50 nm. The injection ratio however gradually drops at higher forward biases as the minority current reaches its injection limitation for a given barrier height. The effect is more pronounced for a lower ϕ_b due to the poor minority carriers supply to sustain the diffusion current level at higher biases. The situation at higher biases is relatively better for a larger ϕ_b with its improved minority carrier supply.

This idea of achieving a high injection ratio even with a nominally high ϕ_b using a sub 100 nm size contact could be interesting for realizing bipolar devices. The upper limit of the operating voltage (current) is however restricted by ϕ_b of the Schottky contact.

Further, the small-size Schottky contact is also a better light emitter than its big-size counterpart. This can be analyzed from Fig. 3.10(a) where at low biases the effective minority (electron) current density, J_e , for the 50 nm contact is shown to be several orders (~ 3) in magnitude higher than that of the 50 μm contact due to a higher perimeter contribution in the former than the latter. Now in Schottky diodes, the light emission (or radiative recombination) is governed by the injected minority current. Therefore, it is expected that the light emission per unit area from the 50 nm contact is also higher than that of 50 μm contact by similar orders in magnitude. This is manifested by Fig. 3.10(b) where indeed a significantly higher (also by ~ 3 orders in magnitude) per unit area light output from the former at low biases can be deduced from the plot of integrated radiative recombination rate (R_{i-rad}) per unit area against the applied bias. This

Figure 3.10: Simulated (a) effective minority (electron) current density (J_e) and (b) integrated radiative recombination rate (R_{i-rad}) per unit area for two different radii (r) of the top Schottky contact shown for $\phi_b=0.78$ V and $\phi_b=0.98$ V. The dotted horizontal lines indicate the upper limit of the minority current density that the Schottky contact with a given ϕ_b can supply.

observation can have important consequences for designing light emitters based on Schottky contacts. Basically, it implies that for a given metal (ϕ_b), the array of nm size contacts when placed sufficiently apart so as not to affect their individual current spreading into the substrate, will as a whole emit more light compared to a μm size single contact with an effective area equal to that of the whole nm size contact array.

However the difference in J_e and therefore light emission among different size contacts fades out at higher biases where the current density is then ultimately capped by its maximum injection limit which in turn is governed by ϕ_b . Again the effect is more pronounced for lower- ϕ_b diodes than higher ϕ_b counterparts as can be noted from Fig. 3.10(a)-(b). Table 3.1 summarizes the TCAD simulation results for various ϕ_b and device geometries.

Table 3.1: Summary of TCAD simulation results for various ϕ_b , substrate thicknesses (t_{Si}), Schottky contact areas (A_E) and temperatures (T) at $V_d \sim -0.2$ V. The term "pp⁺" here refers to the Schottky diode on pp⁺ substrate with the same Gummel number as the bulk 525 μm p-type substrate.

ϕ_b (V)	T(K)	t_{Si} (μm)	A_E (cm^2)	γ	Dominant mechanism
0.58	298	525	7.85×10^{-5}	10^{-7}	TE
0.58	298	0.1	7.85×10^{-5}	10^{-4}	TE
0.78	298	525	7.85×10^{-5}	10^{-4}	TE
0.98	298	525	7.85×10^{-5}	0.6	minority diffusion, TE
0.98	298	0.1	7.85×10^{-5}	0.99	minority diffusion
0.98	398	525	7.85×10^{-5}	0.9	minority diffusion
0.78	298	525 (pp ⁺)	7.85×10^{-11}	0.68	minority diffusion, TE
0.98	298	525 (pp ⁺)	7.85×10^{-11}	0.99	minority diffusion

3.3 Experimental Results

3.3.1 Device Fabrication

p-Si Schottky diodes were fabricated² using Al as a top electrode (Fig. 3.1). The choice of Al is based on its reported low vacuum work function, ϕ_m , of 4.28 eV which ideally should result in a ϕ_b of 0.89 V ($q\phi_b = E_g - \phi_m + \chi_s$), where E_g is the Si bandgap (1.12 eV) and χ_s is the Si electron affinity (4.05 eV). The substrate back was utilized as the bottom electrode. A (111) p-type Si substrate with N_a of 10^{15} cm^{-3} and with a native oxide was used. 200 nm Al was sputtered on the polished surface. The electrodes were then patterned using a standard photolithography process using a positive photoresist. The presence of the thin native oxide between Al and Si surface avoids chemical inter-diffusion and also decouples the electron states in the Si from the metal [83, 151], which might lower the effective ϕ_b . Annealing the wafer was avoided to prevent alloy formation and to keep the as-deposited metallurgical nature of the junction intact. Note that, from view point of ruggedness and reproducibility this annealing step should not be avoided. As a reference, to obtain a low- ϕ_b diode, an n-Si/Al wafer was also fabricated following a similar process.

3.3.2 Electrical characterization: Barrier height extraction

Temperature dependent $I - V$ measurements of the fabricated Al/p-Si Schottky diodes were performed using a Keithley 4200 Semiconductor Characterization System (SCS) with a preamplifier enabling DC measurements with a combined noise level of $\sim 10 \text{ fA}$ for an integration time of 100 ms. The measurements were performed under dark conditions and on a temperature controlled chuck.

A moderately high ϕ_b of 0.77 V with an ideality factor n of 1.09 was extracted from the Richardson plot (see Fig. 3.11(a)) in the exponential region ($V_d = -0.2 \text{ V}$) of the $I - V$ curves. The extracted ϕ_b from $I - V(-T)$ measurements is also in agreement with that obtained from $C - V$ measurements as shown in Fig. 3.11(c). The relatively low value of the extracted A^* ($4.06 \text{ Acm}^{-2}\text{K}^{-2}$) as compared to the reported value of $32 \pm 2 \text{ Acm}^{-2}\text{K}^{-2}$ [1, 152] for a p-Si substrate can be partly caused by the inhomogeneity at the interface [153] as a result of the unannealed electrical contacts. Further, the non-ideality of $n \sim 1.09$ could be attributed to the presence of the interfacial layer (native oxide) and image force effect [1]. However, since the effective $\phi_b > 0.5E_g/q$, some level of surface inversion is expected in this diode. Similar measurements on the n-Si/Al diode results in a low ϕ_b of 0.53 V as desired for comparison. Note that the sum of $q\phi_b$ on p-type and n-type substrate is higher than E_g (1.12 eV). This could be attributed to the presence of native oxide and/or Fermi-level pinning due to interface states.

²The device fabrication part as reported in this chapter was performed by S. Banerjee.

Figure 3.11: (a) Richardson plot of the fabricated Al/p-Si diode ($A_E = 7.85 \times 10^{-6}$ cm²) at $V_d = -0.2$ V forward bias. A ϕ_b of 0.77 V was extracted using this measurement. (b) Measured $I - V$ curves at $T = 298$ K and $T = 398$ K and their fitting using TCAD simulation and the analytical TE model (Eq. (3.1)) with experimentally extracted values of ϕ_b , Richardson's constant A^* and ideality factor n . (c) ϕ_b extraction from $C - V$ analysis in reverse bias.

The extracted ϕ_b of 0.77 V was used as input for the TCAD simulation where excellent agreement with the experimental data was obtained in forward bias operation, as shown in Fig. 3.11(b). ϕ_b of 0.77 V results in a downward band bending near the MS interface with a peak induced electron concentration, n_0 of 3×10^{13} cm⁻³. Note that, this induced electron concentration for the moderately high experimental ϕ_b of 0.77 V is much lower than that for the extremely high ϕ_b of 0.98 V ($\phi_m = 4.2$ eV) adapted for simulations in Section 3.2. Therefore, less pronounced effects on the conduction are expected. Consequently, in our experimental devices the current is largely dominated by TE majority carriers, *i.e.* holes, with $\gamma = 10^{-3}$. This is further evident as experimental and TCAD $I - V$ characteristics are in agreement with the TE analytical model (Eq. (3.1)). The relative contribution of the electron diffusion though increases at higher temperatures to $\gamma = 10^{-2}$. However, J is still governed by TE. Therefore, in this case it is not straightforward to establish the presence of minority carriers experimentally.

Figure 3.12: Schematic of the 2-diode test method and measurement configuration with TCAD simulated current flow lines. The flow lines indicate the current spreading in the device when only D – 1 is biased (forward current bias = 1 μA) for case (a) $\phi_b = 0.98 \text{ V}$ and (b) $\phi_b = 0.58 \text{ V}$. The current spreading due to minority carrier injection is observed near the contact for the high- ϕ_b diode, while less current spreading was observed for the low- ϕ_b diode. The switch S is in closed position when both D – 1 and D – 2 are biased.

3.3.3 2-diode measurements

To study the influence of minority carrier injection in a high- ϕ_b diode, a prior reported 2-diode method [154, 155] was adopted. With this technique, it is possible to distinguish the operation of a (Schottky based) shallow p-n like junction diode from that of a conventional Schottky diode at low injection.

The schematic of the 2-diode test method is illustrated in Fig. 3.12 where two similar diodes, D – 1 and D – 2, are closely spaced ($\sim 2 \mu\text{m}$). Here the current of D – 1 is measured when it is operated in single mode, and in parallel mode along with D – 2. In case of a p-n type diode, there will be a significant contribution of minority carrier injection from the contacts (high γ), and as a result the current will spread outwards from the contacts. When D – 1 is operated in parallel with D – 2, then in case of p-n type diodes, the current of each diode will be less compared to that in single mode operation due to influence of current spreading from the neighboring diode. This influence can be measured from the differential current level in the exponential part of the $I - V$ curve.

While in case of a conventional Schottky diode, the minority carrier injection will be insignificant and therefore there will be hardly any current spreading near the contacts. Hence, for conventional Schottky diodes, the current for both modes (i.e. single mode and parallel mode operation)

Figure 3.13: Simulated electron (I_e) and hole (I_h) currents of diode D – 1 when operated in single mode (I_{D-1}) and in parallel mode ($I_{D-1'}$) for high ϕ_b ($= 0.98$ V) Schottky diodes. $t_{Si} = 525$ μm and $N_A = 10^{15}$ cm^{-3} .

will be the same as it is governed by majority carrier injection from the substrate and depends only on the area of the diode. Therefore then hardly any influence of the neighboring diode will be noticeable in the exponential part of the $I - V$ curve.

Fig. 3.13 shows the TCAD simulated electron (I_e) and hole (I_h) currents in case of high- ϕ_b Schottky diodes when diode D – 1 is operated in single mode (I_{D-1}) and in parallel mode ($I_{D-1'}$) with diode D – 2. As expected, only the minority (electron) current is affected in parallel mode operation while the majority current remains unaffected. Since in case of a high- ϕ_b diode, γ is high, this influence can be measured in the 2-diode test configuration.

Fig. 3.14(a)-(b) shows the experimental 2-diode characteristics for two different ϕ_b diodes. For the p-Si/Al diode with $\phi_b = 0.77$ V, a slight decrease

Figure 3.14: $I - V$ curves showing the measured D – 1 current when operated in single mode and parallel mode at 298 K for (a) $\phi_b = 0.77$ V and (b) $\phi_b = 0.53$ V. The blue solid line indicates an ideality factor $n = 1$ for reference.

in the diode $D - 1$ current ($\Delta I = I_{D-1} - I_{D-1'}$) in the exponential part of the plot when operated in parallel with diode $D - 2$ was observed as shown in Fig. 3.14(a). Here, a current discrepancy ($\Delta I/I$) of 37 % was observed in the forward bias exponential region at $V_d = -0.1$ V. This indicates the influence of minority carrier (electron) injection in the p-type Schottky diode. However, in case of the n-Si/Al diode with a near mid-gap $\phi_b = 0.53$ V, the influence of the minority carrier injection from the metal side into the semiconductor is negligible and thus the $D - 1$ current remains unaffected as shown in Fig. 3.14(b). Here a current discrepancy ($\Delta I/I$) of less than 7 % was observed at $V_d = 0.1$ V. Further, the influence of current spreading increases at higher temperatures where a higher $\Delta I/I = 51$ % was noted at 398 K for diodes with $\phi_b = 0.77$ V. This is expected as an increase in temperature increases the diffusion component more than the TE current and will raise γ , in this case, by one order of magnitude, as observed in our TCAD simulations (Fig. 3.7(b)). The observed lower $I_{D-1'}$ in the series resistance regime for both diodes in Fig. 3.14(a)-(b) is due to the high resistance encountered during parallel mode operation [154, 155].

3.3.4 Electroluminescence (EL) measurements

The light emission in the Schottky diode during its forward bias operation is determined by its injected minority current as discussed in section 3.2.5 (Fig. 3.10) using TCAD simulations. It can be stated that at low bias operation, when the minority current densities in two different ϕ_b diodes are the same then the light emission or radiative recombination rates will also be identical in two diodes. However, in the high bias regime where the series resistance or injection limitation becomes important, the higher- ϕ_b diode shows a higher minority current density and hence more light emission compared to that of a lower ϕ_b diode. Further, for a constant current drive at low bias, the voltage drop across the junction increases with ϕ_b and consequently the diffusion current and $p \cdot n$ product (thus light emission) also increases with ϕ_b in that regime.

In order to support our TCAD findings, the electroluminescence (EL) from our fabricated Si-Schottky diodes was measured. A cooled InGaAs detector based camera (XEVA-320 from Xenics) with a spectral detection range of 950 nm-1700 nm was used for capturing the EL micrograph using an integration time of 30 s. Low-intensity light emission in the infrared (IR) range was observed from our p-Si/Al diodes ($\phi_b = 0.77$ V) at a constant current drive of 20 mA ($J \sim 25$ A/cm²) at room temperature, as shown in Fig. 3.15(a). The light emission occurs via band-to-band recombination of injected minorities (electrons) with background majorities (holes) in the p-type Si substrate. In addition, the emitted light was measured via the short-circuit current (I_{PD}) of an off-chip Si-photodiode [156] as shown in Fig. 3.15(b). The I_{PD} is proportional to the emission intensity which rises steadily with the injected current I_{LED} of the high- ϕ_b Schottky diode.

Circular electrode with hexagonal openings

Figure 3.15: (a) EL IR micrograph (in greyscale) of our fabricated p-Si/Al circular diode ($\phi_b = 0.77$ V) with hexagonal openings (see Fig. 3.1(d)). By using an IR camera a faint glow (white regions) was observed from the hexagonal openings, and from the periphery of the circular electrode, (b) Measured short-circuit current (I_{PD}) in the external photodiode (PD) versus injected forward current (I_{LED}) for the same p-Si/Al diode, (c) Simulated $p \cdot n$ product at injected current density $J \sim 25 \text{ A/cm}^2$ for different ϕ_b . The $p \cdot n$ product increases with ϕ_b as expected in high bias or at constant current drive.

However, no measurable light emission (I_{PD}) was observed from the lower ϕ_b (0.53 V) n-Si/Al diode due to the relatively low minority carrier current.

It should be noted that the maximum injected current density, $J \sim 25 \text{ A/cm}^2$ though in high bias range where series resistance or injection limitation becomes important, is still in low injection regime ($J \ll qNv_{sat} = 1.6 \times 10^3 \text{ A/cm}^2$, where N is the active doping concentration and v_{sat} is the saturation velocity). It is commonly known that at high injection minority carriers do play a role even in a conventional Schottky diode [1, 137, 139] due to their enhanced drift component as also discussed in section 3.1 before. However, the observation of light emission from the higher- ϕ_b Schottky diode at low injection indicates the role of minority carriers in lowering down its series resistance (thus higher injected minority current) as compared to lower- ϕ_b diode. This is also in agreement with our simulations where the emitted light intensity which is proportional to the $p \cdot n$ product [157, 158] increases for a higher- ϕ_b at constant injected forward current drive (at high forward biases) as shown in Fig. 3.15(c). The

Table 3.2: Summary of experimental results.

Diode	ϕ_b (V)	2-diode test	EL
p-Si/Al	0.77	$\Delta I/I=37\%$	Yes
n-Si/Al	0.53	$\Delta I/I=7\%$	No

$p \cdot n$ product hence recombination rate is highest near the MS interface.

The results of our experimental investigations from this chapter are summarized in Table 3.2, all indicating the more prominent role of minority carriers in the higher- ϕ_b diode as compared to lower- ϕ_b diode.

3.4 Discussion

Fig. 3.16 summarizes the ϕ_b dependence of the relative contribution of the diffusion component. As discussed before, for a high- ϕ_b Schottky diode, minority carrier diffusion is important and therefore cannot be neglected particularly for reduced substrate thicknesses or a reduced Gummel number in general, and higher temperatures.

The pronounced effect of the minority carrier transport in high- ϕ_b Schottky diodes at reduced substrate thicknesses could be attractive for next generation dimensionally-scaled CMOS devices where conventional doping is a challenge. There such Schottky based junctions can be used to realize for instance tunnel devices [96], transistors based on 2-D materials [123] or even low-intensity light emitters for applications such as on-chip communication [159]. In addition, a Schottky based p-n type junction

Figure 3.16: (a) Simulated minority carrier injection ratio γ as a function of the barrier height (ϕ_b) of the p-Si Schottky diode for different substrate thicknesses and temperatures (Inset: same plot in linear scale at higher ϕ_b). γ has been calculated at $V_d = -0.2$ V forward bias. The green dashed line indicates our experimentally measured ϕ_b for a 525 μm thick substrate.

could be relevant for optoelectronic applications (for example Schottky based UV LEDs [160]) in direct bandgap materials such as GaN, where conventional doping is also not well matured. Moreover, small (sub 100 nm) size Schottky contact could further be exploited to enhance the minority carrier effects in undoped bipolar transistor or light emitting devices based on MS junctions.

However from a technological viewpoint, there are several limitations to the pronounced minority carriers effects in practical Schottky diodes. The first one is the availability of required high/low metal work functions to realize high- ϕ_b diodes to n-type and p-type semiconductors respectively. This is much of a concern for wider bandgap materials (particularly n-type) as compared to smaller bandgap materials. In this regard, recently popular "carrier selective contacts", such as molybdenum oxide (MoO_x) [126], vanadium oxide (V_2O_x) or tungsten oxide (WO_x) [161, 162] for a "hole selective" and lithium fluoride (LiF_x) [163] or TiO_x [164, 165], for an "electron selective" contact should be explored for realizing extreme- ϕ_b diodes to n-type and p-type semiconductors respectively, which is otherwise difficult with existing elemental metals. The use of a high work function MoO_x material to realize high- ϕ_b diodes will be discussed in the next chapter.

The second limitation are interface traps the effect of which cannot be ignored for realizing a high- ϕ_b Schottky diode. Interface traps influence ϕ_b [1, 83] and particularly in covalent semiconductors, it is only weakly dependent on ϕ_m as the Fermi level is "pinned" at the interface by a large density of surface states. The effective ϕ_b will reduce from its ideal value in presence of interface traps, which in turn will decrease the induced inversion charge concentration near the MS interface [46]. Consequently, minority carrier transport would become less important. Interestingly, for ionic semiconductors such as GaN, CdS and ZnS, the Fermi-level pinning effect is less pronounced and ϕ_b should strongly depend on ϕ_m [1].

The use of a thin interfacial tunneling layer has also been proposed earlier to gain better control over a resultant ϕ_b and thus induced inversion charge [46, 128–130, 151]. The interfacial layers can further be utilized to suppress the majority current as well and thereby offering a high minority carrier injection efficiency at a given applied bias as reported for metal-insulator-semiconductor (MIS) tunnel diodes [166, 167].

Further, in our simulation study, the effect of Schottky barrier lowering [1] has not been considered which may disturb the injection ratio from the ideal scenario where ϕ_b is treated as voltage independent. The barrier lowering is however more pronounced at reverse bias than at forward bias. Moreover, at extreme ϕ_b , the presence of inversion charge results in a sharp drop of the potential near the MS interface and consequently a high surface electric field (see Fig. 3.17). In such scenario, transport mechanisms such as tunneling [1] could be more important than ideally considered TE and diffusion. Previously, Chi *et al.* [168] reported thermionic-field emission as

Figure 3.17: TCAD simulated along with numerically calculated, (a) potential and (b) electric field profile in case of n-type Si Schottky diode with varying ϕ_b at the MS interface. The numerical model is based on the formulations described in [136] (refer to appendix B) for the solution of Poisson's equation taking the inversion charge into account.

the dominant transport mechanism in NiGe/n-(001) Ge Schottky diodes with $q\phi_b$ more than the bandgap. Such formulations should therefore be adapted for more accurate analysis of bipolar charge transport in case of extreme ϕ_b ($\sim E_g/q$) diodes.

3.5 Conclusion

In this chapter, the role of the otherwise negligible minority carrier diffusion in high-barrier ($q\phi_b > 0.5E_g$) Schottky diodes at low injection was discussed using TCAD simulations and experiments with the viewpoint of utilizing such MS contacts for bipolar device applications as an alternative to conventionally doped counterparts. TCAD simulations indicate that in a high- ϕ_b Schottky diode with an induced inversion charge, the diffusion current is comparable (or even higher) to the TE current which imparts bipolar characteristics to otherwise unipolar Schottky diode. The diffusion component and therefore injection efficiency can further be improved by reducing the substrate Gummel number (and increasing temperature) making such concepts more suitable for realizing bipolar devices based on UTB semiconductors. In addition, the geometrical effects in Schottky contacts were discussed where the minority carrier injection is enhanced via current spreading. Small-size (sub 100 nm) contacts could be exploited for bipolar devices even with nominal ϕ_b at lower bias voltages. Moreover, such small-size contacts are more efficient light emitters than their big-size counterparts.

The experimentally observed infrared emission in low injection condition and detected current spreading near the Schottky contact using the 2-diode test methodology all indicate the influence of minority carrier diffusion in a high-barrier Schottky diode, which can be otherwise ignored in a conventional Schottky counterpart.

BIPOLAR CHARACTERISTICS OF HIGH-BARRIER $\text{Pd}/\text{MoO}_x/\text{n-Si}$ DIODES

Abstract

Sub-stoichiometric molybdenum oxide (MoO_x) has recently been investigated for its application in high efficiency Si solar cells as a "hole selective contact". In this work, the electrical and light-emitting properties of MoO_x -based contacts on Si are investigated from the viewpoint of realizing functional bipolar devices such as LEDs and transistors without any impurity doping of the Si surface. The diodes were realized on n-type Si substrates using e-beam physical vapor deposition of Pd/MoO_x contacts and their behavior was compared to that of implanted $\text{p}^+/\text{n-Si}$ diodes. In contrast to a majority-carrier dominated conduction as in conventional Schottky diodes, $\text{Pd}/\text{MoO}_x/\text{n-Si}$ diodes displayed minority-carrier dominated charge transport with $I - V$, $C - V$ and light-emitting characteristics comparable to the implanted $\text{p}^+/\text{n-Si}$ counterparts. Utilizing such MoO_x -based contacts, a lateral bipolar transistor concept without employing any doped junctions is also demonstrated. Finally, the limitations of commonly used characterization methods, such as temperature dependent $I - V$ and $C - V$ measurements, are highlighted for determining the barrier height in case of Schottky diodes with an induced inversion layer at the metal-semiconductor interface.

This chapter is based on the work submitted in Journal of Applied Physics and is built upon the work presented at the 32nd IEEE International Conference on Microelectronic Test Structures (ICMTS), 2019 [169].

4.1 Introduction

The general trend in advanced Si devices is towards lower processing temperatures and more and more shallow junctions. This has shifted the research focus to the development of pn junctions that do not rely on the formation of a heavily-doped surface region on the Si. Ultimately, it would be attractive to form junctions without any chemical doping at all. Schottky diodes fall in this category but conventional Schottky's are unattractive in many situations due to their relatively high saturation currents and poor minority carrier injection. Specifically, for high gain bipolar transistors and in photodiodes where low dark currents are required, other possible solutions should be explored. One solution that has been proposed [55, 56] and discussed in the previous chapter is the use of high-barrier Schottky diodes that significantly suppress the majority carrier injection from the substrate and provide a more favorable minority carrier injection ratio in the diode over a wide voltage range. However, experimentally the search for high-barrier Schottky diodes on Si has not been very successful so far.

