Characterization of High-Resistivity Silicon

Bulk and Silicon-on-Insulator Wafers

by

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ABSTRACT

High-Resistivity Silicon (HRS) substrates are important for low-loss, high-performance microwave and millimeter wave devices in high-frequency telecommunication systems. The highest resistivity of up to ~10,000 ohm.cm is Float Zone (FZ) grown Si which is produced in small quantities and moderate wafer diameter. The more common Czochralski (CZ) Si can achieve resistivities of around 1000 ohm.cm, but the wafers contain oxygen that can lead to thermal donor formation with donor concentration significantly higher (~$10^{15}$ cm$^{-3}$) than the dopant concentration (~$10^{12}$-$10^{13}$ cm$^{-3}$) of such high-resistivity Si leading to resistivity changes and possible type conversion of high-resistivity p-type silicon. In this research capacitance–voltage (C–V) characterization is employed to study the donor formation and type conversion of p-type High-resistivity Silicon-On-Insulator (HRSOI) wafers and the challenges involved in C-V characterization of HRSOI wafers using a Schottky contact are highlighted. The maximum capacitance of bulk or Silicon-On-Insulator (SOI) wafers is governed by the gate/contact area. During C-V characterization of high-resistivity SOI wafers with aluminum contacts directly on the Si film (Schottky contact); it was observed that the maximum capacitance is much higher than that due to the contact area, suggesting bias spreading due to the distributed transmission line of the film resistance and the buried oxide capacitance. In addition, an “S”-shape C–V plot was observed in the accumulation region. The effects of various factors, such as: frequency, contact and substrate sizes, gate oxide, SOI film thickness, film and substrate doping, carrier lifetime, contact work-function, temperature, light,
annealing temperature and radiation on the C-V characteristics of HRSOI wafers are studied.

HRSOI wafers have the best crosstalk prevention capability compared to other types of wafers, which plays a major role in system-on-chip configuration to prevent coupling between high frequency digital and sensitive analog circuits. Substrate crosstalk in HRSOI and various factors affecting the crosstalk, such as: substrate resistivity, separation between devices, buried oxide (BOX) thickness, radiation, temperature, annealing, light, and device types are discussed. Also various ways to minimize substrate crosstalk are studied and a new characterization method is proposed.

Owing to their very low doping concentrations and the presence of oxygen in CZ wafers, HRS wafers pose a challenge in resistivity measurement using conventional techniques such as four-point probe and Hall measurement methods. In this research the challenges in accurate resistivity measurement using four-point probe, Hall method, and C-V profile are highlighted and a novel approach to extract resistivity of HRS wafers based on Impedance Spectroscopy measurements using polymer dielectrics such as Polystyrene and Poly Methyl Methacrylate (PMMA) is proposed.
Dedicated

to

My Parents

Swarnalata Pradhan

Dhruba Charan Nayak
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<tr>
<td>BOX</td>
<td>Buried Oxide</td>
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<tr>
<td>CMOS</td>
<td>Complementary Metal Oxide Semiconductor</td>
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<td>CNLS</td>
<td>Complex Non-Linear Least Square algorithm</td>
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<td>COP</td>
<td>Crystal Originated Particle</td>
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<td>C-V</td>
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<td>CZ</td>
<td>Czochralski</td>
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<td>FTIR</td>
<td>Fourier Transform Infrared Spectroscopy</td>
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<td>FZ</td>
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<td>GaAs</td>
<td>Gallium Arsenide</td>
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<td>GFK</td>
<td>Growth From Knowledge</td>
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<td>GHz</td>
<td>Giga Hertz</td>
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<td>GPSOI</td>
<td>Grounded Plane Silicon-On-Insulator</td>
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<td>Horizontal Magnetic Field Applied</td>
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<td>Integrated Circuit</td>
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<td>MCZ</td>
<td>Magnetic Field Applied Czochralski Crystal Growth</td>
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<td>MOS</td>
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<td>MOS-C</td>
<td>Metal Oxide Semiconductor Capacitor</td>
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<td>NTD</td>
<td>Neutron Transmutation Doping</td>
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<td>RF</td>
<td>Radio Frequency</td>
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<td>RFFE</td>
<td>Radio Frequency Front End</td>
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<td>RFIC</td>
<td>Radio Frequency Integrated Circuit</td>
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<td>Space Charge Region</td>
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<td>Silicon</td>
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<td>System on Chip</td>
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<td>Silicon-On-Insulator</td>
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<td>SHORT-Open-Line-Thru</td>
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CHAPTER 1. INTRODUCTION

1.1. Introduction and Motivation for this Research

High-resistivity (hi-$\rho$) semiconductor substrates are used for low-loss, high-performance microwave and millimeter wave components that are key parts in telecommunication systems [1-7]. Low loss and high performance is essential to keep signal-to-noise ratios at acceptable levels and for maintaining efficient power management in high-reliability systems. Typical devices that benefit from hi-$\rho$ include high-Q inductors and capacitors, transmitters and receivers, GHz mixers, coplanar waveguides, RF MEMS switches, RF LDMOS and BiCMOS devices and others by decoupling of interelectrode capacitances within active devices and low-loss microstrip lines. The most common hi-$\rho$ semiconductor substrates today are semi-insulating GaAs, produced by introducing deep-level traps (antisite AsGa known as EL2) during crystal growth. Such substrates have resistivities in the $10^8$ ohm.cm range. Metal-semiconductor FETs are then fabricated on such substrates. Being GaAs, it is difficult to fabricate ICs of any complexity, however, and MESFETs are depletion-mode devices difficult to implement in CMOS-type configurations. If insulating quartz is used for the substrate, only passive devices can be made on it. Silicon, on the other hand, has the ability for complex ICs, but its resistivity is lower (highest $\rho$ is about $10^5$ ohm.cm) than that of GaAs. High-$\rho$ Si is produced by multiple Float-zone (FZ) passes leading to practical resistivities of about 10,000 ohm.cm. Thermal donors play little role as FZ Si has low oxygen concentrations, but the wafer diameter is limited. Czochralski (CZ) Si, capable of growing larger diameter ingots than FZ,
has resistivities of ~ 1000 ohm.cm, but contains higher oxygen concentrations. This can lead to resistivity shift or type change due to thermal donor formation. Low oxygen concentration or full oxygen precipitation reduces this effect. A further refinement of the Si hi-ρ concept is the use of high-resistivity Si coupled with silicon-on-insulator (SOI) to combine the advantages of SOI (reduced source and drain capacitances, higher transconductance, and dielectric isolation) with the benefits of high-resistivity substrates. With this approach, all the essential elements for low-cost, highly-integrable mixed mode integrated circuits (MMICs) can be obtained using silicon substrates and processing methods and co-integration of high-speed CMOS digital circuitry is possible.

A significant challenge is reliable metrology to measure the low carrier concentrations in the presence of oxygen thermal donors in CZ material. The doping concentration for 1000 ohm.cm Si is around $5 \times 10^{12} - 10^{13}$ cm$^{-3}$ while the thermal donor concentration can be many times this. Traditional thermal donors are formed at temperatures around 450°C and new thermal donors at temperatures around 650°C which is also the temperature at which traditional TDs are annihilated [8-10]. The wafer series resistance of a 500 µm thick wafer with 100 µmx100 µm test structure area is $5 \times 10^5$ ohms, presenting a significant challenge to C-V and other electrical measurements. The combination with SOI to form high-resistivity handle wafers below the BOX leads to additional measurement difficulties of the electrical properties of the high-resistivity wafer/BOX interface.
1.2. What is New in this Research?