Other methods of creating p^+/n -like junctions without doping the n -Si have been found. Besides high-barrier Schottky diodes, the hole injection into the substrate can also be effectuated by forming a hole inversion layer at an insulator-Si interface that is contacted via doped regions, an example of which are photodiodes that need to be sensitive up to the Si surface [170]. In this case, the holes gather at the surface due to the presence of negative charge in an insulating Al_2O_3 layer. Alternatively, an inversion layer at the interface can also be formed by employing a non-insulating layer such as pure boron (PureB). In these "PureB" diodes, the potential responsible for holding the holes at the interface, has been proposed to originate from a high concentration of fixed negative charge created by the B-to-Si bonds [171]. Due to the overall attractive characteristics of this type of junction, it is now widely applied in high performance photodiodes [172].

In this chapter, sub-stoichiometric molybdenum-oxide, MoO_x , with $x < 3$, based contacts on n -Si are studied. MoO_x has been reported before as a high work function (ϕ_m) material [123, 126, 173, 174] that forms a diode to Si with a low electron injection. Due to these properties, it has recently received attention in Si solar-cells research, being termed as a "hole selective" contact [126, 174]. More correctly, MoO_x is a wide bandgap transition metal oxide (TMO) [161] with a bandgap $E_g \sim 3.3$ eV, and a relatively high electron affinity > 6 eV, where an inherent oxygen deficiency results in a defect-band formation near the conduction band [126] (see Fig. 4.1(a)). Thin MoO_x layers were therefore treated as (semi-) metals with a high ϕ_m . If chemical reactions at the interface with the Si do not play a decisive role [176], such a high ϕ_m could be instrumental in the formation of a hole inversion (accumulation) layer on n -type (p-type) Si substrates. Fig. 4.1(b) depicts a schematic energy band diagram of a MoO_x layer on top of n -type Si with an induced hole inversion layer in Si at MoO_x/n -Si interface.

Figure 4.1: Schematic energy band diagram at thermal equilibrium of, (a) a vacuum evaporated MoO_x layer with oxygen vacancies [126, 161], (b) metal/MoO_x/n-Si interfaces [174, 175]. As revealed by TEM analysis, an SiO_x(Mo) interlayer (~ 2 nm) is formed as a result of a chemical reaction between Si and MoO_x during the deposition process.

The presence of a hole inversion layer at the MoO_x/n-Si interface was previously investigated using material characterization approaches such as photoelectron spectroscopy, in conjunction with capacitance-voltage (C–V) measurements [175, 177]. Also, I–V measurements along the Si interface of Pd/MoO_x/n-Si devices were recently performed using dedicated electrical test structures [169] to directly monitor any inversion, but there it was only concluded that if an inversion layer was present it had a sheet resistance higher than ~ 50 k $\Omega/\square$. However, the diode I–V characteristics were found to be similar to that of implanted p⁺/n reference diodes, indicating a strong suppression of the electron injection into the MoO_x. In addition, although the MoO_x was conductive, the resistivity was very high with values greater than about 10^4 Ω -cm.

In this chapter the presence of an inversion layer at the Pd/MoO_x interface to n-Si is confirmed. The origin of the hole inversion layer in the Pd/MoO_x/n-Si and PureB (metal/B/n-Si) diodes may be quite different, but a common property is that the layer on the Si is conductive albeit with a very high resistivity. Therefore, these diodes will be referred here as metal/non-insulator/semiconductor (MnIS) diodes. The bipolar capabilities of experimental MoO_x based MnIS diodes are examined here, among others, by comparing electrical and optical characteristics to that of implanted p⁺/n reference diodes realized on the same wafer. This includes

measurement of proof-of-concept surface barrier transistors [54]. In addition, using TCAD simulations and numerical calculations, it is examined whether or not such MnIS diodes can effectively be modeled as high-barrier Schottky diodes.

4.2 High-barrier Schottky contacts

The high- ϕ_b contact, also referred to as a bipolar-mode Schottky contact [143], can have a significant minority carrier current to total current ratio, γ , in the whole forward voltage range (refer to chapter 3) and therefore may enable applications that cannot be served by conventional Schottky counterparts [55, 56]. Early reports on the application of such a concept can be traced back to 1953 when Bradley proposed the concept of the surface barrier transistor (SBT) in Ge [54]. The SBT utilizes metal-induced inversion charge to obtain bipolar currents suitable for transistor operation without creating any chemically doped regions.

For an n-type semiconductor, the inversion layer is induced and/or minority carrier effects become important provided that [46, 55]:

$$q\phi_{bn} > E_g - kT \ln \frac{N_v}{N_d}, \quad (4.1)$$

where ϕ_{bn} is the barrier height for electrons, E_g is the semiconductor bandgap, k is the Boltzmann constant, T is the temperature, N_v is valence band effective density of states, N_d is the donor doping density and q is the elementary charge. Eq. (4.1) basically states that the induced inversion charge (hole) density should be higher than the background doping density of the substrate.

Despite the early interest, after the invention of the planar silicon bipolar junction technology, inversion-layer-based device concepts have not attracted much attention. Only recently, due to the strong technological advancement in nanoscale semiconductor devices, alternatives to conventional doping are being sought. In this context, high- ϕ_b MS contacts could be relevant for electrostatic doping (ED) [46, 48]. In ultra-thin body (UTB) devices such 2-D surface inversion could effectively result in volume inversion [178]. Both in bulk and UTB semiconductors, such Schottky contacts could be interesting for realizing dopant-free electrical and optical devices. In previous chapter, minority carrier effects were discussed in an Al/p-Si diode where ϕ_b , ~ 0.78 V, was moderately high [56]. It is therefore worthwhile to investigate in this chapter if an extreme work function property of MoO_x can be exploited to realize high-barrier Si diode with bipolar conduction properties.

4.3 Experimental procedure

The basic device structure is shown in Fig. 4.2 for the ring-shaped test structures used for both diode and sheet resistance measurements [169]¹. For $C - V$ measurements, large square-shaped structures with an area of $A_E = 3.1 \times 10^{-3} \text{ cm}^2$ were used. Large structures suitable for measuring lateral bipolar transistors and light-emission were also included. The substrates were n-type (100) Si wafers with a resistivity of 1-10 ohm-cm covered with a 235 nm thick thermal oxide. Implantations of B^+ annealed in argon at 950°C, were used to form p^+ regions with a junction depth of 0.5 μm and a surface doping of 10^{19} cm^{-3} . Windows were then wet-etched in the oxide to give access to both implanted and non-implanted regions. A resist coating suitable for lift-off was used to pattern a layer stack of Pd/MoO_x deposited in an e-beam physical vapor deposition (EBPVD) system. For the MoO_x, a 99.95 % pure material from Kurt J. Lesker in 3-6 mm large pieces was placed in a Fabmate crucible of 99.95% elemental carbon. MoO_x layer with a thickness of $\sim 7\text{-}8 \text{ nm}$ was grown at an evaporation rate of about 0.05 nm/s. Before deposition, the evaporation chamber was pumped down to the base pressure of about $1.5 \times 10^{-7} \text{ mbar}$. The MoO_x layer was then capped with a Pd layer of about 120 nm thick in the same deposition chamber without breaking the vacuum. A lift-off process was used to remove the Pd/MoO_x layer stack from the Si at places other than oxide windows. As a last step, the backside of the substrate was coated with Al.

The Pd has a relatively low resistivity and this prevents the use of the structures described above to measure the sheet resistance of the inversion layer along the surface of the Si. Therefore, another sample was prepared where the Pd was replaced by a 10 nm thick B (boron) layer. The B is known to be chemically very inert in many situations [172] and is expected to protect the MoO_x from oxidation in air. Moreover, the resistivity of B is so high, $> 500 \Omega\text{-cm}$ [179], that it is not likely to influence the sheet resistance measurement. For the B deposition, a 99.5 % pure material from Kurt J. Lesker in the form of cylindrical ingots was utilized. No thermal annealing was performed on any of the prepared samples. The structure of the fabricated layer stacks was examined using transmission electron microscopy (TEM, Philips CM300ST-FEG).

All measurements were carried out in the dark and on a temperature-controlled chuck. The electrical measurements were performed using a Keithley 4200 semiconductor characterization system with a preamplifier. For the optical spectrum measurements, an Avaspec UV-Vis/NIR spectrometer from Avantes was used. IR micrographs were captured using a cooled InGaAs detector based camera (XEVA-320 from Xenics).

¹The device fabrication part reported in this chapter was performed by D.T. Shivakumar.

Figure 4.2: (a) Schematic cross-sections of the fabricated ring-shaped devices, (a) Pd/MoO_x/n-Si diode, and (b) an implanted p⁺/n-Si diode both with a the ring length $L_i=200\ \mu\text{m}$, width $W_i=64\ \mu\text{m}$ and area $A_E=2\times 10^{-3}\ \text{cm}^2$. The vertical axis of symmetry is at the left hand side indicated by a dashed line.

Figure 4.3: TEM cross-sectional images of the fabricated samples, (a) Pd/MoO_x/n-Si and (b) B/MoO_x/n-Si.

4.4 Material analysis

TEM images of the Pd/MoO_x/n-Si and B/MoO_x/n-Si layer stacks are shown in Fig. 4.3. At the interface with the Si, an amorphous interlayer of about 2 nm in thickness is observed in both cases. Such a layer was also reported in other studies [175] where energy-filtered TEM (EF-TEM) analysis revealed a composition of Si, O and Mo atoms, referred to as a hybrid a-SiO_x(Mo) layer. The accompanying SiO_x(Mo) interlayer, which is possibly formed during the deposition of MoO_x on Si, could have multiple roles in the charge carrier transport in our devices such as passivating the Si surface, hence suppressing the electron current and inducing a hole inversion layer. Further, the sub-stoichiometric nature of the e-beam deposited MoO_x thin films was confirmed by X-ray photoelectron spectroscopy (XPS) analysis (not shown) which indicates $x=2.42\pm 0.24$ that is in close agreement with other reports [162, 175]. The bipolar-mode diode characteristics of the MoO_x based MnIS diodes as studied by electrical and light emission measurements will be treated in the following sections.

Figure 4.4: I – V characteristics of a fabricated Pd/MoO_x/n-Si diode and implanted p⁺/n Si reference diode at room temperature. For comparison TCAD simulation data of Si Schottky diode with an identical geometry modeled using $\phi_b=0.90$ V and $S_n=10^3$ cm/s is shown. Other fitting parameters used for simulations: SRH lifetimes, $\tau_n=10$ μ s, $\tau_p=20$ μ s and $N_D=5 \times 10^{14}$ cm⁻³.

4.5 Diode I – V(–T) characteristics

Typical I – V characteristics of the fabricated Pd/MoO_x/n-Si diodes are shown in Fig. 4.4. The diode displays a high rectification of $\sim 10^8$ at $V_d = \pm 1$ V, a very low leakage current density of about 5 nA/cm² and an ideality factor $n \sim 1.14$. The n value close to unity indicates that charge transport in the diode is mainly governed by processes such as drift-diffusion or thermionic emission. The small non-ideality could be attributed to process related defects or contamination.

Also shown in Fig. 4.4 are the I – V characteristics of an implanted p⁺/n reference diode. The current levels of the two diodes are almost identical. In the latter, the current is diffusion limited and the hole injection is dominant because the Gummel number of the p⁺ region is about 10 to 100 times higher than the substrate Gummel number. Moreover, the hole diffusion current of the two diodes should be the same as both are determined by the same substrate Gummel number. This implies that the hole current is dominant even in the Pd/MoO_x/n-Si diode and the electron current is of the same order or lower. The observed high minority carrier injection ratio (γ) in the Pd/MoO_x/Si diodes indicates the role of the high-barrier and associated hole inversion layer at the MoO_x/Si interface. In addition, the passivating nature of MoO_x based contact on Si [175, 180], possibly originating from the observed SiO_x(Mo) interlayer, with a low surface recombination velocity, could also play a role in suppressing the TE further as confirmed by TCAD simulations.

TCAD simulation of the Pd/MoO_x/n-Si diode as a Si Schottky diode shows good agreement with the experimental results as indicated in Fig.

Figure 4.5: (a) Temperature dependent I – V characteristics of the fabricated Pd/MoO_x/n-Si diode and their comparison with those of the simulated Si Schottky diode. (b) Arrhenius plot of the experimental device at $V_d = 0.2 \text{ V}$ forward bias to estimate the activation energy E_a .

4.4 and Fig. 4.5(a). For this purpose, the Schottky electrode and its interface to Si was modeled using the lower limit of the barrier height, $\phi_b = 0.90 \text{ V}$ as extracted from the C – V analysis (section 4.7), and an effective surface recombination velocity for electrons, $S_n = 10^3 \text{ cm/s}$. Such relatively low value of S_n is typical for passivated SiO_x/Si interfaces [181] and is incorporated in our simulations to mimic more complex MoO_x/Si junctions [182]. For a given value of ϕ_b and S_n , I_h determines the I – V characteristics as also observed experimentally, while I_e appears to be one order of magnitude lower than I_h . The I_h is mainly determined by the substrate Gummel number while ϕ_b and S_n affect only I_e . It is possible to model the hole dominated experimental I – V characteristics by other suitable combinations of ϕ_b ($> 0.90 \text{ V}$) and S_n such that I_e falls sufficiently below I_h . Nevertheless, the simulations confirmed the important role of a sufficiently high ϕ_b and well passivated MoO_x/Si interface in the observed I – V characteristics of Pd/MoO_x/n-Si diodes.

As shown in Fig. 4.5(a), temperature dependent I – V measurements were also performed in order to analyze the dominant charge transport mechanism and to extract the activation energy, E_a . In the case of thermionic-emission dominated transport ($I \propto \exp(-q\phi_b/kT)$), as in conventional Schottky diodes, the E_a obtained from Arrhenius plots would give the effective ϕ_b at the MS junction. As opposed to this, in case of diffusion-dominated transport ($I \propto \exp(-E_g/kT)$), an E_a corresponding to the semiconductor bandgap, E_g , is expected. The Arrhenius plot in Fig. 4.5(b) for the Pd/MoO_x/n-Si diode at forward bias ($V_d = 0.2 \text{ V}$) displays an E_a corresponding to the Si E_g . Similar results were obtained for the implanted p^+ /n Si diode. This confirms that hole injection is indeed dominant in our Pd/MoO_x/n-Si diodes at forward bias. These results also underline that it is not possible to determine the actual value of ϕ_b using I – V – T measurements in such high-barrier diodes where diffusion dominates the current rather than TE.

Figure 4.6: Reverse bias $I - V$ characteristics of a fabricated Pd/MoO_x/n-Si diode at room temperature compared to the implanted p⁺/n-Si reference diode.

Furthermore, as shown in Fig. 4.6, the reverse $I - V$ characteristics of the Pd/MoO_x/n-Si diode were also found to be similar to that of implanted p⁺/n-Si diodes with identical breakdown voltages, $V_{br} = -57$ V. This strongly indicates the presence of a hole inversion layer in the Pd/MoO_x/n-Si diode that prevents the expansion of the depletion layer into the MoO_x layer. Moreover, the breakdown characteristics are independent of the MoO_x layer thickness when increased from 5 nm to 33 nm, which further suggests that the depletion width is solely determined by the substrate doping. By calculating the depletion width at breakdown, the charge displaced in the substrate was estimated to be about $8.6 \times 10^{11} \text{ cm}^{-2}$ which is equivalent to the corresponding charge in the p-type region. This value represents a lower limit of the hole concentration in the inversion layer at the MoO_x/n-Si interface.

4.6 Sheet resistance measurements

By using the MoO_x samples prepared with the high-resistivity B capping layer, it was possible to measure the sheet resistance along Si surface under the deposited MoO_x. Following the same methodology as outlined before [169], R_{sh} values in the range of 60-100 kΩ/□ were extracted (refer to appendix D). This is much lower than the sheet resistance of the thin B layer that is at least 1 MΩ/□ and therefore does not contribute in any significant way. Using simulations to translate the R_{sh} into a value for the hole concentration in the inversion layer is not directly possible because the effective mobility at the MoO_x/Si interface is difficult to predict. Nevertheless, the measured R_{sh} does not conflict with the lower limit of $8.6 \times 10^{11} \text{ cm}^{-2}$ found in the previous section.

Figure 4.7: (a) Reverse bias $C - V$ characteristics of the fabricated Pd/MoO_x/n-Si and implanted p⁺/n-Si diodes at room temperature, (b) $(1/C)^2$ as a function of applied voltage indicating the estimated built-in potential, V_{bi} for the Pd/MoO_x/n-Si diode extracted by linear-fitting.

4.7 C – V measurements

In addition to temperature dependent $I - V$ measurements, $C - V$ characteristics measured with reverse biasing are commonly used to extract the ϕ_b of Schottky diodes. The measured $C - V$ profile for a Pd/MoO_x/n-Si diode are shown in Fig. 4.7(a) along with those of the implanted p⁺/n-Si diode. Notably, the two diodes show similar expansion of the depletion region with increasing reverse voltage, with only a small difference that could be attributed to differences in the p to n transition profile of the implanted and MoO_x/n-Si junctions.

Following a conventional approach [1], the built-in potential (V_{bi}) and in turn ϕ_b of the diode can be estimated from the offset voltage, V_{os} , of the $C^{-2} - V$ plot. From the measurements shown in Fig. 4.7(b), V_{bi} of about 0.64 V was extracted for our Pd/MoO_x/n-Si diode with a resulting barrier height ($\phi_{MoOx/Si}$) of about 0.90 V at the MoO_x/n-Si interface. However, this formulation is only valid when there is only depletion charge near an MS interface. Here, the extracted ϕ_b indicates that the interface may be inverted as predicted by Eq. (4.1) which sets the strong inversion condition at $\phi_b > 0.85$ V when $N_d = 10^{15}$ cm⁻³.

When an inversion layer is present, another formulation should be adopted based on the solution of Poisson's equation with the inclusion of the inversion charge [136, 183]. Schwarz and Walsh [136] have previously shown that for a sufficiently high barrier, the measured capacitance is no longer sensitive to the barrier height and is largely determined by the resistivity of the substrate. The inversion charge basically "screens" the depletion charge. Gummel and Scharfetter [184] also reached a similar conclusion for an abrupt (single-sided) p⁺/n junction where the V_{os} was found to be nearly independent of N_a for large N_a/N_d ratios. Therefore, in the presence of inversion charge in a Schottky junction or even in case of a

Figure 4.8: The extracted ϕ_b as a function of the actual ϕ_b , obtained from a numerical solution of Poisson's equation in the presence of a hole inversion layer and compared with TCAD simulations. The black dashed line indicates the position of our experimentally extracted $\phi_{\text{MoOx/Si}}$ value.

single sided p^+/n junction, the V_{os} from the $C^{-2}-V$ plot can no longer be used to accurately determine the V_{bi} or ϕ_b of the junction.

In order to investigate the influence of inversion charge on the extracted V_{bi} for our device, the methodology as outlined in [136] was adapted and the solution of Poisson's equation in presence of a hole inversion layer was re-visited (refer to appendix B), for a more generalized case where $N_c \neq N_v$. From a numerical solution, $C^{-2} - V$ plots were first calculated for various ϕ_b in the reverse bias range of 0 - 1 V. The V_{os} extracted from linear fitting was then used to determine ϕ_b .

Fig. 4.8 shows the extracted ϕ_b using this numerical approach as a function of the actual ϕ_b . The extracted ϕ_b tends to saturate beyond a certain value (~ 0.90 V) where the influence of inversion charge starts to become important. The numerical solution is also in good agreement with TCAD simulations [98]. In a more strict sense, which is practically masked by the experimental and computational inaccuracies, the $C^{-2} - V$ plot in the presence of inversion charge becomes non-linear and V_{os} is then a function of the applied voltage [136, 184]. Therefore, it can be concluded that for a sufficiently high barrier, the actual ϕ_b cannot be obtained using the $C - V$ analysis. In such a scenario, V_{os} at reverse voltages close to zero, could only give an estimate of the lower limit of ϕ_b [184].

Hence, our experimentally calculated $\phi_{\text{MoOx/Si}}$ value of 0.90 V may not correspond to the actual ϕ_b but is an indicator of the lower limit. For $\phi_b = 0.90$ V, a peak hole concentration at the interface was estimated to be about $5 \times 10^{15} \text{ cm}^{-3}$ as given by $p_0 = N_v \exp(-(E_g - \phi_b)/kT)$ which leads to an effective sheet carrier density, $p_{sh} \sim 10^{10} \text{ cm}^{-2}$. The obtained value of p_{sh} here is, however, about two orders of magnitude lower than the one estimated from reverse breakdown characteristics which further indicates that the actual ϕ_b at the $\text{MoO}_x/n\text{-Si}$ interface is indeed higher than 0.90 V.

Figure 4.9: Reverse bias $C - V$ characteristics of a fabricated Pd/MoO_x/n-Si diode, (a) at various frequencies, and (b) for various MoO_x layer thicknesses at fixed frequency of 1 MHz.

In addition, $C - V$ measurements at multiple frequencies were performed as shown in the Fig. 4.9(a). The capacitance remains practically constant for varying frequencies which rules out the possibility of any trapped charge in the MoO_x layer influencing the $C - V$ measurements. Furthermore, the $C - V$ measurements in Fig. 4.9(b) of our samples, show no systematic change in the capacitance for various MoO_x thicknesses. This suggests that the depletion is occurring mainly in the Si, and that the MoO_x layer is behaving more like a metal or degenerate semiconductor with some finite series resistance as was reported earlier [123, 126]. A similar conclusion was drawn before [169], where the diode $I - V$ characteristics hardly changed with the MoO_x layer thickness except at high forward voltages where the series resistance through the MoO_x layer attenuated the current. These experimental observations indicate that only the MoO_x/Si interface is determining the device characteristics and the bulk MoO_x layer is providing the contact to the metal capping layer.

4.8 Light-emission measurements

Forward-bias light emission in Schottky diodes occurs as a result of radiative recombination of injected minority carriers with background majority carriers. The minority current therefore determines the radiative recombination rate in the device. In conventional Schottky diodes, the minority current gets suppressed before it reaches values high enough for any measurable light output due to its poor supply from the contact or series resistance. Therefore Schottky diodes are generally disregarded for light emitting applications. However, a high-barrier diode with an induced inversion layer can sustain a high minority current that, as observed in the previous sections, can become comparable to that of doped junction counterparts.

Light-emission measurements on our fabricated diodes were performed. The Pd/MoO_x/n-Si diodes show clear electroluminescence (EL) during

Figure 4.10: (a) Bright field EL IR micrograph of the fabricated Pd/MoO_x/n-Si diode at a constant forward current drive of 100 mA ($J=165$ A/cm²), (b) Optical spectrum of the emitted light from the same diode at various forward current levels.

forward bias operation as is evident from the IR micrograph in Fig. 4.10(a). The IR emission is centered around the wavelength corresponding to the Si bandgap, *i.e.* 1.12 μ m as shown in Fig. 4.10(b). As expected, the emitted EL intensity increases with the injected current level. The observed full-width-half-maximum (FWHM) in excess of ~ 1.8 kT (Ref. [157]) is attributed to the indirect bandgap in Si where involvement of phonons in the radiative recombination process leads to the EL-broadening.

Moreover, the maximum injected current density ($J=165$ A/cm²) here falls in the low injection regime ($J \ll qNv_{\text{sat}}=1.6 \times 10^3$ A/cm² where N is the active doping concentration and v_{sat} is the saturation velocity). Compared to the p^+ /n reference diodes, the light emission in the Pd/MoO_x/n-Si diode is about the same, being about 1.5 times less bright. Some discrepancy in the observed brightness between the two diodes could be related to a possible difference in their extraction efficiencies caused by their different junction depths, since the $p \cdot n$ product and thus the light emission is highest at the junction. The junction depth in case of the implanted p^+ /n diode is about 0.5 μ m below the surface and would therefore experience relatively low optical losses at the top electrode compared to the Pd/MoO_x/n-Si diode, where light is emitted very close to the electrode. Nevertheless, such a high-barrier Si diode which shows EL comparable to that of the implanted p^+ /n-Si diode could potentially be utilized to realize low-intensity Si based light emitters for applications such as on-chip communication [159].