The aim of this research is to characterize high-resistivity bulk silicon and SOI wafers to understand the doping profile of the substrate using Capacitance-Voltage (C-V) measurements, the effect of thermal donors on the overall substrate resistivity and the doping profile, to determine the challenges in characterizing HR-SOI wafers, to study the substrate coupling effect in High-Resistive Silicon (HRS) and the factors affecting the same, and to compare various resistivity measurement techniques and find the most suitable method to measure the resistivity of bulk HRS wafers.

The *new phenomena and the techniques* proposed in this research are summarized below along with the chapter numbers:

1. A new phenomenon of bias spreading during C-V measurements of HR-SOI using aluminum contact directly on the silicon film without a gate oxide and the challenges it poses to characterize SOI wafers (Chapter 4).

2. Effects of various factors such as: frequency of ac signal, size of film contacts and substrate width, gate oxide, thickness of SOI film, doping concentration of SOI film and substrate, carrier lifetime, Schottky contact barrier heights (type of metal semiconductor contacts), Ohmic contacts, temperature, light, annealing temperature, and radiation (interface traps and oxide charges) on the C-V characterization of HR-SOI, explained using both experiments and simulations (Chapter 4).
3. Study of substrate coupling (crosstalk) in HR-SOI in the presence of thermal donors and how HR-SOI plays a role in minimizing coupling through the substrate, using both experiment and simulation (Chapter 5).

4. Effects of various factors such as frequency of microwave signal, spacing between adjacent devices, substrate resistivity, oxide thickness, radiation (interface traps and charges), annealing, and light on the substrate crosstalk in HR-SOI; explained using both experiments and simulations (Chapter 5).

5. Comparison of various resistivity measurement techniques to measure substrate resistivity of high-resistivity silicon wafers and the challenges involved (Chapter 6).

6. A novel approach to extract resistivity of HRS wafers based on Impedance Spectroscopy using polymer dielectrics such as Polystyrene and Poly Methyl Methacrylate (PMMA) is proposed.

1.3. Background Literature Review for this Research

In this section a brief literature review will be presented addressing the focus areas of this research leading to the new findings. The detailed literature reviews are presented in the respective chapters (Ch. 4, 5 and 6).

Capacitance-Voltage (C-V) is a widely used technique for material characterization of silicon wafers [11]. This technique has also been used to characterize the oxide and the film thickness of SOI wafers [12]. C-V characterization is carried out with various types of devices such as MOS capacitors, pn diodes, and Schottky diodes [11]. In most of the reported C-V
characteristics of SOI wafers using a gate oxide, the maximum capacitance is proportional to the gate area [12-16]. In this research (Ch. 4), during capacitance-voltage measurements using an aluminum contact directly on the SOI film without a gate oxide, very different behavior for such devices is observed compared to devices with gate oxides, under certain bias conditions. After a certain bias the measured capacitance is much higher than that due to the contact area.

In system-on-chip configuration different systems such as analog, digital and microwave are integrated into one chip to reduce size and cost, and achieve greater speed. This complex integration of analog, digital and microwave systems and higher operating frequency give rise to another problem called crosstalk. The digital circuits operate at very high frequencies in the GHz range, but the analog circuits are very sensitive to any noise. At high frequencies some spurious signals from the digital node can pass through the substrate and couple to the analog side and disrupt the analog operation [17-19]. This is termed crosstalk through the substrate. SOI substrates were found to have lower substrate crosstalk than bulk substrates of similar resistivity [20, 21]. High-resistivity silicon (HRS) wafers minimize this coupling compared to low-resistivity substrates (LRS) and specifically high-resistivity SOI wafers are found to have better cross talk prevention capabilities than bulk Si of similar resistivity [22, 23]. Chapter 5 focuses on substrate coupling in HRSOI and effects of various factors, such as: substrate resistivity, separation between devices, buried oxide (BOX) thickness,
radiation, temperature, annealing, light, and device types. And also various ways to minimize substrate crosstalk is discussed.

The low doping concentration of HRS poses challenges in resistivity measurement using commonly used techniques such as four-point probe, Hall measurement method and C-V measurement technique. In the past, researchers have proposed a varieties of approaches to address the challenges in resistivity measurements of high resistivity materials, they are: floating portions of the circuitry [24], ac [25] and dc "bootstrapping" [26, 27], use of differential electrometers [28], double modulation [29], ac guarding [30], and dc guarding [31]. In chapter 6 the challenges in resistivity measurement are highlighted and a novel method based on Impedance Spectroscopy is proposed.

1.4. Organization

This dissertation is divided into seven chapters. Chapter one talks about the motivation and objective of this research. The next two chapters (Ch. 2 and 3) serve as an introduction. Chapter two gives an introduction to high-resistivity silicon wafers, why they are needed and their importance in the current mobile technology era. It also covers the bulk wafer growth techniques such as, Czochralski and float-zone growth techniques, wafer manufacturing processes such as cutting, polishing, lapping etc., and gives an overview of SOI wafer manufacturing methods such as SIMOX, BESOI, Smart Cut, and ELTRAN processes.

Oxygen concentration plays a significant role in HRS substrates due to their low doping concentration and all the research topics are influenced by the
presence of oxygen in silicon, hence the last section of chapter two is dedicated to
discuss “oxygen in silicon”, why oxygen is needed in silicon, how it is
incorporated into silicon, the various effects of oxygen in silicon, and how
oxygen-induced thermal donors affect the electrical properties of silicon.

All the experimental results are bolstered using device simulation and the
additional effects and factors which were not possible to study experimentally
were studied using device simulators. Chapter three highlights the need for device
modeling, gives a brief overview of the popular simulation tool – SILVACO; and
discusses various models used in the simulation related to this research.

Chapters four, five, and six describe the experiments and simulations related to
this research. Chapter four focuses on the experiment and modeling of C-V
characterization of HRSOI and the various factors affecting the same. Here a new
phenomenon of bias spreading is discussed, which was observed during C-V
characterization of HRSOI with an aluminum contact directly on the silicon film
without a gate oxide and with a floating body. The maximum capacitance in
accumulation is much more than what should have been due to the contact area.
Various factors affecting the C-V characteristics are also discussed.

Chapter five covers the topic of reduction of substrate coupling using HRSOI
and effect of various factors on the same. In chapter six, applicability of various
resistivity measurement methods such as four-point probe, Hall measurement
method, and C-V method for HRS substrates are compared and the challenges
involved are highlighted. A novel approach to extract resistivity based on
Impedance Spectroscopy using polymer films such as PMMA (Poly Methyl Methacrylate) and Polystyrene (PS) as dielectric is proposed.
CHAPTER 2. HIGH-RESISTIVITY SILICON FABRICATION

2.1. Introduction – The Need for High-Resistivity Silicon

Traditionally heavily-doped or low-resistivity silicon wafers have been used as substrates in CMOS technology. These wafers have substrate resistivities in the range of 0.05 ohm.cm for heavily doped epi substrate to around 30 ohm.cm for polished wafer [32]. Heavily-doped substrates are useful in preventing latch-up but with recent focus on System-on-Chip (SOC) configuration [33] where both high speed digital circuits and noise sensitive analog circuits are built on the same chip, and with the integration of radio frequency (RF) transceivers operating in the GHz range in the ever growing telecommunication industry; the substrate resistivity plays a crucial role in noise isolation and preventing coupling between devices. As the mobile communication industry moves to higher operating frequencies high-resistivity silicon wafers are needed to improve the performance of the passive components, such as on-chip inductors, and substrate electrical isolation between the integrated digital, RF, and analog components. High-resistivity silicon wafers with substrate resistivity in the excess of 1000 ohm.cm are needed to achieve the required isolation [32].

There has been an unprecedented growth of mobile technology in the last decade (see Fig. 2.1), and it has spurred the consumers’ desire to have both high speed processing and communication capabilities in the same device, such as: smartphones, tablet computers, or laptops. The right semiconductor substrate technology plays a crucial role in achieving higher performing application processors, baseband, memory, imagers, microphones, screens and Mobile RF
components – specifically radiofrequency front-end (RFFE) modules [34]. The quest to achieve optimum performance drives the process technologies and substrates in various RFFE modules, as shown in Fig. 2.2.

![Fig. 2.1. The growth of mobile devices as a percentage of the global consumer electronics market (Source: GFK/CEA) [34].](image1)

![Fig. 2.2. Substrate and process performance versus ideal target [34].](image2)
2.1.1. Gallium Arsenide Substrates

Gallium Arsenide substrates have the highest mobility, high breakdown voltage, low RF loss and high linearity. These properties make them the material of choice for RF application and as a state-of-the-art material for low-noise amplifiers [34]. GaAs is facing challenges in the system-on-chip configuration while integrating both digital and RF systems. To address the integration issues, new GaAs processes such as BiFET or BiHEMT are being developed to enable grouping of different functions on a single die for RFFE module integration [35, 36].

2.1.2. Silicon on Sapphire Substrates

Silicon-on-Sapphire (SOS) is one type of SOI wafer, more significantly it is the first SOI wafer fabricated. SOS substrates are well suited for RF technology as they provide good isolation between devices owing to the insulating substrate and they can easily integrate both high speed digital and RF modules on the same chip for higher performance [37]. This material has all the performance attributes needed for RFFE module integration, combining power amplifiers, switches and antenna tuning on a single chip [36, 38], as shown in Fig. 2.2. There are two types of SOS substrates available: epi SoS [37] and bonded SOS. Bonded monocrystalline SOS is built using transfer processes and direct wafer-bonding expertise to transfer and bond a high-quality, thin silicon layer onto a sapphire substrate. The substrate provides an ideal design landscape for enhanced RFIC performance, functionality and form factor, enabling IC size reduction while increasing performance by as much as 30 percent [34].
2.1.3. High-Resistivity Silicon-on-Insulator Substrates

High-Resistivity SOI (HR-SOI) satisfies almost all the conditions for RF technology and integration of high speed digital and RF circuits on the same chip as shown in Fig. 2.2. It has low RF noise, good linearity, high breakdown voltage, better thermal conductivity than SOS and GaAs, and high programmability as bulk silicon hence is most suitable for SOC configuration integrating multiple functionalities. These improvements in HR-SOI that make them suitable for RF and SOC have been achieved by continuous research as highlighted in [39-43]. Owing to its inherent structure of buried-oxide and high-resistive substrate it provides the best noise isolation, best coupling prevention between the devices and signal integrity among all substrates [23].

2.1.4. Bulk Silicon Substrates

Bulk silicon provides a middle ground solution for integrating high quality digital circuit and standard RF capabilities. The major problems with silicon bulk substrates and their RF properties are poor linearity and high RF signal loss, as shown in Fig. 2.2. To improve system integration using bulk Si various options are suggested such as triple wells and high-resistivity bulk [44]. High-resistivity substrates do help in reducing the crosstalk between devices compared to the regular heavily-doped substrates.

In this chapter, various crystal growth technologies for bulk silicon (CZ and FZ) and SOI wafers will be discussed. HR-SOI wafers have high-resistivity silicon substrate with mostly low resistivity silicon films. The manufacturing process for HRS wafers is similar to normal bulk silicon crystal growth process.
Substrate resistivity of 40-100 ohm.cm are generally classified as high-resistivity wafers and substrate resistivity beyond 100 ohm.cm and into the 1000 ohm.cm range are classified as ultra high-resistivity wafers [32].

2.2. Key Characteristics of High-resistivity Silicon wafers

Key characteristics of a high-resistivity or ultra-high resistivity silicon wafers are (1) a uniform resistivity throughout the wafer, (2) acceptable radial and axial resistivity gradients, and (3) a resistivity that remains stable throughout device processing [32]. These characteristics are dependent on crystal growth and the control of oxygen behavior.

HRS wafers should be available in larger diameters, such as 200 mm and 300 mm for higher device yield and should adhere to all the advanced wafer parameters, such as, site flatness and nanotopography as required by the modern submicron/nano scale RF-CMOS integration technologies. Wafers must also be available in a COP-free (crystal originated particle) form to achieve very low wafer defect density for high yielding, highly integrated devices (COP is vacancy agglomerated defect from crystal growth that intersects final wafer surface). The additional capability for metallic gettering protection via oxygen precipitates is also desirable. The details of oxygen in silicon are discussed in the next chapter.

2.3. High-Resistivity Silicon Crystal Growth

Single crystal silicon was first grown by the crucible pulling method in 1950, three years after the first transistor was discovered, which was made on germanium. There are two main single crystal silicon crystal growth techniques currently in production among many others; they are the float-zone (FZ)
technique and the Czochralski (CZ) crystal growth technique. CZ was the first growth technique to be discovered. FZ is a crucible free technique that can produce very high-resistivity silicon wafers owing to its high-purity growth process. But FZ HRS is not used for regular IC manufacturing due to lower oxygen contents and lower mechanical strengths. CZ is the most commonly used crystal for IC chip fabrication and CZ HRS wafers, up to 100 ohm.cm, can be grown using the existing CZ crystal growth process, but resistivity > 1000 ohm.cm brings challenges in the CZ growth technique because in HRS wafers the background dopant concentration is significantly reduced to achieve the desired resistivity, this emphasizes the precise control of dopants, such as, boron and phosphorous, introduced from the raw materials and components in the crystal puller. These materials and components include the polysilicon source, the quartz crucible, and the graphite heater. In addition, the extremely low dopant concentration in the melt makes the control of dopant mass transfer to, and then through, the boundary layer at the melt-solid interface important for achieving acceptable radial resistivity variation [32].

2.3.1. Czochralski Crystal Growth Technique

Czochralski crystals are named after Czochralski whose crystal pulling technique invented in 1918 is used as the basis for this type of crystal growth [45]. The technique currently used in production is a modified version invented by Teal and Little in 1950 [46]. Today CZ is the most common silicon crystal used in the IC industry because of its manufacturability in large size (300 mm diameter), fast production, inexpensive, ability for internal gettering and higher
mechanical strength. Initial CZ wafers were of smaller diameter, but after 1960s improvements to grow dislocation-free automatic diameter control technology, large diameter crystals could be mass produced.