4.9 Surface barrier transistor (SBT) measurements

A lateral bipolar transistor, referred to as a surface barrier transistor (SBT) [54], was realized using the high-barrier MoO_x contacts. Fig. 4.11(a) shows a schematic cross section of the experimental device where two closely spaced top contact electrodes were utilized as emitter (E) and collector (C), while the metalized substrate back surface served as the base contact (B).

Figure 4.11: (a) Schematic cross-section of the experimental and TCAD simulated device used for bipolar transistor measurements with an inner circle of diameter $d=100\ \mu\text{m}$ as the emitter (E) electrode and outer ring with width $W=50\ \mu\text{m}$ as the collector (C) electrode for two different spacings L_{CE} of $1\ \mu\text{m}$ and $2\ \mu\text{m}$, respectively. (b) $I-V$ characteristics of back-to-back diodes measured between the top emitter and collector electrodes. Inset: Schematic top view of the device used for bipolar transistor measurements.

First the two-terminal back-to-back diode characteristics between the collector and emitter electrode was checked as shown in Fig. 4.11(b). The observed low leakage current between the two electrodes rules out the possibility of any unwanted surface conduction path between the emitter and collector.

The bipolar transistor measurements were performed on devices with two different spacings (L_{CE}) between the emitter and collector electrodes i.e. $L_{CE} = 1\ \mu\text{m}$ and $L_{CE} = 2\ \mu\text{m}$. Fig. 4.12(a) shows the Gummel plot for the device with $L_{CE} = 1\ \mu\text{m}$ where a significant collector current (I_C) comparable to the base current level, I_B , is obtained at $V_{CB} = 0\ \text{V}$. The measured $I_C \sim I_B$ confirms that the improved emitter efficiency of the EB junction as compared to that of conventional Schottky counterparts. The control of the EB junction over the I_C as expected in the bipolar transistor is also clearly visible in the output (I_C - V_{CE}) characteristics of the same device as shown in Fig. 4.12(b).

The I_C further increases while I_B remains unchanged when the reverse bias at the CB junction was raised to $-1\ \text{V}$ which results in the current gain, $\beta = I_C/I_B > 1$. The increased I_C and its non-ideal ($n > 1$) behavior for $V_{CB} = -1\ \text{V}$ is attributed to the widening of the depletion width at the CB junction which eventually results in the punch-through effect, i.e. the depletion regions formed at the EB and CB Schottky junctions gradually start to merge in the gap region between the collector and emitter electrodes. The punch-through effect is also visible in the output characteristics where a low output resistance can be seen. However, for the specified spacing L_{CE} and barrier height (ϕ_b), the punch-through effect is not enough to fully eliminate the potential barrier for holes as there is control of I_B over I_C as expected for the bipolar transistor.

The β becomes less than 1 and the observed punch-through effect is practically reduced when the L_{CE} is increased to $2\ \mu\text{m}$ as can be seen in the

Figure 4.12: Bipolar transistor measurements of the fabricated device. Gummel plot (left) and output characteristics (right) for (a) and (b) $L_{CE}=1\text{ }\mu\text{m}$, (c) and (d) $L_{CE}=2\text{ }\mu\text{m}$. Blue solid line: ideality factor $n=1$ for reference.

Gummel plot in Fig. 4.12(c) and the output characteristics in Fig. 4.12(d).

To further illustrate the working of the SBT, TCAD simulations on the same geometry as shown in Fig. 4.11(a) were performed. The top CE electrodes were modeled as Schottky contacts with the identical ϕ_b and a fixed (default) [98] surface recombination velocity ($S_n = 2.5 \times 10^6\text{ cm/s}$). The base electrode was assumed to be an ohmic (neutral) contact. The ϕ_b of the top electrodes was then systematically varied. The hole inversion charge density below the collector and emitter electrodes increases with ϕ_b as can be observed from the relative position of the Fermi level from the valence band in the energy band diagram in Fig. 4.13(a). Fig. 4.13(a) also shows that the substrate depletion or punch-through effect in the CE gap region increases with ϕ_b at the electrodes. However, for ϕ_b beyond which the inversion layer effect becomes important, as shown in Fig. 4.8, the effective barrier for holes and depletion width does not change anymore with ϕ_b . Further, the punch-through effect even at maximum depletion width is not severe and therefore will not affect the bipolar operation, since the barrier to the hole injection is still sufficiently high as required for the base-controlled collector current. Fig. 4.13(b) re-iterates this point by illustrating the operation of the SBT where the minority (hole) injection into the reverse biased CB junction can be increased by applying a small forward bias at the EB junction which lowers the barrier there.

Figure 4.13: Simulated energy band diagram for the bipolar device shown in Fig. 4.11(a), with $L_{CE} = 1 \mu\text{m}$ in the lateral direction 20 nm below the top electrodes; (a) at thermal equilibrium for 3 different ϕ_b : 0.58 V, 0.78 V and 0.98 V, and (b) for $\phi_b = 0.98 \text{ V}$ at $V_{EB} = 0.5 \text{ V}$ and $V_{CB} = 0 \text{ V}$.

Figure 4.14: Simulated Gummel plots for varying ϕ_b at the CE electrodes with $L_{CE} = 1 \mu\text{m}$, shown for $\phi_b = 0.58 \text{ V}$, $\phi_b = 0.78 \text{ V}$ and $\phi_b = 0.98 \text{ V}$.

The simulated Gummel plots in Fig. 4.14 further elucidate the role of ϕ_b in determining the emitter efficiency of the contacts. The I_B (shown in red) is determined by the TE of majority carriers (electrons) and therefore decreases exponentially with ϕ_b at the emitter electrode. The I_C on the other hand, for a sufficiently high ϕ_b , is determined by the minority carrier (hole) injection at the EB junction which is governed by the Gummel number of the base region. Therefore I_C remains practically unaffected with varying ϕ_b as shown in Fig. 4.14 for $\phi_b = 0.78 \text{ V}$ and $\phi_b = 0.98 \text{ V}$ except at high forward biases where the series resistance becomes important. The relatively small discrepancy in the I_C in the exponential region is attributed to the substrate depletion effect where the effective Gummel number of the base decreases with ϕ_b as also illustrated in Fig. 4.13(a). For low $\phi_b = 0.58 \text{ V}$, I_C is determined by the reverse bias current of the CB junction as it is higher than the corresponding hole injection level of the forward biased EB junction. The β increased to 15 when ϕ_b was further raised to an order of Si bandgap *i.e.* 1.12 V. In general, the improved emitter efficiency, and therefore higher β , with increasing ϕ_b for the SBT device is a result of the

Figure 4.15: (a) Schematic cross-section of the proposed SOI based lateral pnp bipolar transistor [62]. (b) TCAD simulated Gummel plot of the same device. The device dimensions used: $L_E = 10 \mu\text{m}$, $L_B = 0.1 \mu\text{m}$, $L_C = 0.4 \mu\text{m}$ and $L_{EB} = L_{BC} = 0.1 \mu\text{m}$. $\Phi_{mE} = \Phi_{mC} = 5.59 \text{ eV}$ and $\Phi_{mB} = 4.05 \text{ eV}$. Mobility: $\mu_e = 1417 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$, $\mu_h = 470 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ [98] and SOI layer doping: n-type, 10^{13} cm^{-3} .

efficient suppression of I_B . Further, the high ϕ_b and resulting inversion layer ensures an efficient supply of minority carriers for sustaining the I_C till high forward biases and also lowers down the series resistance.

However, it is clear that the chosen device geometry, though interesting for the simple proof-of-concept understanding of the SBT, should be optimized. Alternative device architectures based on UTB SOI, such as the one previously reported by Kumar and Nadda [62] using TCAD simulations, will have more advantages.

To further highlight the potential of such high- ϕ_b contacts in UTB SOI, TCAD simulations were performed to show the working of a scaled-down version of the experimentally realized MoO_x based lateral pnp transistor in SOI. A schematic cross-section of the proposed device architecture is shown in Fig. 4.15(a). Here, the experimentally reported interface work function (ϕ_m) of about 5.59 eV [185] was adopted for the MoO_x based contact (on oxide) for the p-type emitter and collector regions with an induced hole concentration of about 10^{18} cm^{-3} . For the n-type base region, an electrode with ϕ_m of about 4.05 eV was utilized which results in an induced electron concentration of $4 \times 10^{19} \text{ cm}^{-3}$. A relatively low surface recombination velocity for holes (S_p) of $5 \times 10^4 \text{ cm/s}$ was used for the base contact. Note that n-type poly-Si for instance could offer such values for ϕ_m and S_p [186]. The proposed device shows bipolar characteristics with a β of about 400, see Fig. 4.15(b). This result indicates that MoO_x based contacts can potentially replace implanted p^+ regions in the UTB semiconductor for bipolar transistor applications where conventional doping is otherwise challenging. Moreover, such contacts could also be utilized for p-type MOS transistors in undoped UTB semiconductors, specifically narrow bandgap materials. For instance, previously Chuang *et al.* adopted MoO_x based contacts to realize p-type MoS₂ transistors [123].

4.10 Discussion

In this investigation, the behavior of the Pd/MoO_x/n-Si MnIS diodes, with respect to diode $I - V$, $C - V$ and bipolar transistor characteristics, was found to be practically identical to that of the deep-implanted p^+ / n junctions. This is a result of the high minority carrier injection ratio (γ) of both types of diodes with a low hole diffusion current and an electron current that is even lower. The presence of a significant inversion layer was confirmed and can to some degree explain low electron injection into the p-type region. In the research on PureB MnIS diodes fabricated at B deposition temperatures below 400°C, and on the same type of substrates as used in the present study, the inversion layer sheet resistance was lower, $\sim 35 \text{ k}\Omega/\square$, and uniform over the wafer when optimal conditions were applied [187]. Both experiments and simulations supported the conjecture that a layer of fixed negative charge at the interface is responsible for the inversion layer in this case.

For the MoO_x diodes, there can be several reasons why they display such low electron current levels. First, the MoO_x is a high work function material, and the simulations performed here substantiate that for barrier heights higher than about 0.9 eV, a significant inversion layer will be formed. Second, the passivating nature of MoO_x based contact on Si [175, 180], possibly originating from the observed SiO_x(Mo) interlayer that may be partly insulating and is represented by a low surface recombination velocity, could also play a role in suppressing the electron injection even further. Thirdly, a significant amount of negative fixed charge may also be present in the deposited layer. Unlike thermally grown SiO₂ layers that most often contain positive fixed charge near the Si interface, it has been shown before [188] that negative fixed charge may appear in plasma-oxidized Si surfaces. The surplus of oxygen in such layers was proposed to accumulate the negative charge. Similar mechanism may also hold true for the SiO_x interlayer which formed during the MoO_x deposition process.

The partial SiO_x character of the interfacial layer may also be the important feature providing a well-passivated Si surface. A similar mechanism has been developed and well-documented for Al₂O₃ layers that have become popular as passivation layers on n-type c-Si solar cells [189]. As opposed to the Al₂O₃, the MoO_x layers are not insulating and therefore they have generated interest as contact layers. The use of Al₂O₃ for creating an inversion-layer diode requires contacting the negative-charge-induced inversion layer via implanted regions [170].

From electrical analysis on samples with varying MoO_x thicknesses it can be concluded that only the MoO_x/Si interface is playing a dominant role in the charge carrier transport of our devices and the bulk properties of MoO_x only contributes to the series resistance. In other work [190], the MoO_x layer was shown to limit the current only at lower voltages while at higher voltages the current was limited by the barrier. Therefore, for

the situations where the MoO_x layer is not found to limit the current, the charge transport across the MoO_x/Si interface can be effectively modeled assuming a Schottky electrode with a suitable barrier height and surface recombination velocity [123]. For a more generic treatment of charge transport through a transition metal oxide (TMO) layer, taking into the account the density and the energetic distribution of traps inside its bandgap, the methodology as described by Messmer *et al.* [182] should be considered.

The bipolar nature of the MoO_x based diode was clearly established from the measured electrical and optical characteristics. Such MoO_x-based inversion type contacts could also be considered as a possible replacement of doped p⁺ regions for applications where doping is challenging or low temperature processing is required. MoO_x-based contacts could offer a novel dopant-free route for realizing (opto-) electronic devices such as field effect transistors (FETs) [123], bipolar transistors, light emitters, photodetectors [191] or even as Schottky gate contacts [192]. Moreover, for creating an n-type inversion region, a lower work function material such as lithium fluoride (LiF_x) [163] which has been recently reported as an "electron selective contact" should be further explored. In this way, both p-type and n-type regions can be locally created inside a semiconductor body without using any dopants. However, creating a p-type region is more difficult in case of wide bandgap materials such as GaN where even the highest reported vacuum work function of MoO_x i.e. ~ 6.6 eV, is not sufficiently high to reach its valence band.

For many of these potential device applications, the high resistivity of the MoO_x [169, 174] could be a concern. The contact resistivity, ρ_c , of the Pd/MoO_x/p-Si stack, with a ~7 nm thick MoO_x layer, is measured to be around 1.2 mΩ-cm² [169], while this could be an order of magnitude higher on the n-Si interface [174]. In addition to the high ρ_c , the key properties of MoO_x, such as the work function and conductivity, are unstable upon exposure to ambient and high temperatures [193–196]. These concerns need to be addressed before practical applications become feasible.

With the present quality of MoO_x layers, it is important to cap them in-situ with a suitable metal to prevent exposure to air which otherwise may degrade the work function. The choice of the top electrode metal is also important for efficient carrier transport [182] and for a low contact resistivity. In our work, Pd was used for its reported high work function and relative inert nature at room temperature [123]. A few experiments with Au capping layers were also performed and the results were comparable to those with Pd. Reactive metals such as Al are less preferred for capping MoO_x as they may reduce the functional MoO_x layer by forming oxides, thereby creating more oxygen vacancies in the film, and consequently lowering the effective work function [196, 197].

4.11 Conclusion

In this work, MnIS diodes on n-type Si using MoO_x-based contacts were realized. The electrical and light-emitting diode characteristics bore strong functional resemblance to implanted p⁺n-Si diodes rather than to conventional Schottky diodes. The presence of a high potential barrier (>0.90 V) and an hole inversion layer at the MoO_x/n-Si interface was verified with sheet carrier density greater than $\sim 8.6 \times 10^{11} \text{ cm}^{-2}$. The bipolar-mode diode behavior of the MoO_x-based MnIS diodes was further underlined by demonstrating a proof-of-concept Si surface barrier bipolar transistor without any impurity doping of the Si surface.

Theoretically, an inversion layer and efficient suppression of electron injection also appears in very high-barrier Schottky diodes. Simulations that approached the MoO_x/n-Si structure as being a high-barrier Schottky diode could reproduce the experimental findings provided that the surface recombination velocity was set at a relatively low value of 10^3 cm/s . This suggests that the surface was passivated which was supported by the presence of SiO_x(Mo) interlayer.

The very high resistivity of the bulk MoO_x material has not deterred possibly attractive implementations for use as solar cell emitter. In contrast, for nanoscale device applications, the associated series resistance could form a serious bottleneck. Therefore, for such applications, thin layers comprising essentially only the interfacial (tunneling) layer should be investigated. Efforts to significantly improve the reproducibility and robustness of the material would also be necessary. If successful, such an MnIS dopant-free hetero-contact processed at a low temperature would be very interesting for fabricating bipolar devices (BJTs, SBTs and LEDs) in Si and other material systems, as well as UTB devices where actual doping is otherwise challenging.

ELECTRON-HOLE BILAYER LED

Abstract

In this chapter, a novel switched-mode light-emitting device (LED) based on the electrostatically-induced electron-hole bilayer (EHB) concept has been proposed and investigated using TCAD simulations. The proposed ultra-thin-body (UTB) device works on the principle of formation of EHB channels by applying suitable gate biases during the charging-cycle, and their recombination during a discharging-cycle. TCAD simulations show that continuous switching of the gates in an indium arsenide (InAs) based EHB LED with a $\sim 12 \mu\text{s}$ time period leads to radiative recombination of the induced charge carriers with a peak internal quantum efficiency (IQE) as high as $\sim 92\%$ and a time-averaged IQE of $\sim 29\%$. The proposed concept obviates the need for chemically doped p-n junctions in the UTB device for light-emitting applications. However, when relying on the thermal generation alone as a source of charge carriers in a small undoped semiconductor volume, a narrow bandgap semiconductor (such as InAs) is required for the proposed LED which ultimately limits the switching speed. For wider bandgap materials, highly doped regions on either side of the intrinsic UTB layer in the form of a lateral PIN structure could be employed where switching speed is then not limited by thermal generation. TCAD simulations of a silicon (Si) EHB LED based on such a gated PIN structure shows switching capability in the GHz frequency range making it attractive for SOI based optocoupling applications.

This chapter is based on the publication in Solid-State Electronics [57] and EUROSIOI-ULIS conference, 2019 [82]. The work was partly pursued as an undergraduate thesis project, undertaken by F. Mema under the author's supervision.

5.1 Introduction

Light-emitting devices based on ultra-thin-body (UTB) semiconductor-on-insulator technology are interesting candidates for inter-chip and intra-chip optical interconnect [198, 199] as well as for sensing applications [200]. In addition to their attractiveness for integration with SOI technology, the UTB based light sources also benefit from their improved efficiency due to quantum confinement, and weak reabsorption of emitted photons inside their ultra-thin active region [201]. To realize such devices, a sharp junction in the UTB semiconductor is one essential requirement which is technologically challenging [2] in conventional chemical doping approaches. In this direction, electrostatic doping (ED) ([46] and references therein) has been widely explored as a potential alternative to chemical doping for UTB devices in Si and emerging semiconductors. Particularly, the electrostatically induced electron-hole bilayer (EHB) [79] is an interesting concept where charge carriers of opposite polarity are simultaneously induced in a dual gate UTB device. Such a concept has been extensively investigated for tunnel field effect transistors (TFETs) applications in various material systems and geometries [79, 202, 203]. A similar concept has also been reported for capacitor-less DRAM memory [204]. However, so far the EHB concept has not been reported for light emission via electroluminescence. In this work [57, 82], a novel light-emitting device (LED) based on the EHB concept in an undoped UTB channel is proposed.

5.2 Theory and device operation

The schematic cross-section of the proposed device is shown in Fig. 5.1. The proposed device is a dual gate structure with an UTB semiconductor as a channel material. It comprises two different (low-high) work function metals as top and bottom gate electrodes which are oppositely biased during the device operation. In the simulations the semiconductor body is kept floating. In practice the body can be grounded further away from the active gated device region via a side body contact as discussed in Section 5.4.

In the dual gate structure as shown in Fig. 5.1 with different top and bottom gate work functions and opposite biasing, electron and hole channels can be simultaneously induced [79]. To describe the work function and bias-induced charge carriers near each gate in such a fully-depleted UTB channel, the following equations (Eqs. (5.1)-(5.2)) for the vertical electric field (E_s) and surface potential ($\psi_{sT,B}$) at both gate interfaces were derived before [46, 107] (refer to appendix A) assuming negligible charge carrier concentration:

$$E_s = \frac{(V_{GT} - V_{GB}) - (\phi_{mT} - \phi_{mB})}{\frac{\epsilon_s}{\epsilon_{ox}}(t_{oxT} + t_{oxB}) + t_s}, \quad (5.1)$$

Figure 5.1: Schematic cross-section of the proposed electron-hole bilayer InAs LED.

$$\psi_{sT,B} = V_{GT,B} \mp \frac{\epsilon_s E_s}{C_{oxT,B}} - \Delta\phi_{mT,B}, \quad (5.2)$$

where the subscripts T and B refer to the top and bottom gate, respectively. $V_{GT,B}$ is the gate voltage, $\phi_{mT,B}$ is the gate metal work function, $\Delta\phi_{mT,B}$ is gate-body work function difference, $C_{oxT,B}$ is the areal oxide capacitance, t_{ox} and t_s are the oxide and semiconductor thickness, respectively, and ϵ_{ox} and ϵ_s are the oxide and semiconductor dielectric constant, respectively.

Eq. (5.1) expresses the field for the EHB formation in the coupled dual gate system. E_s also determines the field in the gate oxides, and as a result the maximum bias settings in the EHB device can be determined from this equation. Semi-classically, electrons will be induced near the top gate electrode if $\psi_{sT} > 0$ with a density at the interface $n = n_i \exp(\psi_{sT}/u_T)$ where n_i is the intrinsic concentration and u_T is the thermal voltage ($=kT/q$, where k is Boltzmann's constant, T is the temperature and q is the elementary charge). Similarly, if $\psi_{sB} < 0$ holes will be induced near the bottom gate electrode with a density at the interface $p = n_i \exp(-\psi_{sB}/u_T)$. However, since the influence of the mobile charge was neglected for the derivation of Eqs. (5.1)-(5.2), these are therefore not valid for a strong inversion situation. Moreover, quantum effects can modify the carrier densities and their distribution [108]. Further, the effect of interface trap charges can be accounted for as described in [46].

In the proposed EHB structure, which is similar to a parallel plate capacitor, the induced charge carriers remain fixed near their respective gate interfaces in steady state and do not recombine. However, the EHB device becomes electrically active as soon as (one or) both gates are switched between their charged- and discharged-state. During the discharging-cycle, the electron and hole distribution will gradually decay with time via recombination processes. Carrier recombination in a direct bandgap material has

a high chance to be radiative. The result will be then light emission during a switching transient. Steady light output could therefore be obtained by continuously switching the gates.

InAs is an interesting material in this context because of its narrow and direct bandgap ($E_g=0.354$ eV at 300 K) which first makes it more suitable for ED [46]. Second, the small E_g also results in a higher thermal generation rate of charge carriers which along with Shockley-Read-Hall (SRH) lifetime (τ_{SRH}) determines the switching speed in the proposed device. A simplified expression for time t_{th} required to thermally generate n_0 level of carriers from its intrinsic concentration n_i can be derived from the continuity equations as (see appendix C):

$$t_{th} = \frac{n_0}{\frac{n_i}{2 \cdot \tau_{SRH}} + B_{rad} \cdot n_i^2} \quad (5.3)$$

where B_{rad} is the radiative recombination coefficient.

Fig. 5.2 shows t_{th} against E_g , required to thermally generate $n_0=10^{18}$ cm^{-3} carriers for various direct bandgap semiconductors and Si, calculated using Eq. (5.3), from their respective intrinsic carrier level. For narrow bandgap semiconductors such as InAs ($\tau_{SRH} \sim 1$ ns [205]), t_{th} is in a few μs range while for a wide bandgap material such as GaN, it is in order of 10^{17} s, indicating that the proposed device concept will only work for the former case.

Previously, both an electron [206] and a hole [207] inversion layer was observed in InAs MOS capacitors even at frequencies as high as 1 MHz suggesting a t_{th} in the μs range, which agrees well with Eq. (5.3). Further, an UTB InAs-on-insulator (XOI) technology suitable for realizing the proposed device has been experimentally demonstrated [208, 209].

Figure 5.2: Calculated carrier thermal generation time using Eq. (5.3) for various direct bandgap semiconductors (and Si) to reach a carrier concentration of $\sim 10^{18}$ cm^{-3} from their intrinsic level shown for two different τ_{SRH} .

Table 5.1: TCAD simulation parameters for InAs EHB LED at 300 K [98].