The schematic of a modern large diameter CZ crystal grower is shown in Fig. 2.3. Major components of the system are: (a) the hot zone consisting of the graphite susceptor, graphite heater, and the thermal shield, (b) crystal pull and rotation system, (c) crucible lift and rotation system, (d) diameter and temperature sensing devices. The crystal puller is operated under a reduced pressure inert gas ambient. There are three major parts to CZ growth: (1) seeding and necking, (2) body growth, and (3) tang growth and termination. Necking is a very critical and necessary process step for dislocation-free crystal growth and body growth follows the necking process [47].

Fig. 2.3. Schematic of Czochralski silicon growing system [48].
The CZ growth process steps are shown in Figs. 2.4 and 2.5. High-purity polysilicon nuggets are the starting material for the CZ crystal growth. The process begins with melting of the polysilicon nuggets and the doping elements or alloys (n- or p-type) as required depending on the desired substrate resistivity in a quartz crucible at around 1450ºC, Fig. 2.5(a). After the polysilicon is melted the temperature is controlled and stabilized such that the surface temperature of the melt is slightly super cooled. Then a single crystal seed measuring nearly 12 mm diameter attached to a steel cable is lowered to the melt to start the crystal formation. This contact of the seed and melt initiates the most important necking process as described by Dash [49], provided the contact forms a smooth meniscus. The main goal of necking is to begin a dislocation free crystal growth from a dislocation-free silicon lattice i.e. the seed. Even-though the CZ seed is dislocation free, the thermal shock during the contact of the seed with the melt can generate dislocations. And necking is the procedure to outgrow these dislocations to start the dislocation-free single crystal growth. During necking, the seed crystal is gradually decreased in diameter by increasing the pull speed and temperature adjustment to reach a steady state neck diameter of 3-4 mm and a pull rate of 4-6 mm/min. This is normally achieved after few centimeter of growth. The necking process is shown in Fig 2.5(b).

After the dislocation-free growth is achieved via necking, the diameter of the crystal is increased to the desired size by shoulder growth, Figs. 2.4 and 2.5 (c). After the desired diameter is reached the body growth begins. The body growth is controlled by computerized ADC (Automatic Diameter Control) which monitors
the temperature and the pull rate to maintain the desired diameter of the silicon crystal, Figs. 2.4 and 2.5 (d, e). Optical sensors (see Fig. 2.3) monitor the crystal growth diameter and help ADC to maintain the same. After the completion of the body growth the process is terminated by a gradual decrease from full diameter to zero to minimize thermal stress due to diameter change and slip dislocation, Fig. 2.5 (f). After the growth process is complete the heater is turned off but the crystal is allowed to stay in the chamber until it is cooled off. The entire duration the crystal is present in the chamber and the temperature cycles it experiences constitutes its thermal history, which is a very important factor in determining the oxygen precipitation in the crystal. Details about oxygen in silicon are discussed at the end of this chapter. Even though the CZ method used by different manufacturers is the same, the quality of the CZ crystal varies due to variation in operators and variation in the hot zone. A CZ ingot is shown in Fig. 2.4, it can grow up to 2 m in height, have 300 mm diameter and weigh 400 kg.

Fig. 2.4. Schematic of various phases of CZ crystal growth and a silicon ingot
Fig. 2.5. Czochralski crystal growth (g) equipment set up and process steps: (a) polysilicon charge in silica crucible, (b) start of neck, seed is dipped to > 1400°C melt, (c) shoulder growth, after neck is complete, (d) start of body, after completion of shoulder, (e) body growth, (f) conical tail growth after completion of body [51].

2.3.2. Dopant Distribution in CZ crystals

Dopants are added to the polysilicon melt and complete mixing takes place by vigorous thermal convection. The axial dopant distribution follows the normal freezing behavior given by [52]

\[ C_i(x) = C_0 k (1 - x)^{i-k} \]  

(2.1)
where \( C_s \) = crystal dopant concentration, \( C_0 \) = initial dopant concentration of the melt, \( k \) = dopant segregation coefficient, and \( x \) = fraction of melt solidified. The dopant concentration spreads along the CZ crystal depending on the value of the dopant segregation coefficient \( k \); the smaller the \( k \) value the larger is the spread. The yield of the CZ crystals is affected by the segregation coefficient and growth methods, such as; double crucible method [53, 54] and continuous CZ growth technique [55], to eliminate the effect of segregation. The yield of the CZ crystals is affected by the segregation coefficient and growth methods, such as; double crucible method [53, 54] and continuous CZ growth technique [55], to eliminate the effect of segregation. The yield of the CZ crystals is affected by the segregation coefficient and growth methods, such as; double crucible method [53, 54] and continuous CZ growth technique [55], to eliminate the effect of segregation. The axial microscopic uniformity of dopants is controlled by thermal convection, thermal symmetry and pull rate.

The microscopic inhomogeneity in CZ crystals is controlled by growth rate fluctuation and the segregation coefficient during crystal growth. The growth rate fluctuation leads to local variation of impurity concentration, which leads to lattice strains, and causes striation. Large variation in oxygen concentration causes preferential precipitation appearing as ring patterns in etched and heat treated silicon. The sources for microscopic growth variation are: non-centrosymmetric thermal distribution in large silicon melt, thermal convection related temperature fluctuation, and automatic diameter control induced perturbation [47].

### 2.3.3. Unintended Dopants in CZ crystals

There are unintended dopants in the CZ crystals such as oxygen, carbon, metals and transition metals incorporated during crystal growth from the quartz crucible and the vapor above the melt. Oxygen (\( \approx 10^{18} \text{ cm}^{-3} \)) and carbon (\( \approx 10^{16} \text{ cm}^{-3} \)) are the major unintended impurities in CZ crystals. As HRS wafers have
very low background impurities the concentration of these unintended dopants should be kept low enough so that they do not interfere with the intended doping of the wafers. The details of oxygen in silicon will be discussed at the end of this chapter in the section called “oxygen in silicon”.

Carbon in silicon comes from the graphite materials making up the hot zone of the crystal grower [47]. The silicon monoxide evaporated from the melt surface interacts with the hot graphite component creating carbon monoxide (CO) which reenters the melt as a continuous process.

\[
\text{SiO} + 2\text{C} \rightarrow \text{SiC} + \text{CO}
\]

For VLSI/ULSI applications carbon is kept at a minimum level (< 0.5 ppma).

Metallic impurities can enter the CZ crystal from the overheated metal or alloy surfaces of the grower chamber, such as, the steel cable holding the CZ ingot, which can get overheated when it is close to the hot zone. This problem can be avoided by using ceramic or graphite extended seed holding device. Due to low segregation coefficient (<10^{-6}) of metals not much metal can go into silicon [47].

Transition metals can get into silicon during growth as they are fast diffusers in silicon at high temperature. The transition metals are very harmful as they kill the charge carriers, and hence are undesirable. The diffusion of metal into silicon is most effective at the grown crystal surface above the melt.