Parameter	Value
InAs bandgap, E_g , electron affinity, χ	0.354 eV, 5.06 eV
HfO ₂ bandgap, E_g , electron affinity, χ	5.9 eV, 2.05 eV
Electron effective density of states mass, m_c	0.023 m_0
Hole effective density of states mass, m_v	0.48 m_0
Conduction band effective density of states, N_c	$9.3 \times 10^{16} \text{ cm}^{-3}$
Valence band effective density of states, N_v	$8.4 \times 10^{18} \text{ cm}^{-3}$
Radiative recombination coefficient, B_{rad}	$1.1 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$
SRH lifetime, τ_{SRH}	1 ns
Auger recombination coefficient	$10^{-30} \text{ cm}^6 / \text{s}$
Dielectric constant, ϵ_s , ϵ_{ox}	14 ϵ_0 , 22 ϵ_0
Thickness, t_s , t_{ox}	25 nm, 4 nm
Gate work function, ϕ_{mT} , ϕ_{mB}	4.9 eV, 5.4 eV

5.3 Simulation parameters and models

The proposed device (Fig. 5.1) was investigated via 2-D TCAD simulations with cylindrical symmetry around y -axis using Sentaurus [98], applying Fermi-Dirac statistics with doping [210] and field dependent mobility models [211]. For recombination, standard SRH, Auger and radiative models [98] were included without taking into account any surface recombination at semiconductor-oxide interfaces. Also, the density gradient model [109, 212] was used to account for quantum confinement effects. A low/high work function ($\phi_{\text{mT}} = 4.9 \text{ eV}$, $\phi_{\text{mB}} = 5.4 \text{ eV}$) was used for the top/bottom gate for inducing electrons/holes. The chosen gate metal work functions are reasonably symmetric with respect to the mid-gap work function ($\phi_{\text{midgap}} = 5.18 \text{ eV}$) of intrinsic InAs. The InAs body thickness (t_s) of 25 nm was chosen to balance the trade-off between the induced charge carrier concentration and their radiative recombination rate. Moreover the chosen thickness is well-outside the range of supercoupling effect [213, 214], which otherwise becomes dominant at smaller thicknesses and prevent the co-existence of electron and hole channels. Hafnium dioxide (HfO₂) with $t_{\text{oxT/oxB}} = 4 \text{ nm}$ was used for both gate dielectrics which provides a sufficiently high conduction band (ΔE_c) and valence band (ΔE_v) discontinuity as to prevent gate leakage (see Fig. 5.3(a)). Ideal interfaces without any traps or fixed charges were assumed. All simulations were performed at 300 K. Table 5.1 summarizes the parameter values used in this work.

5.4 Device operation: InAs EHB LED

In UTB devices, the electric field inside the semiconductor body is practically constant (see e.g. Fig. 5.3(a)). The electric field inside the InAs body decreases for a larger thickness and increases as the gate biases are raised to higher voltages as shown in Fig. 5.4. The calculated electric field (Eq.

Figure 5.3: TCAD simulations at thermal equilibrium, (a) energy band diagram taken along AA' (see Fig. 5.1). (b) charge carrier profile taken along AA'.

Figure 5.4: Vertical electric field E_s in the InAs layer against the thickness t_s for a different gate bias. The field has been probed at the middle of the InAs body thickness.

(5.1)) for weak inversion condition, i.e. either small body thicknesses or low gate voltages, is in good agreement with the TCAD simulation results. Some deviation between the model and TCAD is observed for strong inversion condition, i.e., when large body thicknesses ($t_s \gtrsim 20$ nm) or high gate voltages ($|V_{GT,B}| \gtrsim 0.25$ V) are used. This can be explained by the influence of the high charge carrier concentration on the electrostatic potential which is not taken into account in Eq. (5.1).

The charge carrier profiles formed by work function induced ED at thermal equilibrium are shown in Fig. 5.3(b). The induced electron layer is relatively thick compared to the hole layer, as also observed experimentally [206], and is attributed to the relatively small electron effective (density of states) mass, m_c , which results in a small conduction band effective density of states, N_c . The carrier concentrations can be further increased by applying a small (~ 0.75 V) positive (negative) bias at the top (bottom) gate as shown in Fig. 5.5(a)-(b). The situation where a high concentration

Figure 5.5: Simulated 2-D cross section of induced charge carriers, (a)-(b) at charged-state ($t=0$ s), (c)-(d) at discharged-state ($t=3$ μs).

($\sim 10^{18}$ cm^{-3}) of both electrons and holes are simultaneously induced at opposite gate interfaces is hereafter referred to as charged-state. Since even at thermal equilibrium an EHB has been formed because of the gate-body work function difference, some opposite biasing ($\sim |\phi_{\text{mT/B}} - \phi_{\text{midgap}}|$) is required to make the body intrinsic. By applying a small (~ 0.25 V) negative (positive) bias at the top (bottom) gate, the body becomes intrinsic ($\sim 10^{15}$ cm^{-3}) as shown in the Fig. 5.5(c)-(d). This situation is hereafter referred to as the discharged-state.

When the EHB is suddenly switched from its charged- to discharged-state, the charge carriers will decay via recombination processes (both radiative and non-radiative) to reach their final steady state value, see Fig. 5.6. The diffusion and recombination of holes can be observed from their transient density profiles in Fig. 5.6 where a spread in their vertical distribution along with a drop in their peak concentration are visible during the discharging-cycle, even when there is still an opposing electric field. However, electrons are mainly recombining and diffusion is less important, possibly because of a smaller slope ($\partial n / \partial y$) of their vertical distribution profile. Fig. 5.7 shows a radiative recombination rate, R_{rad} , (thus light emission) as high as $\sim 10^{24}$ $\text{cm}^{-3}\text{s}^{-1}$ at 0.5 μs after the on-set of discharging-cycle.

By continuously switching the gates, as shown in Fig. 5.8, the charge carriers are first thermally generated to form an EHB during the charging-cycle and later recombine during the discharging-cycle. In this way, steady light output via radiative recombination in the form of short (~ 0.5 μs)

Figure 5.6: Transient electron and hole density (along line AA') at various time instances (t) during the discharging-cycle.

Figure 5.7: (a) 2-D profile of radiative recombination rate at $t_1=0.5 \mu s$ after the on-set of the discharging-cycle. (b) Transient radiative recombination rate (along line AA') at various time instances (t) during the discharging-cycle.

pulses can be maintained. The pulse width here is taken as the time in which the radiative recombination rate falls by about one order in magnitude. In these transient simulations, the voltage pulse was defined as a piecewise linear function with a rise/fall time ($t_{\text{rise/fall}} = 3 \mu s$), an on-time ($t_{\text{on}} = 5 \mu s$) and off time ($t_{\text{off}} = 1 \mu s$). The chosen t_{on} ($5 \mu s$) is sufficiently long for generating charge carriers from their intrinsic value to their high charged-state value.

Moreover, the EHB concentration at the charged-state and consequently R_{rad} can be further increased by applying a bias higher than 0.75 V , but that may degrade the dielectric layer over time. Note that the probed electric field in the HfO_2 layer at the charged-state ($|V_{\text{GT/B}}|=0.75 \text{ V}$) is $\sim 6.5 \times 10^5 \text{ V/cm}$ which is well below its breakdown value [215]. However, the chosen biasing scheme is not the optimized one as it depends on the type of application. Other biasing schemes can also be explored, such as one involving

Figure 5.8: Transient simulations of InAs EHB LED operation showing, (a) the gate voltage switching cycles, (b) the device current, (c) the peak electron density near the top gate interface, (d) the peak hole density near the bottom gate interface, (e) the maximum radiative recombination rate in the device. (charged-state $V_{GT}=0.75$ V and $V_{GB}=-0.75$ V, discharged-state $V_{GT}=-0.25$ V and $V_{GB}=0.25$ V, electrode area, $A_E=7.85 \times 10^{-9}$ cm².)

the continuous switching of electron and hole channel positions between the top and bottom gate interfaces by applying higher positive/negative biases. This scheme will be more suitable for a device where both the top and bottom gate consist of the same metal with $\phi_{mT}=\phi_{mB}-\phi_{midgap}$.

Further, the role of thermal generation in the proposed device can be analyzed from the current vs time ($I-t$) curve shown in Fig. 5.8(b). The switching current here is composed of two parts: the generation/recombination (GR) current and the displacement current. The displacement current is actually a result of the applied voltage switching in the capacitor and is equal to $C \cdot dV/dt$ where dV/dt is constant for the linear voltage ramp and C is the effective capacitance of the dual gate MOS stack which is also constant in the absence of any generation process. The GR current is the measure of carrier generation which in our case is thermal and is affected by parameters such as n_i , τ_{SRH} and B_{rad} . The integral of the GR current over time in the $I-t$ plot (indicated by the red horizontal lines) in Fig. 5.8(b) is equal to the total generated charge in that given time.

In addition, the possible influence of a body side contact on the device operation when placed near the gated region for a ground reference was investigated, and compared that to the previous situation where no such side contact was used. While the device operation remains unaffected,

the peak R_{rad} is however reduced ($\sim$ by one order of magnitude) when a side metal contact with $\phi_m \sim \phi_{\text{midgap}}$ was used. This reduction in R_{rad} is attributed to the carrier leakage via this side contact. The carrier leakage can be suppressed by using a side contact with either a high or low ϕ_m (in reference to ϕ_{midgap}). Moreover in practice, such contact can be placed further away from the gated region of the device which would further minimize the leakage.

5.5 Efficiency estimation

5.5.1 Internal quantum efficiency (IQE)

During the discharging-cycle, both radiative and non-radiative recombination processes such as Auger and SRH occur in the active region of the device. The left vertical-axis in Fig. 5.9 shows the contribution of SRH, radiative and Auger processes to the total recombination across the body thickness. The internal quantum efficiency (IQE) is defined as the ratio of the radiative recombination rate (R_{rad}) to the total recombination rate [216]. The right vertical-axis in Fig. 5.9 shows the variation of IQE across the body thickness at different time instances during the discharging-cycle. As can be seen, a peak IQE as high as $\sim 92\%$ is obtained at $t_1 = 0.5 \mu\text{s}$ which gradually drops to $\sim 60\%$ at $t_2 = 1 \mu\text{s}$ after the on-set of discharging-cycle. The integrated time-averaged IQE over one period across the whole device volume is $\sim 29\%$. Note that both the peak radiative recombination rate and IQE are shifted towards the bottom gate. This is attributed to the asymmetric distribution of electrons and holes, and thus the p-n product (see Fig. 5.6) in the UTB, due to their unequal effective masses.

Figure 5.9: Simulated recombination processes across AA' at $t_1 = 0.5 \mu\text{s}$ after the on-set of discharging-cycle (left vertical-axis). The IQE profile across AA' (right vertical-axis) at $t_1 = 0.5 \mu\text{s}$ and $t_2 = 1 \mu\text{s}$.

5.5.2 Power efficiency

From Fig. 5.8, the power efficiency (η_{power}) of the proposed device, which is the ratio of optical power (energy) output to total electrical power (energy) input, was also estimated. The dynamic energy dissipation during the charging and discharging of a parallel plate capacitor can be expressed as [217]:

$$E_{\text{elec}} = QV = V \int_0^T |I| dt, \quad (5.4)$$

where Q is the total charge generated in one cycle, V is the total voltage swing, I is the current and T is the cycle time. Similarly, the optical energy output during the switching cycle can be expressed as:

$$E_{\text{opt}} = V \int_0^T I_{\text{opt}} dt = qV \int_0^T R_{i-\text{rad}} dt, \quad (5.5)$$

where $R_{i-\text{rad}} = \int \int R_{\text{rad}} dv$ is the integrated radiative recombination rate across the whole device volume.

Therefore,

$$\eta_{\text{power}} = \frac{q \int_0^T R_{i-\text{rad}} dt}{\int_0^T |I| dt} \times 100\%. \quad (5.6)$$

Using Eq. (5.6), the maximum $\eta_{\text{power}} \sim 15\%$ for our device was estimated. For this calculation the light extraction efficiency of our LED was assumed to be 100 % which in practice is difficult to achieve in such a dual gate UTB structure. Measures such as the use of transparent electrodes or electrodes with regular openings should be considered for efficient light extraction.

5.6 Device optimization: Body thickness

The effect of the InAs thickness t_s on the induced charge carrier concentrations and the radiative recombination rate was also checked. As shown in Fig. 5.10(a), the induced electron and hole densities initially increase with the thickness as described by Eqs. (5.1)-(5.2), valid for a fully depleted semiconductor body where the two opposite gate interfaces are electrostatically coupled. The electrostatic coupling gradually reduces for larger thicknesses, and as a result, the carrier concentration at their respective gate interfaces increases. For even larger body thicknesses, the charge carrier concentrations gradually saturate to the value which is mainly determined by the potential of their respective gate only.

Figure 5.10: TCAD simulation for a varying InAs thickness t_s , (a) induced peak electron (n) and hole (p) concentrations at the charged-state condition at their respective gate interfaces, (b) peak radiative recombination rate (R_{rad}) where R_{rad} is noted at $t_1=0.5 \mu\text{s}$ after the on-set of discharging-cycle.

For thicknesses below 10 nm, the sharp drop in carrier density is attributed to a very high electric field and resulting supercoupling effect [213]. Note that in our simulated dual gate structure, which features symmetric gate work functions and equal gate oxide thicknesses, the two gates are of equal strength and consequently the possibility of one gate winning over the other is rather small in the supercoupling regime. This however may not occur in e.g. SOI based devices where generally the top gate with a smaller gate oxide thickness controls the channel in that regime.

The radiative recombination rate on the other hand first increases with the thickness as the induced carrier concentrations increase and thereafter decreases as the spatial separation between the induced electron and hole layer increases as shown in Fig. 5.10(b). The maximum radiative recombination rate is at around $t_s = 20 \text{ nm}$ which also justifies our initial choice for the thickness value used for the device simulations.

Moreover, as discussed, the supercoupling effect can be important in such dual gate UTB devices. Therefore, it is worthwhile to further estimate the critical thickness, t_s^* [213, 214] below which such effect becomes important. The simplified expression for t_s^* as derived before in [213], assuming a strong inversion situation at the top gate ($V_{GT} > V_{TT}$), can be expressed as:

$$t_s^* = u_T \frac{\epsilon_s}{C_{\text{oxB}}(V_{\text{FBB}} - V_{\text{GB}})} \ln \left[\frac{N_a C_{\text{oxT}} C_{\text{oxB}} (V_{\text{FBB}} - V_{\text{GB}})}{q \epsilon_s n_i^2} \right] \quad (5.7)$$

where C_{oxB} , V_{GB} and V_{FBB} are the areal oxide capacitance, applied voltage and flatband voltage at the bottom gate respectively, C_{oxT} , V_{GT} and V_{TT} are the areal oxide capacitance, applied voltage and threshold voltage at the top gate respectively and N_a is the body doping density. To estimate t_s^* for our proposed device structure, Eq. (5.7) was used, which is applicable to long channel devices as in this work but ignores quantum effects. For this estimation in case of our unintentionally doped device, N_a was replaced by the intrinsic carrier concentration ($n_i \sim 10^{15} \text{ cm}^{-3}$). At $V_{\text{GB}} = -0.75 \text{ V}$,

the calculated $t_s^* = 0.8$ nm, which is in fair agreement with our TCAD simulations (including quantum effects) where the supercoupling effect was evident for t_s below 5 nm. Therefore, supercoupling is not much of a concern for our proposed dual gate structure with a symmetric top and bottom gate. It could however be an issue if a thicker bottom gate oxide is used. For example, the calculated t_s^* is about 26 nm for a 200 nm thick back oxide for the same V_{GB} .

As an application note, the proposed In(Ga)As based EHB LED can be monolithically integrated with an InAs photodiode, which could be attractive for a wide range of applications in the mid-infrared spectral region (2-10 μm) such as gas sensing and environmental monitoring [218, 219].

5.7 Diode-mode operation

In addition to the proposed dual gate EHB device shown in Fig 5.1, an alternative device structure, as shown in Fig. 5.11(a), was investigated where the InAs body is now directly sandwiched between two metal electrodes (with $\phi_{mT} = 4.9$ eV and $\phi_{mB} = 5.4$ eV) without any gate oxide in between. For these metal-semiconductor interfaces, a surface recombination velocity of $S_n = 2.5 \times 10^6$ cm/s and $S_p = 1.9 \times 10^6$ cm/s [98] were used in the simulations. All other simulation parameters were kept the same as summarized in Table 5.1.

The simulated energy band diagram for such a device at thermal equilibrium is shown in Fig. 5.11(b). Two Schottky barriers have been formed with different barrier heights (ϕ_b) for electrons and holes at the opposite interfaces. Moreover, the work function induced electron and hole layers are also present at the top and bottom interface respectively. The charge transport in such a device can be considered to be equivalent to a series connection of an n-type and p-type Schottky diode with each having a different ϕ_b . The diode with a lower ϕ_b would then determine the current. The top interface determines the hole current while the bottom interface determines the electron current in the device, both via thermionic emission. The thermionic emission of charge carriers is also evident from the forward bias band diagram (see e.g. Fig. 5.11(c)) where both electron and hole quasi Fermi levels remain flat throughout the whole body [1]. The simulated $I - V$ characteristics of the device is shown in Fig. 5.11(d). Since $\phi_{bn} < \phi_{bp}$, the electron component will determine the total device current at low injection with an ideality factor, n , of unity. At high injection, where $n = 2$, the electron and hole current are comparable.

In such diode-mode operation, a lower steady-state IQE of $\sim 16\%$ at $V_d = 0.5$ V was obtained which is expected to deteriorate further in the presence of tunneling processes, which were not accounted for. The observed lower IQE in the diode-mode operation is attributed to the enhanced SRH recombination rate in the presence of a more uniform distribution

Figure 5.11: InAs EHB device without gate oxides, (a) schematic cross-section, (b) simulated energy band diagram across AA' at thermal equilibrium and (c) at forward bias, $V_d=0.2$ V and (d) simulated I-V characteristics of the same device. Electrode area, $A_E=7.85 \times 10^{-9} \text{ cm}^2$.

($p \sim n \sim \text{constant}$) of charge carriers across the body thickness [158]. This is not the case for the switched-mode operation in the dual gate EHB device where the carrier concentrations gradually drop from their respective gate interfaces leading to $p \neq n$ and therefore a lower SRH rate (for the same SRH lifetime).

Furthermore, in practice, direct metal-semiconductor junctions are prone to the Fermi-level pinning effect [176] and therefore obtaining such Schottky barriers and resulting work function induced EHB is rather difficult. Particularly, in InAs, it has been reported that the Fermi level is normally pinned above the conduction band minimum [220]. In that respect, the proposed dual gate InAs EHB device based on the switched-mode operation is more practical as it is less prone to Fermi level pinning. Moreover it even shows higher IQE.

5.8 Si EHB LED

The EHB LED concept for a wider bandgap material than InAs, such as Si, with a relatively low thermal generation rate, was also investigated. For such a material, the source of charge carriers in the form of highly

Figure 5.12: Schematic cross section of the Si EHB LED with additional highly doped ($\sim 10^{20} \text{ cm}^{-3}$) regions on either side of the UTB intrinsic-Si body. Here, the silicon thickness $t_s=12 \text{ nm}$, $L_i=0.5 \text{ }\mu\text{m}$, $L_d=0.1 \text{ }\mu\text{m}$, $t_{\text{oxT/B}}=4 \text{ nm}$, $\phi_{\text{MT}}=4.1 \text{ eV}$ and $\phi_{\text{MB}}=5.1 \text{ eV}$. For Si, SRH lifetimes, $\tau_n=10^{-5} \text{ s}$ and $\tau_p=3 \times 10^{-6} \text{ s}$ [98] and $B_{\text{rad}}=10^{-14} \text{ cm}^3 \text{ s}^{-1}$ [221] were used.

doped p-type and n-type region on either sides of the intrinsic body, as also originally proposed for the EHB TFET [79], or side metal contacts with a high surface generation velocity should be adopted.

Fig. 5.12 shows the conceptual device architecture for the Si EHB LED with an additional doped region on either side. First, the switched-mode operation of this gated Si EHB device is discussed. During its operation, both gate interfaces are switched between their charged- and discharged-state by applying the voltage pulses while keeping the side contacts to p^+ and n^+ regions grounded all the time, as shown in Fig. 5.12. The proposed device is capable of switching in the GHz frequency range, see Fig. 5.13

Figure 5.13: Simulated switched-mode operation of the Si EHB LED in ns time scale showing the peak electron and hole density at the opposite gate interfaces (left vertical-axis) and the maximum radiative recombination rate in the device (right vertical-axis). (charged-state $V_{\text{GT}}=1 \text{ V}$ and $V_{\text{GB}}=-1 \text{ V}$, discharged-state $V_{\text{GT}}=-0.5 \text{ V}$ and $V_{\text{GB}}=0.5 \text{ V}$, $t_{\text{on/off}} = 2 \text{ ns}$, $t_{\text{rise/fall}} = 3 \text{ ns}$, gate electrode area, $A_E=5 \times 10^{-9} \text{ cm}^2$.)

where the formation and recombination of EHB occurs in ns time period. The Si EHB emits low intensity ($R_{\text{rad}} \sim 2.5 \times 10^{13} \text{ cm}^{-3} \text{ s}^{-1}$) ns light pulses with an IQE of about $\sim 10^{-3}\%$.

Next, the performance of this Si EHB device is compared with a conventional Si PIN diode of the same geometry as shown in Fig. 5.12 but without any provision of the top and bottom gate. The forward biased Si PIN diode shows a much higher light intensity compared to its EHB counterpart, with an IQE $\sim 10^{-2}\%$. However, GHz switching in SOI PIN LEDs is challenging as discussed before in [222]. In this respect, the proposed Si EHB LED could be more attractive for an SOI based opto-coupling application platform for its high speed switching capabilities.

Furthermore, the device efficiency of the Si EHB LED can be improved if the recombination at the p^+ and n^+ regions are effectively suppressed [201]. One way of achieving this is by physically separating the gated EHB regions from the heavily doped regions with an i-Si spacer region. However, the i-Si spacer region would then limit the device speed. So, again there is a trade-off between device speed and its efficiency [222]. Moreover, the carrier transit time through the intrinsic region also affects the device operation when it becomes comparable to the carrier lifetime for a longer diode length (L_i) and therefore the diode length also needs to be optimized for efficient device operation.

5.9 Conclusion

A novel switched-mode light emitting device based on the electrostatically induced EHB concept has been proposed. TCAD simulations show that the InAs based device is capable of switching in the μs range to emit light pulses of wavelengths corresponding to its effective bandgap. Monolithic integration of such an optical device along with (opto-)electronic devices in a UTB III-V on insulator (XOI) technology could be interesting for applications such as on-chip communication and sensing. The proposed device is more suitable for narrow bandgap materials since switching speed is limited by the bandgap through the thermal generation rate. In addition, the EHB LED concept is interesting for wider bandgap materials such as Si in a gated PIN configuration, where high speed switching in the GHz range is possible, which could be explored for SOI based optocoupling applications.

POLYCRYSTALLINE GAN/P-SI HETEROJUNCTION DIODE

Abstract

In this chapter, the charge carrier transport and electroluminescence (EL) in thin-film polycrystalline (poly-) GaN/p-Si heterojunction diodes realized using a plasma enhanced atomic layer deposition (PEALD) process are studied. The fabricated poly-GaN/p-Si diode with a native oxide at the interface showed a rectifying behavior ($I_{\text{on}}/I_{\text{off}}$ ratio $\sim 10^3$ at ± 3 V) with current-voltage characteristics reaching an ideality factor n of ~ 5.17 . The areal (J_a) and peripheral (J_p) components of the current density were extracted and their temperature dependencies were studied. The space charge limited current (SCLC) in the presence of traps is identified as the dominant carrier transport mechanism for J_a in forward bias. An effective trap density of $4.6 \times 10^{17} / \text{cm}^3$ at a trap energy level of 0.13 eV below the GaN conduction band minimum was estimated by analyzing J_a . Other basic electrical properties of the material such as free carrier concentration, density of states in the conduction band, electronic mobility and dielectric relaxation time were also determined from the current-voltage analysis in the SCLC regime. Further, infrared EL corresponding to the Si bandgap was observed from the fabricated diodes. The observed EL intensity from the GaN/p-Si heterojunction diode is ~ 3 orders of magnitude higher compared to that of the conventional Si only counterpart. The enhanced infrared light emission is attributed to the improved injector efficiency of the GaN/Si diode because of the wide bandgap of the poly-GaN layer and resulting band discontinuity at the GaN/Si interface.

6.1 Introduction

Gallium Nitride (GaN) is an attractive semiconductor for both electronic and optoelectronic applications because of its wide and direct bandgap, high breakdown field and stability at high temperature [18–20]. The relatively high substrate cost for GaN based devices may be tackled with GaN-on-Si substrates. These additionally allow the monolithic integration of GaN devices with Si platform technology [21–23]. However, when monocrystalline GaN is to be grown on silicon, a several-micrometer thick buffer layer is required [21, 24] which makes it difficult to form a platform technology combining silicon devices with GaN devices on the same chip. A potential alternative approach is to grow thin-film polycrystalline GaN on silicon. Compared to thick film heteroepitaxy, polycrystalline films bring important fabrication advantages such as lower cost, a lower bill-of-materials and a lower thermal budget. Still, polycrystalline materials generally do not reach the same quality in electrical performance as their monocrystalline counterparts. It is therefore the purpose of this chapter to investigate electrical properties of polycrystalline GaN grown on monocrystalline silicon substrates.

Among the several approaches to grow thin polycrystalline GaN films, atomic layer deposition (ALD) is an attractive solution for applications where excellent wafer-level uniformity, a critical layer thickness control is required, and complex device topologies are involved [36, 37]. An additional advantage of ALD is that it allows to reduce the deposition temperature of many processes [38]. Recently, ALD grown GaN devices such as thin-film transistors have been successfully demonstrated [39–41] with a reasonable performance considering their polycrystalline nature. However so far there have been no reports on vertical devices based on ALD-GaN-on-Si heterojunctions. With this motivation, ALD grown thin-film polycrystalline GaN/Si heterojunction diodes were realized and their charge carrier transport and optical properties have been investigated in this chapter.

6.2 Experimental details

A (111) oriented p-type Si wafer with a background doping concentration of 10^{15} cm^{-3} was used to fabricate the GaN/p-Si heterojunction diodes¹. The native oxide present on the surface of the Si wafer was not removed for this experiment. A thin layer of polycrystalline GaN on Si substrate was deposited using a plasma-enhanced ALD process, in a remote-plasma Picosun R-200 reactor. The precursors were trimethylgallium (TMG) for Ga and ammonia (NH_3) for N. The depositions were done at 400 °C tempera-

¹The poly-GaN thin-film ALD growth, device fabrication and material characterization reported in this chapter were performed by S. Banerjee [223] as part of the joint research project. The chapter though is mainly focused on electrical aspects.

Figure 6.1: (a) Schematic cross-section of the experimental Al/GaN/p-Si diode with circular electrode (area A_E) of diameter $d=100\text{ }\mu\text{m}$, (b) Cross-section TEM image of the fabricated device [42, 223].

ture. The growth of the layers were monitored in real-time using an in-situ spectroscopic ellipsometer (J.A. Woollam Co. M-2000, operating between 245.8 - 1688.5 nm wavelength). All polycrystalline GaN samples studied in this chapter were of $36 \pm 3\text{ nm}$ thickness. For comprehensive account of poly-GaN thin film ALD process, please refer to [223].

Post deposition, the GaN layers were characterized by X-ray photoelectron spectroscopy (XPS, Phi Quantera SXM) for determining the layer composition and by $\theta - 2\theta$ -and grazing incidence angle X-ray diffraction (GIXRD, Panalytical X'Pert Powder) for determining the layer crystallinity. The layer thicknesses that were obtained from the ellipsometer in-situ monitoring were additionally verified by a transmission electron microscope (TEM, Philips CM300ST-FEG).

GaN/Si heterojunction diodes with Al metal electrodes (*i.e.*, Al as a top electrode) were then fabricated using a standard photolithography process. The schematic of experimentally realized device is shown in Fig. 6.1(a). All electrical measurements were performed using a Keithley 4200 semiconductor parameter analyser that was equipped with a temperature-controlled chuck. The bottom of the Si substrate was utilized as the back contact. Optical measurements were performed using a cooled InGaAs detector based camera (XEVA-320 from Xenics) for capturing the IR micrographs. For measuring the emission spectra, an Avaspec UV-Vis/NIR spectrometer from Avantes was used. Further, an off-chip Si photodiode [156] was utilized for photocurrent measurements.

6.3 Material characterization of the GaN layers

The deposition of polycrystalline (poly-) GaN layers was monitored in real time using in-situ spectroscopic ellipsometry (SE). The layers had a growth

rate of ~ 0.095 nm/cycle. Since the layer thicknesses were extracted using an optical model [224], it was necessary to validate the obtained thickness values. This was done with the help of TEM imaging (Fig. 6.1(b)). Both SE and TEM revealed similar thickness values, i.e., ~ 36 nm within an accuracy of ± 3 nm.

The TEM image of Fig. 6.1(b) shows the cross-section of the fabricated device (i.e. Al/GaN/native oxide/Si). The image reveals vertical (columnar) growth of GaN layer at several regions. By performing the fast Fourier transform (FFT) at multiple regions in the GaN layer, d-spacing values typical to (002) planes of hexagonal (wurtzitic) GaN were obtained. Other wurtzitic crystal planes such as (100) and (101) were also observed in small amounts, indicating the polycrystalline nature of the material.

The polycrystalline structure was also reconfirmed with the help of a GIXRD scan (not shown) taken at an incidence angle of 1° . The diffractogram confirmed the wurtzitic structure of the layer and also shows a strong (002) peak, reflecting the abundance of this crystal plane in the polycrystalline layer. The average grain size of the (002) crystal plane from the diffractogram was estimated to be 9.8 nm. This value is slightly higher compared to that observed from TEM images, which showed grain sizes between ~ 5 –9 nm.

The composition and the chemical bonding information in the grown film was determined from XPS, which was equipped with an Al- $K\alpha$ monochromatic X-ray source. The presence of N-Ga bond was confirmed by XPS analysis of the grown poly-GaN films. Further, impurity levels (i.e. C and O) were found to be low inside the film with oxygen content of about 7 % in bulk of the film and ~ 15 % at the surface as revealed from depth profiled XPS analysis. Practically, no carbon was detected inside the film. The XPS depth profile analysis also found the film to be N-rich. For more detailed description of poly-GaN material characterization, please refer to [223].

6.4 Electrical Measurements

The $I - V$ characteristics of the GaN/p-Si diode with native oxide at 298 K (Fig. 6.2) show a rectifying behavior with an $I_{\text{on}}/I_{\text{off}}$ ratio $\sim 10^3$ at ± 3 V. However the semi-logarithmic $I - V$ plot shows a high ideality factor $n \sim 5.17$. An ideality factor of much higher than two indicates a physical transport mechanism other than thermionic emission or diffusion ($n = 1$) and space charge region recombination ($n \leq 2$). The GaN layer could limit the conduction by bulk controlled processes such as space charge limited current (SCLC) or Poole-Frenkel mechanism. Alternatively, the conduction could be limited by interface controlled processes at the GaN/Si heterojunction such as thermionic emission or tunneling.

Fig. 6.3 shows a simulated energy band diagram of the GaN/p-Si heterojunction in which Anderson's model or the electron affinity rule was used [98]. Here, the electron-affinity of GaN was assumed to be 3.3 eV

Figure 6.2: $I - V$ characteristics of fabricated GaN/p-Si vertical diode with native oxide at $T = 298$ K. Inset: schematic cross-section of the experimental device.

which has been reported before both for crystalline GaN [225, 226] and for polycrystalline GaN [31, 33]. The large discontinuity in the valence band ($\Delta E_v = 1.58$ eV) as compared to conduction band discontinuity ($\Delta E_c = 0.7$ eV) makes it less likely for holes to participate in the conduction process, at least at lower voltages (< 1.58 V). Therefore it is very likely that only electrons will determine the current flow in this device.

To further analyze the charge carriers transport, the areal (J_a) from the peripheral (J_p) current density components were first separated via $I - V$ measurement on devices with different perimeter-to-area (P/A) ratio electrodes. The slope of J vs P/A curve yields J_p while the intercept results

Figure 6.3: TCAD [98] simulated energy band diagram of the GaN/p-Si heterojunction diode at thermal equilibrium. The distance is relative to the top Al electrode. The GaN layer thickness is 40 nm and thickness of Si substrate is 525 μm . Filled circles: electrons. Open circles: holes.

Figure 6.4: Current scaling measurement of devices with a varying perimeter-to-area (P/A) ratio of the electrode: (a) at forward bias, (b) at reverse bias. J is the total current density, J_a and J_p are the areal and peripheral current density respectively, P and A are the device perimeter and area respectively.

in J_a as shown in Fig. 6.4 for two different voltage levels. Following this approach, J_a and J_p were separated for the whole measured voltage range as shown in Fig. 6.5. Both J_a and J_p are rectifying in nature.

The extracted J_a and its high ideality factor could be explained in terms of space charge limited current (SCLC) [227, 228] which is a typical conduction mechanism for thin insulating films or lowly doped wide bandgap semiconductors where only a single type of charge carrier participate in the conduction process. This is very likely the case in our devices where no doping was introduced in the GaN layer and conduction is possibly via

Figure 6.5: Extracted J_a and J_p via $J - V$ measurement on devices with different perimeter-to-area (P/A) ratio electrodes using the relationship $J = J_a + (P/A)J_p$. Inset: R^2 residual from the least-square fitting method. The R^2 value of ~ 1 throughout the measured voltage range indicates good linear fitting and therefore uniform current scaling.

Figure 6.6: Log(J)-Log(V) plot of the extracted J_a in the forward bias region.

electrons at lower voltages². The trap-mediated SCLC has been reported before for GaN based films and nanostructures [27, 229–231], GaN/Si heterojunctions [232–234] as well as for other wide bandgap semiconductor based heterojunctions such as ZnO/Si [235, 236] and ZnO/GaN[237].

The observed $J_a - V$ behavior was analyzed in terms of a single type of carrier (electrons) SCLC model [227, 228] in the presence of a single discrete trap level at energy E_t below the conduction band edge. The $\log(J_a)$ - $\log(V)$ plot of the GaN/p-Si diode, see Fig. 6.6, shows four linear regimes with different slopes (α) which are separated by a transition voltage, V_{tr} and a trap-filled limit (TFL) voltage, V_{TFL} . The $J - V$ equations for SCLC in the presence of a single shallow trap level are described as follows [228]:

$$J_{ohm} = qn_0\mu\frac{V}{d}, \quad (6.1)$$

$$J_{Child(trap)} = \frac{9\mu\epsilon_r\epsilon_0\theta V^2}{8d^3}, \quad (6.2)$$

$$J_{Child} = \frac{9\mu\epsilon_r\epsilon_0 V^2}{8d^3}, \quad (6.3)$$

$$V_{tr} = \frac{8qn_0d^2}{9\epsilon_r\epsilon_0\theta}, \quad (6.4)$$

$$V_{TFL} = \frac{qN_t d^2}{2\epsilon_r\epsilon_0}, \quad (6.5)$$

$$\theta = \frac{N_C}{g_n N_t} \exp\left(\frac{E_C - E_t}{kT}\right), \quad (6.6)$$

²The role of device electrical contacts in supplying the required charge carriers for SCLC transport is discussed in chapter 7.

$$\tau_c = \frac{d^2}{\mu V_{tr}}, \quad (6.7)$$

where q is the elementary charge, k is the Boltzmann constant, ϵ_0 is the permittivity of vacuum, d is the thickness of the insulator or space charge region, ϵ_r is the relative permittivity of the medium, μ is the electron mobility, n_0 is the free carrier concentration, θ is the ratio of free carriers to total carriers, E_C is the position of conduction band edge, E_t is the trap energy level with respect to E_C , g_n is the degeneracy of the states in the conduction band (~ 2) [238], N_C is the conduction band effective density of states, N_t is the effective trap density of the medium and τ_c is the carrier transit time.

At low bias ($0 < V < V_{tr}$, region I), there is ohmic conduction (Eq.(6.1)) with $\alpha \sim 1$ where the thermally generated free carrier density (n_0) is larger than the injected carrier density (n). In this region, the carrier transit time (τ_c) is greater than the material dielectric relaxation time (τ_d) and material remains in quasi-neutral state [238]. At $V = V_{tr}$, a transition from ohmic conduction to SCLC occurs as n becomes larger than n_0 and τ_c just becomes equal to τ_d .

In region II ($V_{tr} < V < V_{TFL}$) the electron quasi-Fermi level (E_{Fn}), which is a function of injected charge in case of extrinsic type conduction, is still below the shallow trap energy level E_t . In this regime, most of the injected charge does not contribute to the current and a part of it occupies the traps. Further, the fraction (θ) of the free charge to the total charge (*i.e.* free and trapped charge) remains constant and doesn't vary with the applied voltage as long as E_{Fn} is below E_t [228]. The conduction (in region II) follows Child's law however with a current density reduced by a factor θ (Eq.(6.2)).

Further increasing the injected free carrier density by biasing a higher voltage, moves E_{Fn} further up and eventually at $V = V_{TFL}$, E_{Fn} just passes over E_t . Thus, V_{TFL} is defined as the threshold voltage required to fill the traps. Shortly beyond V_{TFL} , *i.e.* region III, a steep rise in the current ($\alpha = 6.6$) occurs as it rapidly recovers from its low trap-limited value to a high trap-free SCL value. Therefore region III is the transition from a trapped I – V behavior to a trap-free behavior. Finally beyond this transition region, when all traps are completely filled, they no longer affect the charge injection. Hereafter, any injected charge fully contributes to the current (region IV) and an ideal trap-free square law ($\alpha = 2.06$) is followed (Eq.(6.3)).

Using Eqs.(6.1)-(6.7) [228] and following the methodology as previously described by Chiu *et al.* [238], the basic electrical properties of the poly-GaN material were extracted and are summarized in Table 6.1. For the calculations, $d=36$ nm (GaN thickness) and the literature reported value of $\epsilon_r=8.9$ for GaN [239] were used. $V_{tr}=0.31$ V and $V_{TFL}=0.61$ V were estimated from Fig. 6.6. Further, temperature dependent measurements

Table 6.1: Extracted electrical properties of poly-GaN material at 300 K from the $J_a - V$ analysis.

Properties	Values
Transition voltage from ohmic to SCLC regime, V_{tr}	0.31 V
Trap-filled-limited voltage, V_{TFL}	0.61 V
Effective trap density, N_t	$4.6 \times 10^{17} / \text{cm}^3$
Trap energy level, $ E_C - E_t $	0.13 eV
Free carrier concentration, n_0	$4.4 \times 10^{15} / \text{cm}^3$
Fermi level, $ E_C - E_{Fn} $	0.18 eV
Conduction band density of states, N_C	$4.6 \times 10^{18} / \text{cm}^3$
Ratio of free carriers to total carries, θ	0.03
Electronic mobility, μ	$1.7 \times 10^{-8} \text{ cm}^2 / \text{V-s}$
Dielectric relaxation time, τ_d	$2.4 \times 10^{-3} \text{ s}$

(see Fig. 6.7(a)) were used to estimate the effective E_t from the Arrhenius plot. The energy levels E_{Fn} and E_t are relative to E_C .

The Arrhenius plot of J_a at a range of voltages in the forward bias is shown in Fig. 6.7(b) indicating a rate-limited thermally activated process ($J_a \propto \exp(-E_a/kT)$) where E_a is the thermal activation energy. The estimated E_a is constant throughout the measured temperature range. This also indicates that a single trap level is dominant over the statistics of majority carriers throughout the measured temperature range [240]. Further, no significant variation ($\sim kT$) in E_a from ohmic conduction to SCLC regime at different voltage ranges was observed. According to Roberts and Schmidlin [240], this suggests that the conduction is largely extrinsic in nature, as also expected in wide bandgap materials. The estimated E_a from Arrhenius plot can then be interpreted as the dominant trap energy level E_t as long as $\theta \ll 1$. Hence, $E_t = 0.13 \text{ eV} \pm 0.0259 \text{ eV}$ below E_C was estimated from the extracted E_a in the trap filling region (II) of the $\log(J_a)$ - $\log(V)$ curve (Fig. 6.6). In this region, E_{Fn} lies below the E_t and therefore θ which

Figure 6.7: (a) Temperature dependent $J_a - V$ characteristics of the fabricated Al/GaN/p-Si diode. (b) Arrhenius plot of J_a for various forward bias levels.

Figure 6.8: (a) Modeled Arrhenius plot of θ' using Eq. (6.8) for various N_t . (b) Estimated E_a against N_t for a fixed $E_t = 0.13$ eV.

contains the E_a for J , can be described by Eq. (6.6).

It should however be noted that Eq. (6.6) is only accurate when $\theta \ll 1$ and therefore the interpretation of E_a from the Arrhenius plot as E_t may be erroneous otherwise. A more generalized expression for θ as given by Eq. (6.8) [228] offers better insight into the interpretation of Arrhenius plot.

$$\theta' = \frac{N_c \cdot \exp\left[\frac{(E_c - E_{Fn})}{kT}\right]}{N_c \cdot \exp\left[\frac{(E_c - E_{Fn})}{kT}\right] + \left(\frac{N_t}{1 + (1/g_n) \cdot \exp\left[\frac{-(E_t - E_{Fn})}{kT}\right]} \right)}, \quad (6.8)$$

From Eq. (6.8) various cases depending on the relative positions of E_{Fn} and E_t within the bandgap can be analyzed. The impact of Eq. (6.8) on our results was investigated further by inserting the estimated E_t , N_c and E_{Fn} values from Table 6.1 there and varying the N_t from 10^{14} till 10^{19} / cm^3 . The modeled Arrhenius plot along with extracted E_a for different N_t is shown in Fig. 6.8. It was noted that the extracted E_a values agree with given E_t only in a region where $N_t \sim N_c$. Since in our case, N_t is expected to be very high because of the polycrystalline nature of the film, as also reported before [27], the measured E_a corresponds to E_t .

Further, the role of any other possible conduction mechanism in our diodes were also investigated. It is possible that the steep slope region in the mid-voltage range ($-1 < V < -0.5$ V) in Fig. 6.6 could also be partly originating from the recombination tunneling mechanism [241]. This type of conduction mechanism has been reported before for wide bandgap heterojunctions [235, 236] in the presence of deep level traps. For a single step tunneling recombination pathway where the electrons from the conduction band of an n-type wide band gap material falls into the empty deep level trap, and subsequently tunnel into the valence band of the p-type material, the forward current density is described as $J = C_1 N_t \exp(B \cdot V)$ where C_1 is a constant and N_t is the trap density [241]. The temperature

independent exponential pre-factor B is given as [241]:

$$B = (8\pi/3h)(m_h^* \epsilon_r \epsilon_0)^{1/2} N_D / [N_A^{1/2} (N_A + N_D)], \quad (6.9)$$

where m_h^* is the hole effective mass, ϵ_r is the relative permittivity of the wide band gap material, N_D and N_A are donor and acceptor concentration respectively and h is Planck's constant. The estimated B value ($\sim 7.3 \text{ V}^{-1}$) from Fig. 6.7(a) via curve fitting is temperature independent in the said voltage range. However J_a does show a temperature dependency in the same range unlike expected for the tunneling mechanism [241]. This suggests that recombination tunneling is not the dominant mechanism there.

Other related trap assisted tunneling (TAT) processes such as two-step TAT [242, 243] or even multi-step TAT [244] are also shown to have a weak temperature dependency. However our $J_a - V - T$ characteristics clearly suggest a rate-limited thermally activated process (Fig. 6.7(b)). Therefore the TAT current contribution to the forward J_a , though possibly present, is not significant and consequently does not affect our SCLC analysis.

The possibility of Poole-Frenkel type of conduction in our diodes [245, 246] was also considered. The $\ln(J_a/V)$ vs. $\sqrt{V}$ plot showed a straight line in the mid-forward voltage range as expected for Poole-Frenkel type conduction. However, the decrease in its slope with increase in temperature as also expected for Poole-Frenkel conduction was not manifest in our data. In addition, E_a also did not decrease with the applied bias unlike in case of Poole-Frenkel conduction where the applied field reduces the effective trap ionization level. Therefore it appears that Poole-Frenkel conduction is not the dominant transport mechanism in our diodes as well.

Our $J_a - V$ analysis along with its temperature dependency strongly suggest the single level shallow trap mediated SCLC as the dominant mechanism. As a sanity check on the proposed SCLC model, N_t value was also independently estimated from the intercept of the Arrhenius plot (Fig. 6.7(b)) using Eq. (6.2) and assuming $N_c \sim 1.2 \times 10^{18} \text{ /cm}^3$ for GaN [239]. This was found to be consistent with the previously calculated value from the $J_a - V$ analysis using Eq. (6.5). Moreover, the conduction was analytically modeled using Eqs.(6.1)-(6.7) along with the extracted parameters from Table 6.1 and a good fit with the $J_a - V$ plot was obtained.

6.5 Optical Measurements

Infrared (IR) electroluminescence (EL) was observed from the fabricated Al/GaN/p-Si (Fig 6.9(a)) diode. The measured spectrum (Fig 6.9(b)) is centered around the $1.12 \mu\text{m}$ wavelength corresponding to the Si bandgap ($E_{g-\text{Si}} = 1.12 \text{ eV}$) with a full-width-half-maximum (FWHM) $\sim 96 \text{ meV}$ at 300 K. The observed FWHM is in excess of $\sim 1.8kT$ [157] because of light being emitted from silicon, an indirect band gap semiconductor where interaction with phonons during the radiative recombination process leads

Figure 6.9: (a) Bright field IR micrograph of the fabricated GaN/p-Si diode at a constant forward current drive of 15 mA ($J=19 \text{ A/cm}^2$), (b) Optical spectrum of the emitted light from the same diode.

to the broadening of the EL-spectrum compared to that in direct band-gap semiconductors [247, 248]. Both the peak wavelength and the FWHM are in good agreement when compared with standard p-n junctions in silicon [249].

For reference sake, an Al/p-Si (with native oxide) Schottky diode [56] was also realized. From this device, faint IR emission was observed which was too weak to be detected by our spectrometer as reported before [56]. This is also in line with the detected photocurrent (I_{PD}), Fig. 6.10(a), using an off-chip Si photodiode (PD) [156] which is a measure of the emission intensity corresponding to the injected diode current (I_{LED}). For the same I_{LED} , the measured I_{PD} and therefore emission intensity for the Al/GaN/p-Si diode ($I_{PD} \sim 1 \text{ nA}$) is ~ 3 orders of magnitude higher than for the Al/p-Si diode ($I_{PD} \sim 1 \text{ pA}$). The emission intensity in the GaN/p-Si diode was also found to gradually increase with the injected power as expected from the LED behavior [157].

Figure 6.10: (a) Measured short-circuit current (I_{PD}) in the photodiode (PD) versus injected forward current (I_{LED}) for the Al/GaN/p-Si diode and Al/p-Si diode [56]. (b) I_{PD}/I_{LED} ($\propto \eta_{LED}$) versus I_{LED} .

Further, the I_{PD}/I_{LED} ratio, is proportional to the internal quantum efficiency (IQE) of the LED. This is so because $I_{PD}/I_{LED} = \eta_{PD} \cdot \eta_{ext} \cdot \eta_{LED}$, where $\eta_{PD/ext./LED}$ is the IQE of detection in the PD/extraction efficiency of light/IQE of the LED, respectively [249]. Out of the three efficiencies, only η_{LED} is a function of I_{LED} . Thus, the trend in η_{LED} versus I_{LED} is reflected in the trend in I_{PD}/I_{LED} versus I_{LED} . As shown in the Fig. 6.10(b), in the low injection regime, η_{LED} was found to be increasing for higher I_{LED} and no droop was observed up till an injected current density $\sim 25 \text{ A/cm}^2$.

Based on our measured I_{PD} (with a η_{PD} of 0.2 at $\sim 1120 \text{ nm}$ free-space wavelength [156]), the external quantum efficiency of our LED (at $I_{LED}=10 \text{ mA}$) was estimated to be 3.5×10^{-7} . Further, from an estimate of the optical extraction efficiency ($\sim 1.5 \times 10^{-3}$) of our measurement set-up [250], the lower limit of the η_{LED} of our LED was calculated to be $\sim 2 \times 10^{-4}$ (at $I_{LED}=10 \text{ mA}$) without taking into account losses at the top electrode which blocks majority of emission, allowing only light from the periphery of the hexagonal openings (Fig 6.9(a)) to be detected.