2.3.4. Magnetic Field Czochralski Crystal Growth (MCZ)

Good quality high-resistivity silicon wafers require low and precise control of oxygen concentration. Thermal convection is known to play a significant role in the quality of CZ crystals as it affects the concentration and uniformity of the
dopants and oxygen in the crystal, apart from other factors. Fortunately the irregularities in the thermal convection in an electrically conductive fluid can be suppressed by magnetic field as described by Utech and Flemings in 1966 [56]. MCZ is the processes of CZ crystal growth by suppressing the thermal convection and the related temperature fluctuations in the silicon melt by applying magnetic field and thereby reducing impurity striation. The applied magnetic field can be either vertical (VMCZ) or horizontal (HMCZ). MCZ is based on the principle described by Chandrsekhar in 1952 [57], according to his principle when a magnetic field is applied across an electrically conductive melt, it increases the effective kinematic viscosity of the melt and hence suppresses the thermal convection and associated temperature fluctuations in the melt.

It has been shown by various studies that HMCZ is a preferable approach over VMCZ from growth controllability and crystal quality. VMCZ is found to have poor control over oxygen incorporation, impurity segregation and radial uniformity of impurity concentration in large diameter CZ growth [58, 59]. HMCZ method can be used to grow large diameter crystals with finer control of oxygen concentration from few ppm to 20 ppm and with good axial concentration uniformity. *High-resistivity CZ silicon with low oxygen and low micro-defects can be grown with the HMCZ method* [60-62]. Figure 2.6 shows an MCZ crystal growth set up.
2.3.5. Continuous Czochralski Crystal growth

As the diameter of the CZ wafer increases the height of the silicon ingot is limited by the amount of the charge i.e. polysilicon melt present in the crucible. In order to address this problem and grow large diameter longer CZ ingots, the continuous Czochralski growth technique was invented, where polysilicon and dopant mixture is continuously added into the quartz crucible and a constant level of the melt is maintained during crystal growth. The process is similar to the double crucible method, the raw material is added to an outer chamber of the crucible or in a primary crucible and the melt is supplied into an inner or a secondary smaller crucible where the crystal growth takes place from the melt maintained at a constant level [47]. Fiegl in 1983 first demonstrated the concept of continuous CZ growth using a two-container system, as shown in Fig. 2.7. This
“feed-pull” system with two containers can also be implemented as shown in Fig. 2.8 (a, b). If the total melt volume is kept constant then the partition between the two crucibles is not necessary (see Fig 2.8(c)) but still retains some of the advantages of the double crucible method. But this single crucible arrangement contains a physical barrier separating melted and unmelted silicon and a silica baffle to reduce thermal convection.

Fig. 2.7. Schematic showing a generalized continuous CZ growth from a two-container system with a constant melt volume maintained by constant feed [47].
Fig. 2.8. Crystal growth from double crucible arrangements. (a) Constant melt level, (b) constant inner crucible melt volume maintained by continuous feed and (c) crystal growth from a single container equipped with a circular silica baffle. In all cases the melt level is maintained constant by continuous feed [47].

Apart from facilitating the growth of longer silicon ingots, the continuous growth method also ensures axial uniformity in dopant and oxygen concentration in the crystal. Additionally, in this method, the oxygen concentration incorporated into the crystal can also be controlled by the volume and the aspect ratio of the melt in the growing crucible [47]. *This helps in achieving low oxygen concentration which is important in high-resistivity silicon wafers.*

**2.3.6. Float Zone Crystal Growth Technique**

Float Zone crystal growth technique is based on the zone melting technique developed by Pfann at Bell Labs in 1952 [64]. Zone melting is a method of purifying crystals, in which a narrow region of a crystal is molten, and this molten zone is moved along the crystal (in practice, the crystal is pulled through the heater). The molten region melts impure solid at its forward edge, since impurities are usually more soluble in the liquid than in the solid, they are carried
forward with the molten zone so that the recrystallized material is purified at the end where the zone starts its traverse and the impurities concentrated in the melt move to one end of the ingot. If the process is repeated a number of times a high degree of purification can be achieved. The zone melting process is shown in Fig. 2.9(a) where the molten zone moves from left to right in the direction of the movement of the hot zone.

In 1950s many researchers were working simultaneously on the crucible free crystal growth technique [63] called the float zone method based on the zone melting process, namely: (a) Keck and Golay (Bell Laboratories) [65]; (b) Theuerer (Bell Laboratories) [66][16]; (c) Sieberts and Henker (Siemens); and (d) Emeis (Siemens). Figure 2.9 (d) describes the method invented by Theuerer (patent applied in 1952 and issued in 1962). This is a bottom seed FZ growth approach where the single crystal silicon seed is brought up from the bottom to make contact with the melt at the tip of the polysilicon rod. The polysilicon rod is mounted in a growth chamber maintained at high vacuum or inert gas. A needle-eye coil placed around the polysilicon rod; this coil provides radio frequency power to the polysilicon rod causing it to melt and maintains a stable melting zone. The levitation effect of the radio frequency field helps to support the large melting zone. To begin the growth process the melted polysilicon is first contacted with the single crystal seed brought up from below and a necking process is carried out, as shown in Fig. 2.9(b). Necking process creates a dislocation-free feature before the “neck” is allowed to increase in diameter to form a taper and reach the desired diameter for the steady-state body growth. The
molten zone is moved along the length of the polysilicon rod, as it moves, the molten silicon solidifies to single crystal silicon and the impurities are carried forward in the direction of coil movement and the silicon is purified in the process, as shown in Fig. 2.9(c). The coil is moved up and down several times until the desired level of purity is achieved. During the growth the molten zone and the crystal diameter is monitored by infrared sensors and are adjusted by the RF power input to the coil and travel speed [47].

Even though 200 mm Czochralski grown material is available since the mid 80's, the technical limit in crystal pulling of FZ was seen at 150 mm for a long time. In 2002, Siltronic succeeded to pull 200 mm FZ ingots and to produce 200 mm FZ wafers as the first silicon manufacturer worldwide [67].

Doping of FZ Si crystals is achieved by the gas phase doping method by adding phospine (PH₃) gas for n-type and diborane (B₂H₆) gas for p-type to the inert gas ambient of the growth chamber. Alternatively the polysilicon rods used as starting material can also be pre-doped by gas phase doping method and the dopant redistribution is achieved during FZ crystal growth by the zone melting process [47]. Since the doping is by gas phase interaction with the molten silicon, axial dopant uniformity is achieved. However, due to the very nature of FZ growth configuration, the small “hot-zone” lacks thermal symmetry. As a result, the temperature fluctuations, remelting phenomena and dopant segregation cause FZ silicon to display more microscopic dopant inhomogeneity or dopant striations than that observed in the CZ crystals.
Fig. 2.9. (a) Liquid moves forward from left to right in zone melting process in FZ crystal growth [68], (b) silicon crystal at the beginning of FZ growth process [68], (c) growing silicon crystal [68], and (d) schematic diagram of the FZ crystal growth process [69].

Wafers with dopant non-uniformity are not suitable for certain high-resistivity applications such as power electronics that requires uniform resistivity throughout the wafer. For these devices to work at the designated power and voltage level the doping should be uniform without any non-uniformities [70]. This dopant micro-
inhomogeneity can be overcome only in n-type FZ crystal by NTD (Neutron Transmutation Doping). Neutron transmutation doping is the process of creating non-radioactive impurity isotopes from the host atoms of a material by thermal neutron irradiation and subsequent radioactive decay. This technique is particularly applicable to doping semiconductors in cases of: (1) better control on the spatial uniformity of doping, and (2) addition of a very small amount of dopant.

The basic concept of doping silicon (Si) by creating phosphorous (P) atoms by the absorption of thermal neutrons was discussed in 1961 by Tanenbaum and Mills [71]. Significant commercial use of NTD Si started in the mid 1970s. In NTD high-purity (undoped) FZ crystal is subjected to thermal neutron bombardment, causing some of the silicon isotopes $^{30}$Si (~3.1% of Si) to form the unstable isotope $^{31}$Si, which decays to form stable phosphorous isotope $^{31}$P as described below:

$$^{30}\text{Si}(n, \gamma) \rightarrow ^{31}\text{Si} \rightarrow ^{31}\text{P} + \beta$$

There are secondary reactions as below:

$$^{31}\text{Si}(n, \gamma) \rightarrow ^{32}\text{P} \rightarrow ^{32}\text{S} \quad \text{Radioactivity}$$

$$^{28}\text{Si}(n, 2n) \rightarrow ^{27}\text{Si} \rightarrow ^{27}\text{Al}$$

$$^{28}\text{Si}(n, \alpha) \rightarrow ^{25}\text{Mg}$$

$$^{29}\text{Si}(n, \alpha) \rightarrow ^{26}\text{Mg}$$

The radioactivity produced from the $^{31}$P transmutation, or any other trace impurity initially in the silicon, can lead to abnormally long half-life activities, which may require that the doped material be held from device production until
sufficient decay has been reached. Neutron bombardment (both thermal and fast neutrons) induces radiation damage; the irradiated crystal must be annealed at about 700°C for defect annihilation and to restore resistivity due to the phosphorous doping [47]. The dopant striations in FZ silicon are greatly reduced by NTD. The NTD method is feasible only for high-resistivity phosphorous doped FZ. Low-resistivity doping of FZ by NTD would require excessive long irradiation (more lattice damage) and is not feasible. NTD process is not available for p-type doping of FZ.

Table 2.1 Phosphorus doping concentrations and the corresponding neutron doses required for typical resistivity range of NTD silicon [72].

<table>
<thead>
<tr>
<th>Resistivity (Ω-cm)</th>
<th>Dopant Conc. (10^{13} \text{ atoms/cm}^3)</th>
<th>Phosphorus ppba</th>
<th>Neutron Dose (10^{16} \text{ cm}^{-2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>14.5</td>
<td>2.9</td>
<td>86</td>
</tr>
<tr>
<td>100</td>
<td>4.3</td>
<td>0.85</td>
<td>24</td>
</tr>
<tr>
<td>200</td>
<td>2.1</td>
<td>0.42</td>
<td>10.5</td>
</tr>
<tr>
<td>300</td>
<td>1.4</td>
<td>0.28</td>
<td>7</td>
</tr>
<tr>
<td>500</td>
<td>0.85</td>
<td>0.17</td>
<td>4</td>
</tr>
<tr>
<td>1000</td>
<td>0.45</td>
<td>0.086</td>
<td>2</td>
</tr>
</tbody>
</table>

2.3.7. Silicon Wafer Manufacturing

After the crystals are grown either by CZ or FZ process, the silicon ingots go through several subsequent process steps to manufacture the circular discs of silicon wafers, as shown in Fig. 2.10 [73]. First the silicon crystal ingot is ground all around to have a uniform diameter all along the ingot, Fig. 2.10(b). Then the
two conical ends of the ingot are sawn off by a diamond saw, Fig. 2.10(c). The ingot is then sawn off into wafers with approximately ½ mm to ¾ mm in thickness, Fig. 2.10(d). The edges of the wafers are ground to round off the sharp edges, Fig. 2.10(e). Edge grinding minimizes chipping of wafer edges during subsequent steps. Then both surfaces of each wafer are lapped to flatten out the faces and make both faces parallel, Fig. 2.10(f). After lapping, a special wet etch is used to etch surface damage remaining after lapping, Fig. 2.10(g). Then the wafers are polished to remove any residual damages on the wafer surface to obtain the mirror like finish, Fig. 2.10(h). Wafers can have both or only one face polished. At the end a final cleaning step removes any contaminants left on the wafer surface from previous steps, Fig. 2.10(i). Now the wafers are ready to be shipped.

Fig. 2.10. Silicon wafer manufacturing process [73].
2.3.8. Comparison between CZ and FZ crystals

Even though CZ and FZ processes grow single-crystal silicon but due to their different growth mechanisms the crystals have different properties. FZ being a crucible-free process can achieve high purity and lower oxygen content than CZ crystals. FZ crystals can easily have very high resistivity (as high as 10,000 ohm.cm), higher than CZ (up to 1000 ohm.cm). But the low oxygen content in FZ crystals (< $10^{16}$ cm$^{-3}$) has its drawbacks; due to this low oxygen concentration, which is below the solid solubility in silicon, FZ crystals lack internal oxygen precipitation and hence internal gettering ability and have lower mechanical strength [74, 75] leading to greater thermal stress and associated wafer bow, wrap and crystal plane slips [76, 77], hence they have limited application in IC device fabrication. CZ crystals with higher oxygen concentrations are mechanically stronger and have very good internal gettering capabilities, making them the most common crystals in IC fabrication. Oxygen and nitrogen doping during FZ growth has been proposed to improve the mechanical strength of FZ crystals. Sumino et al. in 1980 [78] showed that FZ silicon crystals doped with 1.0~1.5×$10^{17}$ atoms/cm$^3$ oxygen have higher mechanical strength than undoped ones and Abe et al. [79] showed that FZ crystals doped with around $1.5\times10^{17}$ atoms/cm$^3$ nitrogen also have higher mechanical strength. Table 2.2 shows a comparison between CZ and FZ crystal growth.
Table 2.2 Comparison of Czochralski and Float Zone growth [80].

<table>
<thead>
<tr>
<th>Characteristics</th>
<th>Czochralski</th>
<th>Float zone</th>
</tr>
</thead>
<tbody>
<tr>
<td>Growth Speed (mm/min)</td>
<td>1 to 2</td>
<td>3 to 5</td>
</tr>
<tr>
<td>Dislocation-Free?</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Crucible?</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>Consumable Material Cost</td>
<td>High</td>
<td>Low</td>
</tr>
<tr>
<td>Heat-Up/Cool-Down Times</td>
<td>Long</td>
<td>Short</td>
</tr>
<tr>
<td>Axial Resistivity Uniformity</td>
<td>Poor</td>
<td>Good</td>
</tr>
<tr>
<td>Oxygen Concentration (atoms/cm$^3$)</td>
<td>&gt; $10^{18}$</td>
<td>&lt; $10^{16}$</td>
</tr>
<tr>
<td>Carbon Concentration (atoms/cm$^3$)</td>
<td>&gt; $10^{17}$</td>
<td>&lt; $10^{16}$</td>
</tr>
<tr>
<td>Metallic Impurity Concentration</td>
<td>Higher</td>
<td>Lower</td>
</tr>
<tr>
<td>Bulk Minority Charge Carrier Lifetime ($\mu$s)</td>
<td>5-100</td>
<td>1,000-20,000</td>
</tr>
<tr>
<td>Mechanical Strength</td>
<td>$10^{17}$ Oxygen</td>
<td>$10^{15}$ Nitrogen</td>
</tr>
<tr>
<td>Production Diameter (mm)</td>
<td>200-300</td>
<td>150-200</td>
</tr>
<tr>
<td>Operator Skill</td>
<td>Less</td>
<td>More</td>
</tr>
<tr>
<td>Polycrystalline Si Feed Form</td>
<td>Any</td>
<td>Crack-free rod</td>
</tr>
</tbody>
</table>