The observed infrared EL from the GaN/p-Si device is attributed to the recombination of the injected minority carriers (electrons) with the background majority carriers (holes) at the silicon side of the GaN/p-Si interface as illustrated in Fig. 6.3. Therefore the electron current component determines the light emission. Further, no ultra-violet (UV) emission originating from the GaN band-edge was observed due to high valence band offset at GaN/p-Si interface which indicates negligible hole concentration in the GaN layer. The role of the single type of charge carrier (*i.e.*, electrons) in the conduction in GaN layer is also confirmed by the observed SCLC behavior. Higher IR emission in case of GaN/p-Si diode can be attributed to the wide band gap of the (n-type) GaN layer and resultant band discontinuity at the GaN/p-Si interface which improves its (minority) injection efficiency compared to Al/p-Si diode. Previously, enhanced emission from Si in the presence of native oxide has been reported [251]. However, in our case, no conclusive evidence of any possible role of the native oxide in the observed EL could be established. Both our diodes *i.e.* Al/GaN/p-Si and Al/p-Si had a native oxide.

Fig. 6.11 which shows measured $I - V$ characteristics of two different devices; the Al/p-Si and Al/GaN/p-Si diode, sheds more light on the observed EL characteristics. The data indicate that for the same injected current level I_{LED} , as subjected to our EL measurements, the internal junction voltage V_j increases for devices with a reduced current level. Moreover, for the GaN/p-Si diode the electron current is its actual current depicted in Fig. 6.11. Since it is limited by the GaN layer that component will be less than in the Al/p-Si diode. As a result, $V_{j-pSi} < V_{j-pSiGaN}$. Consequently, the product of the hole and electron density (*i.e.*, $p \cdot n$) in Si (light emitting region in both the cases) which is exponentially dependent on V_j , also follows the same order ($p \cdot n_{pSi} < p \cdot n_{pSiGaN}$). This explains the enhanced emission from the GaN/Si diode compared to that of the Si-only diode,

Figure 6.11: Measured I-V characteristics of Al/GaN/p-Si diode and Al/p-Si diodes.

since a higher $p \cdot n$ -value yields a higher radiative recombination rate (*i.e.*, light emission) [158].

6.6 Discussion

From the analysis discussed before, it can be concluded that the current flow in our ALD-grown thin-film poly-GaN/Si diode is largely limited by the GaN layer³. This allowed us to estimate the basic electrical properties of the polycrystalline layer via $I - V$ analysis using the single shallow trap SCLC model [228]. The relatively large trap density in the unintentionally doped thin film of the wide band gap material could be the reason for the observed SCLC behavior. However, in a good heterojunction [252], for electronic applications such as bipolar transistors, the current should be limited by diffusion in the narrow band gap material.

Despite this, the optical measurements indicate that such engineered poly-GaN based heterojunctions, realized at low temperature, could be interesting for fabricating efficient Si based IR emitters using a relatively simple process. Such heterojunctions can also be investigated for Si based solar cells with an improved injector efficiency [234, 253, 254]. Heterojunction diodes utilizing wide bandgap materials as an emitter are interesting for enhancing the injector efficiency, for example, of the electroluminescent diode [1] and have been reported before for different materials [251, 255–259]. For instance, Favennec *et al.* [255] reported the improved luminescence from Er when implanted in a wide band gap materials matrix. More recently, near IR emission peaking at 826 nm from GaN/Si heterojunctions was also reported by Han *et al.* [259, 260], where unlike in our process,

³More detailed discussion on electrical properties of ALD-grown poly-GaN thin films will be followed in chapter 7.

a 500 nm thick GaN nanocrystalline film was grown at 1050 °C with a CVD process on an Si nanoporous pillar array (NPA). The difference in the observed peak EL wavelength with that obtained from our GaN/Si devices is due to the reported higher energy bandgap ($E_{g-Si-NPA}=2$ eV) and electron affinity ($\chi_{Si-NPA}=3.6$ eV) of the Si NPA and therefore resulting in different band alignment and heterojunction properties. Interestingly, the conduction mechanism reported for the GaN/Si-NPA device [260] was also attributed to an SCLC process.

6.7 Conclusions

It was shown that heterojunction diodes can be realized at a low temperature by adopting ALD of poly-GaN on an Si wafer. The fabricated heterojunction devices showed good rectification and also infrared EL. The current transport in the forward bias is explained by SCLC in the presence of traps as possible dominant transport mechanism. Following the single trap SCLC model along with temperature dependent $J - V$ analysis, a minimum trap density of $4.6 \times 10^{17}/\text{cm}^3$ at an energy level 0.13 eV below the conduction band minimum was estimated in the polycrystalline film. Other electrical properties of the poly-GaN layer such as free carrier concentration, density of states in the conduction band, electronic mobility and dielectric relaxation time were also determined using the SCLC analysis. The observed IR emission from EL is attributed to band-to-band recombination in the Si near the heterojunction interface because of a high $p \cdot n$ -value. The presence of a thin polycrystalline GaN significantly improves the IR emission. The introduction of such engineered heterostructures could be a way forward for making efficient optoelectronic devices such as IR emitters and solar cells realized in bulk Si. The study of such thin-film ALD GaN on Si is also promising for future nanoscale (opto)electronics based on this platform.

ELECTRICAL PROPERTIES OF ALD-GROWN POLY-GaN THIN-FILMS

Abstract

This chapter deals with the basic electrical conduction properties of polycrystalline gallium nitride (poly-GaN) thin films. These films were fabricated by means of two different atomic-layer deposition (ALD) processes namely plasma-enhanced ALD and thermal ALD. Their electrical properties were systemically investigated and compared using electrical measurements on simple device test structures. Based on this study, potential applications of such materials are proposed and discussed.

7.1 Introduction

Polycrystalline (poly-) GaN is an interesting material for various thin-film device applications and also from GaN-on-Si integration perspective as outlined previously in chapter 1 as well as in chapter 6. It is expected that the electrical properties of poly-GaN thin-films are different from their crystalline counterparts. Therefore it is imperative to investigate the electrical properties of these films in order to predict their possible applications in semiconductor technology.

In this work, two different types of atomic-layer deposition (ALD) techniques, as developed by S. Banerjee [223] in the joint research project, were utilized to grow poly-GaN thin films. The first technique, referred to as plasma-enhanced ALD (PEALD), utilizes a plasma source to dissociate NH_3 for creating reactive nitrogen radicals during an ALD cycle for the GaN formation. The use of a plasma source enhances the reaction rate by creation of radicals and/or ions and allows it to proceed at a relatively low temperature which otherwise would have been energetically unfavorable. The PEALD process has been utilized to realize GaN/p-Si heterjunction diodes as described in chapter 6.

The second technique, referred to as thermal ALD, relies on pure thermal-mode for GaN formation via the surface adduct mechanism as described in more detail in [223, 261]. The NH_3 precursor is then not dissociated by striking a plasma, instead the reaction proceeds by forming a so-called TMG: NH_3 surface adduct. These surface adducts subsequently link together and convert into GaN units by releasing CH_4 .

In both techniques, the GaN film is grown at 400°C using trimethyl-gallium (TMG) and NH_3 as precursors. From hereafter, the poly-GaN thin-films grown by PEALD and thermal ALD will be abbreviated as P-GaN and T-GaN respectively. The material characterization results of P-GaN film has been briefly discussed in chapter 6. The layer was found to be N-rich with negligible carbon and about 7% oxygen inside the film. In comparison, T-GaN film is Ga rich with an average composition estimated as $\text{Ga}_{0.53}\text{N}_{0.39}\text{C}_{0.01}\text{O}_{0.07}$ [223]. Both films confirm to polycrystalline wurzitic structure. Table 7.1 summarizes the key features of the P-GaN and T-GaN growth techniques and their respective film qualities. Next, the basic electrical properties of both P-GaN and T-GaN are investigated and compared using simple device test structures. To obtain better insight into the conduction properties of the poly-GaN material in vertical as well as lateral direction, both T-GaN and P-GaN layers were grown on Si, SiO_2 and sapphire substrates.

The polycrystalline GaN thin-film ALD growth and device fabrication as reported in this chapter were mainly performed by S. Banerjee as part of the joint research project.

Table 7.1: Comparison of key features of P-GaN and T-GaN ALD growth techniques [223].

Key features	P-GaN	T-GaN
Tool	Picosun R-200 remote plasma	Cluster ALD
Precursors	TMG + NH ₃	TMG + NH ₃
Growth temperature	400°C	400°C
Process	NH ₃ -plasma activated	surface adduct mechanism
Composition	N-rich	Ga-rich
H-content	low	high
Crystallinity	polycrystalline	polycrystalline
Crystal structure (dominant)	wurtzite	wurtzite

7.2 Experimental details

The P-GaN films were deposited using a commercial remote plasma R-200 Picosun reactor, while T-GaN was grown in a home-made ALD cluster system. Both films were deposited at $\sim 400^\circ\text{C}$ using TMG and NH₃ as precursors. In addition, the AlN film (wherever mentioned) was deposited using the same reactor without breaking the vacuum. Poly-GaN films deposited on sapphire substrates were utilized for lateral electrical measurements. For back-gated TFT realization, highly doped ($\sim 10^{18} \text{ cm}^{-3}$) p-type Si substrates (4-inch) with $\sim 50 \text{ nm}$ thermally grown silicon dioxide (SiO₂) layer on top were used. For investigating the vertical current component, p-type Si(111) substrates (with native oxide) with a background doping concentration of 10^{15} cm^{-3} (as reported in chapter 6) were utilized.

Before the film deposition, sapphire substrates were cleaned in acetone, while SiO₂/Si substrates were cleaned using 99 % and 69 %-by-vol. HNO₃ sequentially to remove organic and metallic contaminants respectively. For electrodes, Al metal (low work function) electrodes were realized on the top poly-GaN surface using a standard photolithography and wet etch process. For realizing Pd (high work function) electrodes, a lift-off process was utilized instead of wet etching. The substrate bottom was used as a back contact for vertical measurement. Surface passivation (wherever mentioned) was done using a $\sim 165 \text{ nm}$ PECVD grown silicon nitride (Si₃N₄). Finally, unless mentioned otherwise, no heat treatment was given to any of the prepared samples after contact metalization.

7.3 Electrical properties of P-GaN

7.3.1 Vertical conduction in P-GaN

Vertical conduction is possible in P-GaN thin-films, as evident from the results discussed in the previous chapter where a rectifying behavior was observed in the P-GaN/p-Si heterojunction diode. The charge transport was found to be largely limited by the space charge limited current (SCLC) mechanism in the P-GaN layer. Both the areal (J_a) and peripheral (J_p) current component in the vertical diode were studied. The root cause of the significant J_p could not be established before. The high J_p could be due to the presence of a surface conductive channel in the P-GaN film as analyzed further in this chapter.

7.3.2 Lateral conduction in P-GaN

Hall measurements

Hall measurements [262] were performed¹ in order to estimate the charge carrier density and their polarity *i.e.* n-type or p-type, in the P-GaN film. The P-GaN/sapphire sample with a film thickness of 40 nm was used for this purpose. The sample was first diced into 8 mm x 8 mm pieces using a laser cutting tool and then point contacts were formed at four edges of the square samples by depositing Al metal via a shadow mask as shown schematically in Fig. 7.1(a). The Hall measurements were performed for a varying magnetic field strength, B , from -9 T till 9 T at various temperatures (100 K - 300K). The excitation current, I , was in the range of 0.8 μ A. The relation between the Hall voltage, V_H , and sheet carrier density, n_{sh} of the

¹The measurements were performed using Quantum Design Physical Properties Measurement System (PPMS) in temperature-controlled environment and under dark conditions.

Figure 7.1: (a) Schematic top view of P-GaN (40 nm)/sapphire sample used for Hall measurements and (b) Measured resistance, R , for a varying magnetic field strength at 300 K.

film can be described as [262]:

$$\frac{V_H}{IB} = \frac{R}{B} = \frac{-r}{n_{sh}q}, \quad (7.1)$$

The r is the scattering factor and is assumed to be unity in our measurements [262]. Here, we consider this relation in terms of effective measured resistance, $R (=V_H/I)$, instead of Hall voltage, V_H , as the former is independent of the measurement current. The sheet carrier density, n_{sh} and carrier type can then be determined (using appropriate units) from the slope of measured resistance (R) against the magnetic field (B) using Eq. (7.1). Other than reducing the uncertainty of relying over two data points ($\pm B$) in conventional Hall analysis, the slope method [263] also eliminates the unwanted contribution of any constant offset voltage which appears across the diagonally opposite terminals at $B=0$ T independent of the measurement current. The finite offset voltage may originate from thermoelectric effects or asymmetry of the contact electrodes or measurement sample itself. In addition to Hall measurements, the van-der-Pauw measurements were performed at zero magnetic field for the sheet resistance (R_{sh}) calculation.

The negative slope of the R vs B plot in Fig. 7.1(b) suggests that electrons are involved in the conduction process. The sheet carrier density, n_{sh} , as extracted from the slope of this curve is $\sim 10^{14} \text{ cm}^{-2}$ at 300 K. Assuming that the carriers are uniformly distributed across the film layer thickness then for the 40 nm film it would be equivalent to a (volume) carrier concentration of $\sim 2.5 \times 10^{19} \text{ cm}^{-3}$. The sheet resistance, R_{sh} , obtained from resistivity measurements, is $\sim 433 \text{ k}\Omega/\square$ at 300 K. For the 40 nm film it is equivalent to a "bulk" resistivity $\rho \sim 1.7 \text{ }\Omega\text{-cm}$. Using the n_{sh} and R_{sh} values, the carrier Hall mobility, μ_n is calculated to be $\sim 0.16 \text{ cm}^2/\text{V-s}$ at 300 K. The observed noise (scattered data) in the measured data can be attributed to the relatively high resistance (low carrier mobility) of the experimental sample which limits the excitation current to be below 1 μA .

Electrical measurements were performed for several temperatures to analyze the conduction properties as shown in Fig. 7.2. The sheet resistance (conductance) decreases (increases) with the temperature. The positive temperature coefficient of the conductance also suggests a semiconductor-like behavior of the channel and rules out the possibility of a metal like film (e.g. metallic Ga). This is confirmed by the fact that no signature of elemental Ga *i.e.*, Ga-Ga bonds was observed in the X-ray photoelectron spectroscopy (XPS) analysis of P-GaN film as reported by S. Banerjee [223]. The sheet carrier density, n_{sh} , shows a decreasing trend with temperature. For a semiconductor, n_{sh} should either increase or remain constant with the temperature. Therefore, considering the relatively large error ($\sim 7 \times 10^{13} \text{ cm}^{-2}$) in the n_{sh} extraction for lower temperatures, the small variation in measured n_{sh} with temperature are ignored and it is treated as a constant ($\sim 10^{14} \text{ cm}^{-2}$) for our further analysis. However, Hall measurements should be repeated at more temperatures for confirmation. The mobility, μ_n , on

Figure 7.2: P-GaN layer properties extracted from Hall measurements at various temperatures, (a) sheet resistance, R_{sh} , (b) sheet conductance, R_{sh}^{-1} , (c) sheet carrier density, n_{sh} and (d) Hall mobility, μ_n . The thermal activation energy, E_a , of μ_n estimated from its Arrhenius diagram i.e. $\ln(\mu_n) - T^{-1}$ plot (not shown) is ~ 0.02 eV.

the other hand, clearly increases almost linearly with the temperature. The trend of mobility and inverse of sheet resistance (measure of conductance) against the temperature are further reflected in the $I - T$ characteristics, as discussed in the next section (ref. Fig. 7.6(b)).

The extracted layer properties (at room temperature) of the P-GaN film grown on a sapphire substrate are also in good agreement with our less extensive measurements on various other P-GaN samples both on sapphire and SiO_2/Si substrates.

It is however important to note that such a standard dc Hall measurement procedure is prone to possible errors due to the polycrystalline nature of the film with a low mobility ($< 1 \text{ cm}^2/\text{V}\cdot\text{s}$) and therefore should be taken with some caution [263]. For a higher accuracy, the procedures as outlined by Werner [263] should be followed. Interestingly, a reasonably good fits to measured $I - T$ (ref. Fig. 7.6 (b)) and $I - V$ (ref. Fig. 7.11(b)) characteristics were obtained using the n_{sh} and μ_n information obtained from Hall measurements.

Figure 7.3: Schematic cross-sections of experimental P-GaN/sapphire devices, (a) with Al contacts and Si_3N_4 surface passivation, (b) with Pd contacts and no surface passivation.

I – V – (T) characteristics

Figure 7.4: I – V characteristics of P-GaN/sapphire devices with Al (Si_3N_4 passivation) and Pd contacts. Device width $W=400\ \mu\text{m}$, $T=300\ \text{K}$.

Fig. 7.3 shows the schematic cross-sections of the experimentally realized devices for studying lateral conduction properties of P-GaN thin films. The P-GaN thin-film grown on sapphire substrate showed linear I – V characteristics in the lateral direction irrespective of using metal electrodes with a high (Pd) and low (Al) work function, as shown in Fig. 7.4. Interestingly, even a point-contact using a (tungsten) probe tip directly on the P-GaN film showed a linear behavior. The observed linearity in the I – V characteristics sustained even after passivating the P-GaN surface with an Si_3N_4 layer ($\sim 165\ \text{nm}$) suggesting that the conduction is determined by intrinsic properties of the P-GaN film. Similar linear I – V characteristics were also observed for various other P-GaN samples grown on sapphire as well as SiO_2/Si substrates with good reproducibility.

The observed conduction behavior irrespective of the metal electrode work function, surface passivation condition and substrate type, suggests the possibility of a high carrier density near the electrode which facilitates tunneling at the metal-semiconductor (MS) interface. This is confirmed

Figure 7.5: (a) $I - V$ characteristics of Pd/P-GaN/sapphire devices for varying spacing, S , between the contacts. (b) Current vs inverse of contact spacing ($1/S$) at a fixed voltage $V_d = -3$ V ($W=400$ μm , $T=300$ K).

with the Hall measurements where a high sheet electron density, $n_{\text{sh}} \sim 10^{14}$ cm^{-2} , was obtained before. The channel conductivity remains unaffected even in the presence of UV light ($\lambda=255$ nm) which once again indicates the presence of a high electron density in the grown film. Moreover this type of conduction behavior was observed for various electrode spacings (2-200 μm) as shown in Fig. 7.5(a), which indicates that the observed conduction behavior is not a local effect. Further, the current scales linearly with inverse of the distance between the electrodes (see Fig. 7.5(b)) which also suggest the pure resistive (ohmic) nature of the conduction channel and can simply be described as:

$$I = qWn_{\text{sh}}\mu_n \frac{V_d}{S}. \quad (7.2)$$

where V_d is the applied bias, W is the width of the contact and S is the contact spacing.

Temperature dependent $I - V$ measurements of the P-GaN/sapphire

Figure 7.6: (a) Temperature dependent $I - V$ characteristics of Al(P-GaN)/sapphire device, (b) $I - T$ plot at a fixed voltage $V_d = -3$ V. Here Eq. 7.2 is used to model the measured $I - T$ curve using temperature dependent mobility and carrier sheet density data obtained from the Hall analysis.

sample were also performed, as shown in Fig. 7.6(a), where a similar linear $I - V$ behavior was observed for $T=248$ K-398 K. The current scales linearly with the temperature as shown in Fig. 7.6(b). The observed positive temperature coefficient of the conductance reveals the semiconductor nature of the channel and rules out the possibility of a metal like film as also concluded previously from the Hall analysis. Interestingly, the observed $I - T$ variation in Fig. 7.6(b) correlates well (both qualitatively and quantitatively) when modeled with Eq. 7.2 and using μ_n , n_{sh} and their temperature dependencies as obtained from the Hall measurements (refer to Fig. 7.2(c)-(d)). This implies that the observed (linear) temperature dependency of the current is mainly caused by the change in the carrier mobility with the temperature. In other words, both current (conductivity) and mobility have an identical temperature dependence. Here, the n_{sh} ($\sim 10^{14} \text{ cm}^{-2}$) is considered to be largely temperature independent as discussed before in respect to Fig. 7.2(c).

Note that the observed temperature dependency of μ_n can not be attributed to the thermal annealing effect where the film quality has possibly improved during temperature dependent measurements. The μ_n is found to vary uniformly with temperature even down to 100 K where no such annealing is expected to occur.

In order to get further deeper insight into the temperature-dependent conduction property of the film, it is important to discern the dominant charge transport mechanism. Random surface potential fluctuations in the polycrystalline film could lead to carrier localization as illustrated in Fig. 7.7 [264]. Such carrier localization could result in 2-D transport properties as reported before for inversion layers in an Si-MOSFET [265]

Figure 7.7: Graphical representation of random surface potential fluctuations in the conduction band of the polycrystalline material. (a)-(c) short-range fluctuations and (d) long-range fluctuations (after [264]).

Figure 7.8: (a) $\ln(I) - T^{-1}$ and (b) $\ln(I) - T^{-1/3}$ at a fixed voltage $V_d = -3$ V obtained from the measured $I - T$ dependence in Fig. 7.6(b).

and other material systems, such as hydrogen-terminated diamond [266], where transport takes place via a surface channel.

According to the ideal Anderson mobility-edge model [267], thermally activated transport takes place as a result of disorder-induced localization of carriers. For a high electron density, such that $E_F > E_C$, metallic conduction in extended states is predicted as shown in Fig. 7.7(a). While, for the case where $E_C > E_F$, at a sufficiently high temperature, charge transport proceeds via thermal excitation of electrons from a localized state to an extended state as shown in Fig. 7.7(b). In this situation, the current (hence conductivity), $I \propto \exp(-E_a/kT)$, where $E_a = (E_C - E_F)$ is the activation energy and k is Boltzmann's constant. At very low temperatures, thermally-activated tunneling between the localized states, *i.e.* variable range hopping (VRH) is dominant, where $I \propto \exp(-(T_0/T)^{1/3})$ as illustrated in Fig. 7.7(c).

In our devices, the $I - T$ characteristics show compliance with both thermal emission and VRH transport mechanisms (see Fig. 7.8) where $\ln(I)$ is linearly dependent on both T^{-1} and $T^{-1/3}$ possibly due to the relatively small measured temperature range (248 K–398 K). However, for the "ideal" Anderson-Mott model, Hall effect measurements should then result in a temperature activated carrier density while the mobility should show a weak temperature dependency (from scattering mechanisms such as involving interface roughness or phonons) [266]. Therefore, our results which on the contrary show a practically temperature independent carrier density (ignoring a variation possibly due to a measurement error) and a mobility with an identical temperature dependence as that of the current (conductivity), cannot be simply explained by the "ideal" Anderson-Mott model based on short-range potential fluctuations, associated with microscopic inhomogeneities in the material. Similarly, the possibility of VRH transport can be ruled out since it predicts both the Hall mobility and carrier density to be thermally activated ($\propto \exp(-(T_0/T)^{1/3})$) as described in [266]. This also explains the unrealistically high characteristic hopping temperature, T_0 , obtained from the $I - T$ curve fitting (see Fig. 7.8(b)).

Figure 7.9: Modeled curve for measured $I - T$ dependence (ref. Fig. 7.6) using three different temperature dependent functions i.e. linear, $\exp(-E_a/kT)$ and $\exp(-(T_0/T)^{1/3})$. Experimentally extracted parameter values were used for all functions.

Similar results have been reported before ([266] and references therein) and are explained using a long-range potential fluctuations (due macroscopic inhomogeneities in the material) model and the percolation theory [268]. According to this model, "insulating" regions ($E_C > E_F$) exist side-by-side with "metallic" regions ($E_F > E_C$), as shown graphically in Fig. 7.7(d). In this situation, increasing the carrier density (by shifting E_F upwards), makes the "metallic" regions larger and the potential barriers separating them lower. At a certain percolation threshold, which occurs when the fraction of "insulating" area equals the fraction of "metallic" area, a continuous conduction path is established between the "metallic" regions. Above this threshold, thermally activated transport persists where the excitation of carriers over insulating barriers leads to a further reduction in the resistance of the percolation path. The channel conductivity, mobility and their temperature dependence can then be derived using the effective medium theory [268]. In this situation, as described in [266], the conductivity and Hall mobility show the same thermally activated behavior, i.e. $\exp(-E_a/kT)$ dependence. However, the Hall coefficient (R_H) that determines the carrier density ($n=1/qR_H$) corresponds to that of the metallic region and therefore is temperature independent.

The long-range fluctuation model with a carrier density above the percolation threshold best describes our results where the current ($E_a=0.04$ eV, see Fig. 7.8(a)) and Hall mobility ($E_a=0.02$ eV, see Fig. 7.2(d)) show similar thermal activation energy, E_a , while the carrier density is largely temperature independent.