2.4. Silicon On Insulator (SOI) Wafers

In an MOS transistor, only the very top region (0.1 - 0.2 $\mu$m thick) of the silicon wafer is actually useful for electron transport. The inactive volume, more than 99.9% of the wafer, induces only undesirable parasitic effects [81]. This knowledge of active upper region and the undesirable influences of the substrate showed the way for SOI structures. They are created with the idea of isolating the active device overlay from the detrimental substrate. SOI structures consist of a film of single crystalline Si separated by a layer of SiO$_2$ called the BOX (Buried
Oxide) from the bulk substrate [16, 81]. Recent studies have shown that high
resistivity SOI wafers have the best crosstalk prevention abilities compared to all
other substrates [23].

2.5. SOI Fabrication Methods

Researchers around the world have pioneered various fabrication methods for
SOI wafers. Some of them are new and some are improvements to the existing
processes to reduce occurrences of defects, expand the knowledge base of crystal
growth and bring new ideas. All these fabrication techniques are summarized in
Table 2.3. Not all of these techniques made their ways into industrial
manufacturing due to certain limitations and challenges. In this chapter, four
important fabrication methods which were adopted for commercial production
namely: Separation by Implanted Oxygen (SIMOX), Bonding and Etchback
(BESOI), Smart Cut™, and Epitaxial layer transfer (ELTRAN) method will be
discussed. The main challenge in all these techniques is to create a very thin
uniform layer of single crystal silicon over the buried oxide.

Table 2.3 Various SOI wafer fabrication methods [82].

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DI - dielectric isolation</td>
<td>Oxide isolated “tubs” of monocrystalline Si supported by a polycrystalline “handle” wafer.</td>
</tr>
<tr>
<td>SOS - Si-On-Sapphire</td>
<td>Si film epitaxially grown on sapphire substrates.</td>
</tr>
<tr>
<td>SOZ - Si-On-Zirconia</td>
<td>Si film epitaxially grown on ZrO₂ substrates.</td>
</tr>
<tr>
<td>Recrystallization from the melt:</td>
<td>Rapid melting of polysilicon films deposited over a SiO₂ layer grown on a Si wafer, followed by</td>
</tr>
<tr>
<td>Method</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>(a) Laser - seeded [86]</td>
<td>CW laser beam raster-scanned across the surface, with via holes that connect the polysilicon film with the single crystalline substrate.</td>
</tr>
<tr>
<td>(b) Laser - unseeded [87]</td>
<td>As above, but no seeding vias in the oxide.</td>
</tr>
<tr>
<td>(c) ZMR—zone melt recrystallization with a hot wire [88]</td>
<td>A long and narrow molten zone is swept once across the entire wafer.</td>
</tr>
<tr>
<td>(d) LEGO - lateral epitaxial growth over oxide - stationary lamp heater [89]</td>
<td>A thick Si film is melted simultaneously across the entire wafer. Gradients due to seeding vias control crystallization.</td>
</tr>
<tr>
<td>ELO - Epitaxial Lateral Overgrowth [90]</td>
<td>Selective Si epitaxial deposition, starting from via holes in SiO₂ and spreading laterally over the oxide.</td>
</tr>
<tr>
<td>SPE - Solid Phase Epitaxy [91]</td>
<td>Oxidized Si wafers with via holes through the SiO₂ are coated with amorphous Si, which is epitaxially crystallized.</td>
</tr>
<tr>
<td>FIPOS - Full Isolation with Porous Oxidized Silicon [92]</td>
<td>Porous Si is formed locally under islands of crystalline Si, then it is oxidized to form isolation.</td>
</tr>
<tr>
<td>Heteroepitaxy of crystalline insulators, followed by single crystalline Si [93]</td>
<td>CaF, ZrO₂, Spinel, and other crystalline insulators have been used.</td>
</tr>
<tr>
<td>SIMOX - separation by implantation of oxygen [94]</td>
<td>Buried oxide layer is synthesized in situ from implanted oxygen.</td>
</tr>
<tr>
<td>Wafer bonding and etch-back [95]</td>
<td>Two wafers are bonded with an oxide layer in between. One of the wafers is thinned by grinding and etching.</td>
</tr>
<tr>
<td>Smart-Cut™ process - layer transfer facilitated by ion implantation [96]</td>
<td>One wafer is implanted, typically with H or noble gas ions. The Si layer above the implanted region is transferred to a “handle” wafer by wafer bonding and splitting along the implanted region.</td>
</tr>
<tr>
<td>ELTRAN process - layer transfer facilitated by porous silicon [97]</td>
<td>Epitaxial layer is grown on a porous Si region and transferred by bonding and splitting to a “handle” wafer.</td>
</tr>
</tbody>
</table>
2.5.1. SIMOX

SIMOX stands for “Separation by IMplanted OXygen”. The principle of SIMOX material formation consists in the formation of a buried layer of SiO$_2$ by implantation of very high dose of oxygen ions beneath the surface of the silicon wafer followed by an annealing step, as depicted in Fig. 2.11. A TEM cross section of a SIMOX wafer is shown in Fig. 2.12. Processing must be such that a thin layer of single crystal silicon is maintained over the buried oxide. This implantation of oxygen into silicon is similar to the ion implantation method used to introduce dopant atoms into silicon to form source and drain. But here the dose of oxygen is very high, of the order of $10^{18}$ cm$^{-2}$ to produce the buried oxide layer, whereas the dose for dopant introduction is around $10^{16}$ cm$^{-2}$. The annealing temperature is around 1350°C or more.

The earliest reported SIMOX technique is by Watanabe and Tooi in 1966 [99], implantation of about $1.5 \times 10^{18}$ cm$^{-2}$ oxygen at 60 keV appears to have produced a surface layer of SiO$_2$. Izumi et al. in 1978 [94], demonstrated a 19-stage CMOS ring oscillator made in the new material called SIMOX. In 1985, SIMOX structures annealed at 1300°C for several hours [100] or at 1405°C in a lamp furnace for 30 min [101] demonstrated that an atomically sharp and planar interface between Si and the buried oxide is feasible. Currently all SIMOX wafers
are annealed in furnaces with either polysilicon or SiC tubes at temperatures ~ 1350°C.

In SIMOX technology the wafer cost is a strong function of the implant dose. The feasibility of thinner BOX film of the order of 56 nm has been demonstrated with oxygen ion implantation of just $2 \times 10^{17}$ cm$^{-2}$ at 65 keV, followed by 4 hour anneal at 1350°C [102]. But the SIMOX process creates more defects due to the high implant dose.