Further, it should be noted that the observed linear as well as the $\exp(-(T_0/T)^{1/3})$ dependence of the measured current with temperature, in addition to proposed $\exp(-E_a/kT)$ dependence, is purely mathematical

Figure 7.10: $I - V$ characteristics of P-GaN/sapphire devices for varying P-GaN layer thicknesses ($T=300$ K).

in nature. Fig. 7.9 shows that for the extracted parameters in the given measured temperature range, the three functions show practically identical $I - T$ relations.

P-GaN layer thickness variation

In order to understand whether the lateral conduction takes place at the surface or in bulk, electrical measurements on devices for various P-GaN layer thicknesses² were performed, as shown in Fig. 7.10.

All three samples showed linear $I - V$ characteristics however the current level of the 25 nm sample is at least three orders of magnitude less compared to that of other two (30 nm and 40 nm) devices, implying that the current scales, but not linearly, with the thickness. The sheet resistance, R_{sh} , measured using CTLM test structures confirmed this behavior. The measured R_{sh} neither remained constant with varying thickness nor it scaled linearly making it difficult to distinguish the surface contribution from that of the bulk type of conductance. It appears that the film quality (hence lateral conductance) improved with layer thicknesses. The fact that the $I - V$ is linear even for a 25 nm thickness suggests that the electron concentration could be equally high in all three devices while their mobility improved with the thickness due to possible reduction in defect density or grain boundaries that affect the lateral charge transport.

Table 7.2 summarizes the extracted electrical properties of the P-GaN layer on various samples using Hall measurements and circular transmission line measurements (CTLM) [262]. For a nominal layer thickness in the range of 30-40 nm, $R_{sh} \sim 400$ -500 $k\Omega/\square$ with specific contact resistivity, ρ_c of $\sim 10^{-3}$ - 10^{-4} $\Omega\text{-cm}^2$. The transfer length is in the range of 1 μm for all measured samples.

²ALD of poly-GaN films for this experiment were performed by B.Y. van der Wel and R.O. Apaydin.

Table 7.2: Electrical properties of the P-GaN layer at 300 K for various samples as obtained from Hall analysis. CTLM specifically refers to the data obtained from circular transmission line measurements [262].

Sample	n_{sh} (cm^{-2})	R_{sh} ($k\Omega/\square$)	μ_n ($cm^2/V\cdot s$)	ρ_c ($\Omega\cdot cm^2$)
Al/P-GaN (40 nm)/sapphire	10^{14}	433	0.16	---
Al/P-GaN (20 nm)/sapphire	---	440 (CTLM)	---	3.5×10^{-2} (CTLM)
Al/P-GaN (35 nm)/SiO ₂ /Si	10^{14}	68, 185 (CTLM)	0.23	10^{-4} (CTLM)
Al/P-GaN (30 nm)/sapphire	---	476 (CTLM)	---	6.8×10^{-4} (CTLM)
Al/P-GaN (40 nm)/sapphire	---	98 (CTLM)	---	10^{-5} (CTLM)

7.3.3 Back-gated P-GaN TFT

Back-gated P-GaN thin-film transistors (TFTs) (see Fig. 7.11(a)) were also fabricated in order to investigate the effect of field on the channel conductivity. Linear $I_{DS} - V_{DS}$ characteristics were again observed between the drain and source, similar to that observed before for the P-GaN/sapphire devices. The channel conductivity however remains unaffected by the gate voltage, V_{GS} , as shown in Fig. 7.11(b). A similar conclusion was also drawn

Figure 7.11: (a) Schematic cross-section of the experimental back-gated P-GaN TFT structure, (b) Measured $I_{DS} - V_{DS}$ characteristics for a varied back-gate bias in the same device.

from measured $I_{DS} - V_{GS}$ characteristics (not shown) where a constant I_{DS} was observed when V_{GS} was swept from -30 V to 30 V at the fixed $V_{DS}=3$ V. Moreover, identical results were obtained for different geometries such as rings and rectangular structures and for various drain/source spacings. These observations ascertain the elevated level of carrier density in the P-GaN film which is too high to be depleted by the applied gate bias. Note that the vertical gate leakage for these measurements was in the range of $\sim 10^{-12}$ A.

To further improve the understanding, TCAD simulations of the device shown in Fig. 7.11(a) were performed. To emulate the possible n-type surface accumulation channel, a high carrier sheet density, $n_{sh} \sim 10^{14} \text{ cm}^{-2}$ was incorporated in the top 2 nm of the GaN film. The rest of the GaN layer was assumed to be lightly n-doped to 10^{15} cm^{-3} . The channel mobility ($\mu_n=0.23 \text{ cm}^2/\text{V-s}$) as obtained from the Hall analysis was used. TCAD simulation results (see Fig. 7.11(b)) were found to be in good agreement with the experiments. Moreover they did not show any gate induced field effect for such a high channel density which is in accordance with the experimental observation.

However, similar results could be obtained even if the whole GaN layer would have been uniformly doped with a carrier density $>10^{19} \text{ cm}^{-3}$ instead of having a localized surface channel. Therefore, the actual spatial distribution of the charge carriers inside the P-GaN film, whether accumulated only near the surface or distributed throughout the bulk, cannot be determined from this measurement as well as the TCAD analysis.

7.4 Electrical properties of T-GaN

7.4.1 Lateral (photo-) conduction in T-GaN

For studying lateral conduction properties of the T-GaN film, three different types of T-GaN devices on sapphire were realized as schematically shown in Fig. 7.12. The first sample had only a T-GaN (45 nm) film directly on sapphire, the second one had a thin AlN (44 nm) layer between the sapphire and T-GaN (26 nm), while the third had AlN (11 nm) on top of the T-GaN (31 nm) layer. This was purposefully done to study whether the AlN layer has any effect on the lateral conductance of the GaN layer.

All three devices showed no electrical conduction in the lateral direction under dark condition, see Fig. 7.13(a). Similar conduction behavior has also been observed for T-GaN layers grown on SiO_2 substrates (not shown). Thermal annealing at 400°C for 30 minutes in the N_2 environment also did not improve the conduction properties of the T-GaN films. Even measurements at high temperature till 150°C did not show any electrical conduction. All T-GaN films, irrespective of the substrate or inclusion of the AlN layer, were found to be electrically insulating in the lateral direction.

Figure 7.12: Schematic cross-sections of experimental T-GaN devices, (a) T-GaN/sapphire, (b) T-GaN/AlN/sapphire, (c) AlN/T-GaN/sapphire.

Figure 7.13: $I - V$ characteristics of (a) T-GaN/sapphire and (b) AlN/T-GaN/sapphire lateral device samples in dark and under UV illumination condition. A UV LED ($\lambda=255$ nm) with a variable optical power was used for illuminating the samples during the measurements ($T=300$ K).

The poor lateral conduction in the T-GaN films is likely to be related to its bulk property (*i.e.* poor carrier concentration and/or high defect density) rather than being limited by the metal-semiconductor contact. Vertical conduction has been observed through a similar Al contacted T-GaN film on Si with a reverse leakage current of more than 10^{-10} A (section 7.4.2). The measured lateral current in the range of 10^{-13} A ($\sim$ noise level of the measurement system) with no clear voltage dependent therefore cannot be explained based on the back-to-back Schottky diode characteristics of the device.

All T-GaN samples grown on sapphire however showed photo-conductive behavior in the presence of a UV LED light source of 255 nm wavelength (also for 280 nm), as shown in Fig. 7.13(a). The optically generated electron-hole pairs are responsible for the observed photo-conduction behavior. As expected, the measured photo-current also scales with the optical power (of the UV light source) and is shown for the AlN capped T-GaN sample in Fig. 7.13(b). Moreover, the photo-conduction in the AlN capped sample was three times higher in magnitude compared to that of its counterparts. AlN may be preventing the GaN surface from being oxidized in the air and thereby keeping the intrinsic properties such as the bandgap, of the

Figure 7.14: Time (history)-dependent $I - V$ characteristics of the AlN/T-GaN/sapphire sample, (a) at different times after switching off the UV light and (b) at different times when the UV light is on ($T=300 \text{ K}$).

as-grown layer preserved. It could also be that the AlN helps in preventing reflection losses at the surface, thereby leading to more light absorption inside the GaN layer. The observed photo-conductance in the T-GaN sample also highlights that the film bulk properties, mainly its low carrier concentration, is responsible for its observed electrically insulating nature in the lateral direction under dark condition.

Further, the samples also showed the persistence photo-conductivity (PPC) effect [269] where the conductivity decays gradually with time and not immediately after switching off the exciting light source, see Fig. 7.14(a). The quick recovery to the initial unperturbed dark state is delayed by the presence of charge carriers (hence current) higher than their steady dark level. Moreover the samples also showed a higher photocurrent when excited for a consecutively second time with UV light before it was fully recovered from the first excitation (see Fig. 7.14(b)). The photo-generated electron-hole pairs remain in the sample for some time after switching off the light source and do not immediately extinct. This phenomenon is common in wide bandgap materials with a high defect density where the probability of the electron capture exceeds that of recombination [269]. This property is however undesirable for photodetector applications where a fast photo response is needed. The time to full recovery or the time between subsequent excitation, though not thoroughly investigated, was estimated to be in order of few minutes.

7.4.2 Vertical conduction in T-GaN

A T-GaN/p-Si diode (see Fig. 7.15(b)) was also realized to examine the vertical electrical conduction properties of the grown T-GaN film. Rectifying $I - V$ characteristics were observed as shown in Fig. 7.15(a). This measurement shows that the T-GaN film, although restricting the lateral conduction, allows the current to flow vertically. The T-GaN/p-Si diode

Figure 7.15: (a) Measured $I - V$ characteristics of the T-GaN/p-Si diode compared to that of the P-GaN/p-Si diode. Schematic cross-section and illustrated current flow lines for, (b) the T-GaN/p-Si diode and (c) the P-GaN/p-Si diode.

also showed higher rectification and a lower leakage current compared to its P-GaN counterpart (refer to chapter 6). Moreover, no peripheral current component (J_p) was observed in case of the former unlike its counterpart where a significant J_p was measured. The observed lower leakage current in the T-GaN/p-Si diode can be attributed to the absence of J_p .

The schematic cross-section in Figs. 7.15(b)-(c) illustrate the possible current flow lines in both diodes. For the T-GaN/p-Si diode there will be hardly any current spreading from the contact due to the poor lateral conductivity of the T-GaN film. While in the P-GaN/p-Si diode, the current spreads laterally away from the contact (hence significant J_p), possibly due to the presence of a surface conductive channel, before entering into the Si substrate. More electrical measurements as discussed below will further clarify the current flow lines illustration as depicted in Figs. 7.15(b)-(c).

In order to further highlight the possible role of a surface conductive channel in the observed electrical properties of the grown P-GaN film, and its comparison to that of T-GaN film, a dedicated test structure comprising two parallel diodes was utilized. In this test structure the first vertical diode ($D - 1$) is surrounded by the second vertical diode outer ring ($D - 2$) as shown schematically in Fig. 7.16(a). The latter, when biased in parallel, acts as a guard ring for the former and thereby inhibit any surface current flow in the region between the two diodes.

For the P-GaN/p-Si device, Fig. 7.16(b) shows the measured vertical current of the $D - 1$ when operated alone (I_1) and in parallel (I'_1) with $D - 2$. The strong reduction in the current (both forward and reverse) of $D - 1$ when operated in parallel with $D - 2$ suggest the presence of surface conduction channel between the two diodes which is responsible for the relatively high leakage current. Note that this is even true for a 20 μm spacing between the two diodes. Therefore, the measured difference between I_1 and I'_1 for the P-GaN device can not be explained solely based on the minority current spreading phenomenon, as discussed in chapter 3 using the "2-diodes" measurements. Moreover, the current in $D - 2$ remains

Figure 7.16: (a) Schematic device cross-section and test configuration for measuring the inner diode (D – 1) current, with and without connecting outer diode ring (D – 2) in parallel. Measured I – V characteristics for, (b) the P-GaN device and (c) the T-GaN device. I_1 and I_1' refers to the current through D – 1 when the D – 2 ring is disconnected and connected in parallel, respectively (T=300 K).

unaffected irrespective of whether D – 1 is operating in parallel or not as it remains unguarded in either situation. Note that the poor rectification and the higher leakage current observed on this sample compared to other measurements (ref. to chapter 6) on the same sample is possibly due to its aging with time.

Conversely, no discrepancy is observed between I_1 and I_1' for the T-GaN diodes. This confirms that there is no dominating surface leakage path and no current spreading in the T-GaN film due to its poor lateral conductivity.

The lateral current transport in a T-GaN/p⁺-Si structure as shown schematically in Fig. 7.17(a) is examined next. Provided that the metal contacts on top of the T-GaN film do not limit the current, it is expected to scale with the spacing, S , between the contacts but is not influenced by the contact length, L . However the current scales with varying L (see Fig. 7.17(b)) and remains unaffected with a change in S (see Fig. 7.17(c)). The measured non-linear current was limited by the vertical leakage of the heterojunction diode. These measurements indicate that the current first flows vertically through the T-GaN film before crossing the heterojunction to the reach p⁺-Si region. There it flows laterally (via diffusion) and then finally returns back to the other contact again via the vertical path through the T-GaN film. This current path is indicated using flow lines in Fig. 7.17(a). These results reconfirm that the T-GaN has a poor lateral conductivity and

Figure 7.17: (a) Schematic cross-section of the T-GaN/p⁺-Si structure. Measured I – V characteristics of the same structure in the lateral direction, (b) with varied contact length, L and (c) with varied spacing, S, between the contact. The substrate contact was electrically isolated during these measurements.

therefore the current doesn't spread sideways when injected via the contact. Note that, instead of diffusion in bulk p⁺-Si, the lateral current inside p⁺-Si could also flow via possible electron inversion layer (ref. Fig. 6.3 in chapter 6) in the Si at the GaN/p-Si interface.

Conversely, similar measurements on the P-GaN/p-Si structure showed that the current clearly scaled with the contact spacing, but does not change with the contact length, as expected from a lateral current flow via the P-GaN film.

7.5 Discussion

From the elaborate analysis, it can be concluded that there is high electron density in the P-GaN layer. It is however not established whether these electrons have been distributed across the film thickness or are more concentrated near the surface, though some measurements hint more towards the latter. The observed SCLC limited charge transport in the vertical diode, as discussed in the previous chapter 6, suggests the presence of low electron density ($\sim 10^{15} \text{ cm}^{-3}$) in the bulk P-GaN layer. At the same time, the discerned SCLC mechanism also indicates good ohmic contacts (hence high electron density) where the electron injection is not contact limited in the measured voltage range. Both conditions are satisfied by the surface channel model where a high electron density is located near the interface

promoting an ohmic contact while the electron concentration is relatively low inside the bulk of the film with high trap density. Further, the presence of surface channel could also underline the main reason for the observed high peripheral component, J_p , in the measured diode current.

The observed striking contrast in the lateral conductance of the two types of poly-GaN films could be related to the possible difference in their crystal structure, stoichiometry and/or impurity (C, H, O) concentrations. The crystallinity of PEALD films have been known to be generally better than that of thermally-grown films [223]. P-GaN films are also found to be N-rich while T-GaN is more Ga-rich. The observed Ga richness attributed to the accumulation of unreacted TMG-chemisorbed sites, which had actually not converted into GaN, could also possibly explain the poor lateral conductance of the T-GaN layer [223]. Moreover, the higher hydrogen content in the T-GaN layer could also be responsible for its insulating nature.

In addition, the (effective) electron concentration (unintentional doping) in the two films could also be different. The problem of unintentional doping in GaN films has been well articulated by Zhu and Oliver before [270]. It is argued that the role of native defects, such as nitrogen vacancies, (unlike originally thought by early crystal growers) is less important for possible n-type shallow donors due to their high formation energy. This prohibits their spontaneous creation during film growth. On the contrary, the impurities (mainly oxygen) are responsible for the observed n-type conductance in undoped GaN films [270]. Oxygen, can act as a shallow donor by substituting nitrogen from its site, a reaction which is also energetically favorable. Carbon impurity on the other hand is more likely to result in p-type doping as suggested by the first principal calculations. If conductive channel formation is indeed due to the substitution of N by O, the origin of which is either due to surface oxidation or from the bulk oxygen content, then O may be substituting N in somewhat different manner in P-GaN and T-GaN. This could arise from differences in their lattice structure, for example. Further study is needed to clarify this.

Previously, PolyGaN based FETs have been reported by several groups [39, 41, 271–273]. Their process often involved doped source/drain junctions, high temperature annealing or a GaN/AlN heterojunction to improve the channel conductivity. High temperature annealing ($\sim 800^\circ\text{C}$) may also help in improving the T-GaN film conductivity by reducing the defect density and the contact resistance [272] and therefore could be interesting to experiment in the future.

With the present knowledge of the electrical properties of the grown poly-GaN layers presented in this chapter, various potential applications of these materials can be proposed. P-GaN could be attractive for improving the efficiency of Si based IR emitters, or even solar cells without the need of any doped junction, as discussed in the chapter 6. Further, the lateral (surface) conductive channel in the P-GaN film, if optimized (for gate

control, channel mobility), could also be promising for FET applications again without requiring any additional doping. A similar concept has been widely exploited in hydrogen-terminated diamond for realizing surface channel FET [274].

T-GaN films can be utilized to realize self isolating vertically functioning devices owing to its poor lateral conductivity. T-GaN films could also be interesting for UV-detection applications as observed from the photo-conduction measurements. However, the response time which is plagued by persistence photo-conductivity effect could be of a concern for certain applications. T-GaN could also be attractive for realizing the EHB-LED as proposed in chapter 5 using a combination of high-low gate work functions and AlN as a gate dielectric. Such a dual gate GaN/AlN stack can be easily realized by ALD without breaking the vacuum ensuring good quality interfaces. Further, the polycrystalline nature of the GaN film, though adversely affect light emission, could benefit from its possibly high thermal generation rate as required for the undoped EHB LED operation.

Finally, with regard to possible ED-based poly-GaN devices (switches, LED), P-GaN films in the present form are less suitable as they contain a high density of electron charge which is difficult to deplete or invert either via a Schottky contact or by a applied gate bias. The T-GaN film on the other hand could be interesting for ED-based vertical devices, for *e.g.* EHB LED as discussed above. Extreme work function contacts such as MoO_x, which appears to be very promising on Si, could also be explored for realizing undoped bipolar devices in poly-GaN material. However more experiments and optimizations of poly-GaN films properties are required to evaluate their true potential for ED based device applications.

7.6 Conclusion

An electrical analysis of ALD grown poly-GaN layers was carried out in this chapter. It was found that P-GaN is both vertically and laterally conductive. The vertical conduction in the P-GaN layer is limited by the SCLC mechanism while linear $I - V$ characteristics were obtained in the lateral direction. Hall measurements confirm the presence of a high electron sheet density ($\sim 10^{14} \text{ cm}^{-2}$) which was found to be practically independent of the temperature. The Hall mobility (μ_n) was however found to be temperature dependent with a similar thermal activation as that of conductivity. This observation was explained in the framework of the long-range potential fluctuations model and the percolation theory.

The T-GaN film on the other hand was found to be vertically conductive but laterally insulating under dark condition. The T-GaN film also showed the persistence photoconductivity effect under UV illumination suggesting a low free carrier density and a high trap density inside the layer.

Based on these observed electrical properties of the poly-GaN films various possible applications were proposed.

CONCLUSIONS AND RECOMMENDATIONS

In this chapter, general conclusions of the work presented in this thesis are summarized and the key original contributions of this thesis are listed. Finally, recommendations and directions for possible future work are proposed.

8.1 General conclusions

Electrostatic doping is a potential solution to the problems connected with chemical doping in UTB devices and emerging semiconductors. With performance at par with conventionally doped counterparts, ED based devices offer additional benefits such as low temperature realization and reconfigurable functionality that could be interesting for future CMOS devices. Moreover ED offers an opportunity to realize innovative device concepts such as EHB-LEDs. Among various reported ED devices, high-barrier Schottky diodes based on extreme work function contacts are a potentially attractive solution for realizing bipolar devices (such as BJTs, LEDs) without adding any doping. Hetero-contacts using extreme work function materials such as MoO_x offers a possible dopant-free, low temperature route of realizing such high-barrier diodes with bipolar conduction capabilities. Such extreme work function contacts when applied to UTB semiconductors could lead to the formation of localized n-type or p-type regions via volume inversion which can be exploited for various applications.

Thin-film ALD grown poly-GaN on Si is also an interesting technology platform and could open up a new route towards future nanoscale (opto-)electronic devices. For example, engineered poly-GaN/Si heterostructures could be a way forward for making efficient optoelectronic devices such

as IR emitters and solar cells realized in bulk Si. Realization of functional devices based on this material would in general benefit from ED approaches developed in this work, particularly for realizing an n-type region. For p-type ED in such wide bandgap material, high work function materials such as MoO_x should be explored. Moreover, such contact if optimized can also be employed to lower down the contact resistance of p-type contacts. Further, the EHB-LED concept as proposed in this work could also be utilized in poly-GaN technology platform for light emitting applications.

However, more experiments are needed to access the true merits of poly-GaN thin films and proposed ED solutions.

8.2 Original contributions of this thesis

The work presented in this thesis contains several original contributions:

- ED has been previously reported for various material systems and different device geometries. However this approach has never been treated holistically and in a more generalized way using a common theoretical platform. This thesis reviews, defines and discusses the ED approaches for their applicability and adaptability to different material systems and geometries using simple 1-D electrostatics.
- Minority carrier injection in conventional Schottky diodes has been discussed previously, mostly as a high injection phenomenon. This thesis revisits the physics of a high-barrier diodes from an ED perspective and differentiates the operation from conventionally Schottky devices. The modeling/simulation work shows the possibility of using high-barrier Schottky diodes with a high minority-carrier injection ratio as a possible replacement of doped junctions for various bipolar device applications such as light emitters and transistors.
- The high work function property of MoO_x has previously been reported for realizing a "hole-selective contact" in Si solar cells. However its application to realize an undoped Si diode with bipolar current characteristics was discussed and demonstrated for the first time in this work. Alongside high-barrier property of such contact to Si, the role of SiO_x interlayer and resulting reduced surface recombination velocity was shown to play a key role in suppressing the electron injection from the substrate. Using such MoO_x based contacts, bipolar transistor action and light emission were also demonstrated in bulk undoped Si substrates for the first time paving the way forward for undoped transistors and LEDs.
- A one to one comparison between the electrical and optical properties of high-barrier $\text{Pd}/\text{MoO}_x/\text{n-Si}$ diodes and implanted $\text{p}^+/\text{n-Si}$ reference diodes (realized in the same technology) is presented for the first time in this work.

- A light emitting device concept based on electrostatically induced electron-hole bilayer in undoped UTB channel semiconductor has been proposed and investigated using TCAD simulations for the first time.
- Polycrystalline GaN based heterojunction diodes to silicon has been realized and studied for the first time in this work. The heterojunction to poly-GaN layer improved the infrared light emission from bulk Si by almost three orders in magnitude. Further, the electrical properties of poly-GaN thin films has also been investigated and analyzed in this work for their possible device applications.

8.3 Recommendations and future work

- Electrical measurements on $\text{MoO}_x/\text{n-Si}$ diodes reported in this work showed that the electron current is relatively low compared to the hole current but the actual level of the former is still unknown. Experiments on MoO_x based vertical bipolar transistor test structures in bulk Si will be needed for individually extracting the electron and hole components of the current. The minority carrier injection ratio, γ , can be determined from these electrical measurements which would shed more light on the bipolar conduction in such diodes.
- In this work, the proof-of-concept SBT has been demonstrated on a bulk Si substrate with unoptimized device geometry for its ease of experimental realization. However for obtaining a high gain bipolar transistor, such a concept should be tried experimentally on SOI or other UTB semiconductor technology as shown with TCAD simulations in this work.
- The surface inversion in a semiconductor (in our case Si) when contacted with extreme work function materials such as MoO_x , was confirmed experimentally from its sheet resistance and diode characteristics. Such contacts when applied to UTB layers could lead to volume inversion. However experiments are needed to assess the true potential of such contacts. Further, the use of proposed $C - V$ technique [275] can be explored to obtain the signature of induced ED in UTB devices.
- In this work the EHB-LED concept is proposed and investigated via TCAD simulations. However, experimental realization of such a device is a must to assess its true potential and therefore should be the focus of future work. It will be interesting to investigate the EHB LED based on poly-(In)GaN material for UV/visible light applications. EHB formation in such polycrystalline materials may benefit from possibly high thermal generation rate while light emission in general would profit from its direct bandgap. Moreover, a dual gate stack

(e.g. AlN/GaN/AlN) as required for EHB LED can be realized using an ALD process without actually breaking the vacuum ensuring high quality interfaces. Further, MoO_x along with LiF_x can be explored as high/low work function gate electrodes.

- In this work it was theoretically established that an array of small nm-size Schottky contacts are better light emitters than a single big μm -size contact. This concept could be interesting when designing light emitters based on Schottky contacts and therefore should be experimentally investigated in the future.
- Most ED ideas developed in this work have been initially investigated on Si. Such ideas should however be ultimately investigated on (poly-)GaN. The EHB-LED is one example proposed above. Other ideas such as MoO_x based (high-)barrier diodes on n-type (intrinsic) GaN could be interesting for light emission. A similar contact if optimized on p-type (poly-)GaN could help in forming a good ohmic contacts with a low contact resistance.
- Along with the high work function MoO_x contact for p-type ED, a low work function material such as Hf, Cs or even LiF_x should be explored for n-type ED. An experimental toolbox equipped with such complimentary work function electrodes would be convenient for designing any ED based device application in different semiconductors.
- Other applications of poly-GaN thin films should also be explored. For example, the highly conductive channel in P-GaN should be investigated for FET or even power applications. In general, poly-GaN/Al(Ga)N heterostructures or even their superjunction should be investigated in more detail for polarization induced 2-DEGs and 2-DHGs which was not the focus of this work.
- Last but not the least, adhesion issues (on GaN), temperature stability and high resistivity of extreme work function contacts such as MoO_x should be addressed for reliable technology application. In addition, systematic annealing experiments which were avoided throughout this work should be the part of future work for optimized, reproducible and robust contact properties.

ELECTRIC FIELD AND CARRIER CONCENTRATION IN THE ELECTRON-HOLE BILAYER SYSTEM

A case of electrostatically induced electron-hole bilayer (EHB) in dual gated UTB channel is considered and a closed-form analytical expressions for its formation are derived based on 1-D electrostatics. For doing so, quantum mechanical effects as reported before by Trivedi and Fossum [276] for dual gate SOI MOSFETs and more recently, Alper *et al.* [108] for EHB-TFET systems are neglected.

From Fig. 2.11, it can be written that

$$V_{GT} = V_{oxT} + \Delta\phi_{mT} + \psi_{sT} \quad (A.1)$$

$$V_{GB} = V_{oxB} + \Delta\phi_{mB} + \psi_{sB}, \quad (A.2)$$

where V_{GT} and V_{GB} are top and bottom gate voltages, V_{oxT} and V_{oxB} are voltage drops across top and bottom oxides, $\Delta\phi_{mT}$ and $\Delta\phi_{mB}$ are top and bottom gate-body work function difference and ψ_{sT} and ψ_{sB} are top and bottom surface potentials. Now applying Gauss' law at both surfaces of the semiconductor body it can be written that

$$V_{oxT} = \frac{1}{C_{oxT}}(\epsilon_s E_{sT} - Q_{fT} - Q_{iT}) \quad (A.3)$$

$$V_{oxB} = \frac{1}{C_{oxB}}(-\epsilon_s E_{sT} - Q_{fB} - Q_{iB}) \quad (A.4)$$

where C_{oxT} and C_{oxB} are the top and bottom areal oxide capacitances, E_{sT} is the electric field in the body at the top surface, ϵ_s is the semiconductor

The derivations were performed by R.J.E. Hueting.

dielectric constant, Q_{fT} and Q_{fB} are fixed charge densities, and Q_{itT} and Q_{itB} are the interface trapped charge densities at top and bottom surfaces respectively. Since full depletion is assumed, the electric field is constant inside the body:

$$\psi_{sT} - \psi_{sB} = E_{sT}t_s = -E_{sB}t_s \quad (A.5)$$

where t_s is the thickness of the body and E_{sB} is the electric field in the body at the bottom surface. Now for simplicity sake, neglecting fixed charge at both surfaces and a relatively small inversion charge, it can be written that

$$\psi_{sT} = V_{GT} - \frac{\epsilon_s E_{sT}}{C_{oxT}} - \Delta\phi_{mT} \quad (A.6)$$

$$\psi_{sB} = V_{GB} + \frac{\epsilon_s E_{sT}}{C_{oxB}} - \Delta\phi_{mB}. \quad (A.7)$$

Subtracting Eq. (A.7) from Eq. (A.6) and replacing the term $\psi_{sT} - \psi_{sB}$ with $E_{sT}t_s$ and substituting $C_{oxT} = \epsilon_{ox}/t_{oxT}$ and $C_{oxB} = \epsilon_{ox}/t_{oxB}$ it can be obtained that

$$E_s = \frac{(V_{GT} - V_{GB}) - (\phi_{mT} - \phi_{mB})}{\frac{\epsilon_s}{\epsilon_{ox}}(t_{oxT} + t_{oxB}) + t_s}. \quad (A.8)$$

The effect of the interface traps on the electrostatics of the EHB system can also be incorporated here. Consider a device in which $t_{oxB} = t_{oxT} = t_{ox}$ with the same uniform interface trap charge density at both semiconductor surfaces, then there is a constant areal interface capacitance C_{it} , and consequently $Q_{itT} = C_{it} \cdot \psi_{sT}$ and $Q_{itB} = C_{it} \cdot \psi_{sB}$. Then it can be obtained that

$$E_s = \frac{(V_{GT} - V_{GB}) - (\phi_{mT} - \phi_{mB})}{\frac{2\epsilon_s}{\epsilon_{ox}} \cdot t_{ox} + \left(1 + \frac{C_{it} \cdot t_{ox}}{\epsilon_{ox}}\right) \cdot t_s}. \quad (A.9)$$

Hence for the same biasing conditions it can be concluded that the higher the C_{it} , *i.e.* the higher trap density, the lower the E_s and therefore the effectiveness of the EHB concept.

SOLUTION OF POISSON'S EQUATION IN THE PRESENCE OF INVERSION LAYER

A high-barrier n-type Schottky diode where a hole inversion layer has formed at the MS interface as shown in Fig. B.1 is considered. Here $\phi(x)$ is the electron potential from the bottom of the conduction band edge E_c with boundary conditions $\phi(0) = \phi_b$ and $\phi(\infty) = \phi_e$.

Figure B.1: Schematic energy band diagram for a high-barrier n-type Schottky diode [136]. + sign denotes a hole, - sign denotes an electron and circle with a + sign denotes a donor charge.

By adapting the methodology as outlined in [136] and considering unequal conduction band (N_c) and valence band (N_v) effective density of states in this work, the electron density, n , at thermal equilibrium at any distance x from the interface can be written as:

$$n(x) = N_d \exp \left(\frac{-(\phi(x) - \phi_e)}{u_T} \right). \quad (B.1)$$

Similarly, assuming Boltzmann's approximation, the hole density, can be written as:

$$p(x) = \frac{n_i^2}{n(x)} = \frac{n_i^2}{N_d} \exp \left(\frac{\phi(x) - \phi_e}{u_T} \right), \quad (B.2)$$

where n_i is the intrinsic carrier concentration, and u_T is the thermal voltage ($=kT/q$, where k is Boltzmann's constant, T is the temperature and q is the elementary charge).

At any applied voltage, V_d :

$$n(x) = N_d \exp \left(\frac{-(\phi(x) - \phi_e - V_d)}{u_T} \right), \quad (B.3)$$

and

$$p(x) = \frac{n_i^2}{N_d} \exp \left(\frac{\phi(x) - \phi_e}{u_T} \right). \quad (B.4)$$

Note that $p(x)$ is independent of V_d in the space charge region as it is determined by ϕ_b which is constant. For such an MS junction, the 1-D Poisson's equation can be written as:

$$\begin{aligned} \frac{d^2\phi}{dx^2} &= \frac{q[N_d + p(x) - n(x)]}{\epsilon_s} \\ &= \frac{q}{\epsilon_s} \left[N_d + \frac{n_i^2}{N_d} \exp \left(\frac{\phi(x) - \phi_e}{u_T} \right) - N_d \exp \left(\frac{-(\phi(x) - \phi_e - V_d)}{u_T} \right) \right] \\ &= \frac{qN_d}{\epsilon_s} \left[1 + \frac{n_i^2}{N_d^2} \exp \left(\frac{\phi(x) - \phi_e}{u_T} \right) - \exp \left(\frac{-(\phi(x) - \phi_e - V_d)}{u_T} \right) \right] \end{aligned} \quad (B.5)$$

Now, let's define

$$\frac{qN_d}{\epsilon_s} \left[1 + \frac{n_i^2}{N_d^2} \exp \left(\frac{\phi(x) - \phi_e}{u_T} \right) - \exp \left(\frac{-(\phi(x) - \phi_e - V_d)}{u_T} \right) \right] = F(\phi) \quad (B.6)$$

and

$$\frac{d\phi}{dx} = E(\phi) \quad (B.7)$$

Therefore,

$$\frac{dE}{dx} = F(\phi), \quad (B.8)$$

$$\begin{aligned} dE &= F(\phi) dx \\ &= \frac{F(\phi) d\phi}{d\phi/dx}, \end{aligned} \quad (B.9)$$

and

$$E dE = F(\phi) d\phi. \quad (\text{B.10})$$

Integrating Eq. (B.10) on both sides

$$\int E dE = \int F(\phi) d\phi \quad (\text{B.11})$$

yields

$$\frac{E^2}{2} + C_1 = f(\phi) + C_2, \quad (\text{B.12})$$

where $f(\phi)$ is the anti-derivative of $F(\phi)$ and C_1 and C_2 are constants of integration. Using the boundary condition that $d\phi/dx = E = 0$, at $\phi = \phi_e + V_d$, it can be obtained that

$$C_1 - C_2 = f(\phi_e + V_d). \quad (\text{B.13})$$

Combining Eqs. (B.7), (B.12) and (B.13) it can be obtained that

$$\frac{1}{2} \left(\frac{d\phi}{dx} \right)^2 = f(\phi) - f(\phi_e + V_d). \quad (\text{B.14})$$

After taking the square root and integrating on both sides, Eq. (B.14) can be rearranged as

$$\int_0^x dx = \int_{\phi_b}^{\phi} \frac{d\phi}{\sqrt{2(f(\phi) - f(\phi_e + V_d))}}. \quad (\text{B.15})$$

Now, using Eq. (B.6)

$$f(\phi) = \frac{qN_d}{\epsilon_s} \left[\phi + \frac{n_i^2}{N_d^2} u_T \exp \left(\frac{\phi(x) - \phi_e}{u_T} \right) + u_T \exp \left(\frac{-(\phi(x) - \phi_e - V_d)}{u_T} \right) \right] \quad (\text{B.16})$$

and

$$f(\phi_e + V_d) = \frac{qN_d}{\epsilon_s} \left[\phi_e + V_d + \frac{n_i^2}{N_d^2} u_T \exp \left(\frac{V_d}{u_T} \right) + u_T \right]. \quad (\text{B.17})$$

Therefore, integrating Eq. (B.15) yields

$$x = \int_{\phi_b}^{\phi} \frac{d\phi}{\sqrt{2(f(\phi) - f(\phi_e + V_d))}}. \quad (\text{B.18})$$

The shape of barrier or plot of ϕ as a function of distance x can be obtained by numerical integration of Eq. (B.18) after inserting $f(\phi)$ from Eq. (B.16) and $f(\phi_e + V)$ from Eq. (B.17).

The capacitance of the diode can be obtained from calculating the change in the number of electrons in the conduction band with change in the applied bias and therefore can be expressed as follows [136]:

$$C = q \frac{dN}{dV_d}, \quad (\text{B.19})$$

where N represent the change in the number of electrons in the conduction band with the applied bias which is equivalent of calculating the total number of unneutralized donors in the conduction band and can be expressed as:

$$N = \int_0^{\infty} (N_d - n) dx. \quad (B.20)$$

Now, using n from Eq. (B.3)

$$(N_d - n) = N_d \left(1 - \exp \left(\frac{-(\phi(x) - \phi_e - V_d)}{u_T} \right) \right). \quad (B.21)$$

Therefore,

$$\begin{aligned} C &= q \frac{dN}{dV_d} = q N_d \frac{d}{dV_d} \int_0^{\infty} \left[1 - \exp \left(\frac{-(\phi(x) - \phi_e - V_d)}{u_T} \right) \right] dx \\ &= q N_d \frac{d}{dV_d} \int_0^{\infty} \left[1 - \exp \left(\frac{-(\phi(x) - \phi_e - V_d)}{u_T} \right) \right] \frac{d\phi}{d\phi/dx} \quad (B.22) \\ &= q N_d \frac{d}{dV_d} \int_{\phi_e + V_d}^{\phi_b} \frac{\left[1 - \exp \left(\frac{-(\phi(x) - \phi_e - V_d)}{u_T} \right) \right]}{\sqrt{2(f(\phi) - f(\phi_e + V_d))}} d\phi. \end{aligned}$$

The capacitance of the diode as a function of applied bias can therefore be numerically computed using Eq. (B.22).

DERIVATION OF CHARGE CARRIERS THERMAL GENERATION TIME

In the absence of impact ionization and under dark conditions, the carrier generation will be mainly via thermal processes. The thermal generation rate can be distinguished by four processes: bulk space-charge (scr) generation (G_1), band-to-band generation (G_2), quasi-neutral bulk generation (G_3) and surface generation (G_4). G_1 is characterized by the generation time (τ_g) [262] and G_2 is characterized by the radiative recombination coefficient (B_{rad}) which is equally important for direct bandgap semiconductors. For the UTB based EHB concept G_3 can be ignored. Further, ideal interfaces are assumed here hence surface generation (G_4) is absent.

For convenience sake, let's focus on a 1-D system with uniform concentrations. Using the continuity equation for electrons (ignoring holes) it can be written [262]:

$$\frac{dn}{dt} = G = G_1 + G_2 \quad (C.1)$$

where G is the net generation rate due to various mechanisms.

For bulk scr generation when $pn < n_i^2$, which is actually the inverse of SRH recombination, the generation rate can be expressed as [262]:

$$G_1 = -R_{SRH} = \frac{n_i^2}{\tau_p n_1 + \tau_n p_1} = \frac{n_i}{\tau_g} \quad (C.2)$$

Assuming SRH lifetimes $\tau_n = \tau_p = \tau_{SRH}$ and defect level (E_T) coinciding with the intrinsic Fermi level (E_{Fi}), Eq. (C.2) can be re-written as:

$$G_1 = \frac{n_i}{2\tau_{SRH}} \quad (C.3)$$

The derivations were performed by R.J.E. Hueting.

The band-to-band generation can be expressed as:

$$G_2 = \frac{n}{\tau_{\text{rad}}} = B_{\text{rad}} n_i^2, \quad (\text{C.4})$$

So, substituting Eqs. (C.3)-(C.4) in Eq. (C.1), it can be written that:

$$\frac{dn}{dt} = \frac{n_i}{2\tau_{\text{SRH}}} + B_{\text{rad}} n_i^2. \quad (\text{C.5})$$

Now, the number of electrons, n_0 , generated in the total time t_{th} can be determined as:

$$n_0 = \int_0^{t_{\text{th}}} G dt = \int_0^{t_{\text{th}}} \left(\frac{n_i}{2\tau_{\text{SRH}}} + B_{\text{rad}} n_i^2 \right) dt. \quad (\text{C.6})$$

In principle the generation components do not have a strong time dependence, and consequently:

$$t_{\text{th}} = \frac{n_0}{\left(\frac{n_i}{2\tau_{\text{SRH}}} + B_{\text{rad}} n_i^2 \right)}. \quad (\text{C.7})$$

From the above simplified expression, it can be concluded that the generation time t_{th} rises exponentially with the bandgap through n_i and therefore narrow (and direct) bandgap materials are more effective for the thermally generated EHB concept.

INVERSION LAYER IN HIGH-BARRIER Pd/MoO_x/N-Si DIODES

The systematic electrical investigation of Pd capped MoO_x contacts on Si, both n-type and p-type, using dedicated ring-shaped test structures has been reported before in [169]. On those test structures, inversion layer went undetected as current choose to flow via top Pd layer instead of inversion layer. In order to satisfactorily establish the presence of the hole inversion layer at the MoO_x/n-Si interface and to measure its sheet resistance, insulating capping layer is more beneficial instead of conductive layer. For this purpose, another sample with similar test structures was prepared in which conductive Pd capping layer was substituted with a thin insulating boron (B) layer of ~10 nm following the same (in-situ B/MoO_x e-beam deposition) procedure as described before [169]. For boron, 99.5 % pure material from Kurt J. Lesker in the form of cylindrical ingots was utilized. No thermal annealing was performed on any of the prepared samples.

A series of electrical measurements were performed on boron capped MoO_x test structures to check whether there is lateral conduction via the inversion layer. In this case, contact to the inversion layer is made via doped regions after scratching away the few nm of boron layer from top (see inset of Fig. D.1). Unlike on Pd capped samples, clear downscaling of measured resistance was observed with decreasing ring width confirming the lateral conduction via inversion layer.

The inversion layer sheet resistance was extracted using differential measurements on ring structures to exclude the contact resistance using

This appendix is supplementary to the work presented at the 32nd IEEE International Conference on Microelectronic Test Structures (ICMTS), 2019 [169]. The device fabrication for this work was performed by D.T. Shivakumar.

the methodology as described in [277, 278]. The sheet resistance, R_{sh} , can be estimated as [277, 278]:

$$R_{sh} = \frac{R_{ij}}{\alpha_{ij}} = \frac{R_{mj} - R_{mi}}{\alpha_{ij}}, \quad (D.1)$$

where R_{ij} is the differential resistance between two ring structures of indices i/j with different ring width, $L_{i/j}$. $R_{mi/j}$ is the measured resistance across the ring and α_{ij} is the coefficient associated between ring pair $i - j$ and can be expressed as:

$$\alpha_{ij} = \frac{1}{2\pi} \ln \left(\frac{(r_g - \frac{1}{2}L_i) \cdot (r_g + \frac{1}{2}L_j)}{(r_g + \frac{1}{2}L_i) \cdot (r_g - \frac{1}{2}L_j)} \right), \quad (D.2)$$

where r_g is the ring radius which is fixed and equal to $164 \mu\text{m}$. Using, Eqs. D.1-D.2, the sheet resistance of inversion layer is extracted as shown in Fig. D.1. From measurements across different ring pairs (shown for only 6 pairs), $R_{mi/j}$ in the range of $60\text{--}100 \text{ k}\Omega/\square$ was extracted. Similar measurements on p-substrate (with n^+ doped regions) did not showed any conductance which further confirms that the measured resistance is indeed associated with the hole inversion layer. Moreover, the sheet resistance of as deposited boron layer is around $1 \text{ M}\Omega/\square$ and therefore doesn't contribute to the measured sheet resistance.

Table D.1 summarizes the results of electrical measurements from [169] and their comparison to values reported in literature. The investigation of the conductance along the Si surface on B/MoO_x/n-Si test structures did reveal the presence of a hole inversion layer as has been reported in the literature albeit with relatively high sheet resistance in the range of $60\text{--}100 \text{ k}\Omega/\square$. The extracted sheet resistance of inversion layer in the

Figure D.1: Extraction of inversion layer sheet resistance using differential resistance measurements of lateral S3 ring structures with various ring widths, L_i .

Table D.1: Electrical properties of the Pd/MoO_x stack on silicon as extracted from the measurements on ring-shaped test structures [169] and compared to literature values. Inversion layer sheet resistance reported here is extracted from the measurement on B/MoO_x/n-Si test structures instead.

	contact resistivity, Pd/MoO _x to p-Si, ρ_c ($\Omega\text{-cm}^2$)	resistivity, MoO _x ρ_{MoO_x} ($\Omega\text{-cm}$)	sheet resistance, inversion layer $R_{\text{sh-inv}}$ ($\text{k}\Omega/\square$)	sheet resistance, p ⁺ implant $R_{\text{sh-p}^+}$ ($\Omega/\square$)
our work [169]	1.2×10^{-3}	1.5×10^4	60-100	25
literature values	1.0×10^{-3} [174]	5×10^4 [174]	12 [174]	25 [278]

range of 60-100 $\text{k}\Omega/\square$ is in contrast to the reported sheet resistance value of $\sim 12 \text{ k}\Omega/\square$ in [174]. High sheet resistance value indicates that either the MoO_x/Si bonding structure that supposedly is responsible for the inversion of the n-Si interface only occurs in electrically separated islands, or if the interface has high defect density that seriously deteriorates the carrier mobility. Both explanations are consistent with the fact that the hole injection from the MoO_x into the Si is similar to that measured on fully-implanted p⁺-n diodes. Further, the role of the thermal annealing step, which has not been explored in our work due to the known temperature instability of MoO_x [193–195], could also be interesting for a future study. Finally, though MoO_x readily forms an ohmic contact to p-Si without any thermal annealing step, the contact resistivity of Pd/MoO_x/Si stack as also reported before [174] is too high for any device application. The contact resistivity, $\rho_c = 1.2 \text{ m}\Omega\text{-cm}^2$, was measured on the p-Si interface which could be an order of magnitude higher on the n-Si interface [174] making it suitable only for large area devices such as solar cells.

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LIST OF PUBLICATIONS

Journal articles

1. G. Gupta, D.T. Shivakumar, L.K. Nanver and R.J.E. Hueting, "Investigation of Pd/MoO_x/n-Si diodes for bipolar transistor and light-emitting device applications", (submitted to Journal of Applied Physics)
2. G. Gupta, F. Mema and R.J.E. Hueting, "Electron-hole bilayer light-emitting device: Concept and operation", Solid-State Electronics, vol. 168, 107726, June, 2020.
3. G. Gupta, S. Banerjee, S. Dutta, A.A.I. Aarnink, J. Schmitz, A.Y. Kovalgin and R.J.E. Hueting, "Charge carrier transport and electroluminescence in atomic layer deposited poly-GaN/c-Si heterojunction diodes", Journal of Applied Physics, vol. 124, no. 8, August, 2018.
4. G. Gupta, S. Dutta, S. Banerjee and R.J.E. Hueting, "Minority carrier injection in high-barrier Si Schottky diodes", IEEE Transactions on Electron Devices, vol. 65, no. 4, April, 2018.
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1. G. Gupta and R.J.E. Hueting, "Characteristic C – V profile as a signature for electrostatic doping in FD-SOI", Joint International EUROSOI Workshop and International Conference on Ultimate Integration on Silicon (EUROSOI-ULIS), 2020, Caen, Normandy, France (accepted).
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3. G. Gupta, D.T. Shivakumar, R.J.E. Hueting and L.K. Nanver, "In search of a hole inversion layer in Pd/MoO_x/Si diodes through I-V characterization using dedicated ring-shaped test structures", International Conference on Microelectronic Test Structures (ICMTS), 2019, Kita Kyushu, Japan.

Book chapter

1. R.J.E. Hueting and G. Gupta, "Electrostatic Doping and Devices", Springer Handbook of Semiconductor Devices (under-revision).

Others

1. G. Gupta, F. Mema and R.J.E. Hueting, "InAs Electron-Hole Bilayer LED", oral presentation at SAFE 2019 Workshop, Delft.
2. G. Gupta and R.J.E. Hueting, "Polycrystalline GaN: Material and Devices", oral presentation at the MESA+ Symposium 2018, Enschede.
3. G. Gupta and R.J.E. Hueting, "Electrostatic Doping in Dimensionally-Scaled Semiconductor Devices", poster presentation at the SAFE 2018 Workshop, Enschede. (Best poster award)
4. G. Gupta and R.J.E. Hueting, "Electrostatic Doping in Semiconductor Devices", poster presentation at the MESA+ Symposium 2017, Enschede.

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