![Principle of SIMOX](image)

Fig. 2.11. Principle of SIMOX: a heavy dose of oxygen ion implantation followed by an annealing step produces a buried SiO$_2$ layer below a thin Si film.

![SIMOX wafer](image)

Fig. 2.12. SIMOX wafer [Courtesy of D. Esseni, University of Udine, Italy].
2.5.2. Bonding and Etchback (BESOI)

J. Laski at IBM [95] and Frye et al. [103] at Bell Labs independently proposed the fabrication of SOI structures by means of wafer bonding. Frye’s method requires an electric field to press the wafers together in order to initiate the bonding process. Laski showed that bonding only required applying slight mechanical force. Two very flat and very clean surfaces are held together by Van der Waals forces, which depends on polarizability of atoms and molecules on two surfaces placed very close (< 1 nm) to each other. In the bond-and-etch-back SOI (BESOI) process two clean oxidized wafers are brought close together. An etch stop is introduced in the donor wafer prior to bonding typically by implanting a high dose of boron to produce a buried layer. Epitaxial layer growth on top of a boron-doped surface is another alternative. Germanium or a combination of Ge and B can also be used. The wafers are bonded together and annealed at 1100°C, the thin uniform silicon film is produced by a combination of mechanical wafer thinning followed by selective etch, which stops at the boron or germanium rich region and the final step is the removal of the doped region. In the BESOI technique much of the donor wafer is wasted during the thinning process which incurs additional cost and also some contamination of the thin film is introduced by the etch-stop dopant. The BESOI process is described in Fig. 2.13.
Fig. 2.13. Principle of BESOI process: two oxidized wafers are bonded together and the donor wafer is etched and polished to get the final thin silicon film.

2.5.3. Smart Cut™ Process

The Smart Cut™ process is the commercial version of the process for SOI formation by wafer bonding and ion implantation induced weakening or splitting. Smart Cut™ process was developed by the French wafer manufacturing company Soitec. The wafers manufactured by this process are called Unibond wafers. This technique has become industry standard for thin-silicon-layer transfer.

The method of forming SOI wafer by wafer bonding followed by splitting of a thin layer was originally patented by Bruel of LETI in 1991 [104]. In Bruel’s method, hydrogen gas is used as an atomic scalpel to cut through silicon wafers to produce a thin layer. When hydrogen atoms are implanted to a dose of > 5x10^{16} cm^{-2} they produce fine microcavities in the silicon lattice. Some hydrogen ions bond to the dangling silicon bonds in the microcavities, while others fill these voids. If such an ion implanted wafer is heated to 400–500°C, more hydrogen segregates into the voids in the form of molecular hydrogen H_{2}, the pressure builds up to a point of fracture, and also the silicon surface is blistered with
pockmarks. In the past, these blisters were not desirable and efforts were made to avoid them. The beauty of Bruel’s method was to use this undesirable effect to create a weakened plane or zone that makes it possible to attain a controlled cut through the crystalline lattice. The key to the new method was to introduce a stiffener, a thick and very stiff layer that prevents blistering and redirects the pressure that builds up in the microcavities in a lateral direction. Heating of the wafer can split this weakened plane or zone or it can be cleaved by application of mechanical or other stress. In the Smart Cut™ process for making SOI wafers, the stiffener is a handle wafer.

The Smart Cut™ process to manufacture SOI wafers using implanted hydrogen ions is illustrated in Fig. 2.14. A donor wafer from which a layer of silicon will be removed is oxidized to a desired thickness. This oxide becomes the buried oxide after bonding. In the next step, hydrogen ions with dose typically $5 \times 10^{16} \text{ cm}^{-2}$ are implanted through the oxide layer. After implantation, the handle wafer and the donor wafer are carefully cleaned to remove any particles and surface contaminants and to make both surfaces hydrophilic. Wafer pairs are aligned and contacted so that the fusion wave can propagate across the entire interface. A batch of bonded wafer pairs is loaded into a furnace and heated to a temperature of 400-600°C, at which point the wafer is split along the hydrogen implanted plane. The as-split wafer surface has a mean roughness of a few nanometers. A light touch polish brings the same surface roughness as the standard bulk silicon wafer, i.e. $R_a < 1 \text{ Å}$ across $1 \times 1 \mu\text{m}$ square [82]. The donor wafer is reclaimed and, if necessary, repolished so that it can be used again.
The thickness of the silicon film transferred to the handle wafer and the thickness of the buried oxide can be controlled over a wide range by tuning the ion implantation energy and oxidation time. This approach makes it possible to reuse the donor wafer. The handle wafer can be of lower quality as it only serves as a mechanical support; the quality of the SOI film is decided by the donor wafer. All these benefits reduce the overall cost of SOI wafer manufacturing [82].

Fig. 2.14. Principle of Smart Cut™.
2.5.4. Porous Si Based Process: ELTRAN

“Epitaxial Layer TRAnfer” or ELTRAN developed by Yonehara et al. [105] is another approach to define a thin layer, which is transferred from a seed (donor) wafer to a handle wafer utilizing the properties of porous silicon. ELTRAN SOI wafers were developed and produced by Canon Inc. Japan in 1990. Porous silicon is formed by an electrochemical reaction where silicon constitutes the anode of an electrolytic cell with an HF solution as electrolyte. The etching process cuts random network of nanometer scale pores in silicon producing a porous layer that has a fraction of the density of silicon and very large surface to volume ratio (200 – 1000 m$^2$cm$^{-3}$) [106, 107].

Porous silicon is mechanically weak but still retains the single crystal quality of the wafer on which it is formed, ELTRAN technique uses this property of porous Si to form SOI wafer. Fig. 2.15 illustrates the ELTRAN process flow. Two layers of porous silicon with different pore morphology are formed on top of a seed wafer. By suitably changing the current flow conditions during anodic etching, a layer with very fine pores is formed at the surface and a second layer having coarse pores is formed deeper in the substrate. This double porous layer structure, an improvement over single porous layer, enables a more uniform and smoother fracture along the planar surface during the water jet cutting process. An epitaxial layer of silicon is grown on top of this porous silicon layer. Yonehara et al. [108] improved the epitaxial silicon growth on top of the porous silicon layer, which was previously shown by Baumgart et al. [109] by sealing the pores at the top of the porous silicon layer using high temperature annealing.
in a hydrogen ambient. A thermal oxide is grown on top of the epitaxial silicon layer and the wafer is bonded to a handle wafer. Since porous silicon layer is mechanically weak, it can be easily cut. In ELTRAN a powerful fine water jet uniformly cuts the porous silicon layer along the planar surface as there is considerable interfacial stress at the boundary between the two porous layers. After cutting by water jet, the residual porous silicon in the SOI wafer is etched and the newly exposed SOI wafer surface is smoothed by a second application of hydrogen annealing at about 1100°C. The remaining part of the seed wafer that donated the epitaxial film, can be reclaimed, polished and then used again.
Fig. 2.15. ELTRAN process flow [110].
2.6. Oxygen in Silicon

Oxygen is present in both float-zone and Czochralski crystals but the background oxygen concentration in FZ silicon is $\sim 10^{13}$ cm$^{-3}$ which is much lower than that in the CZ crystal of the order of $10^{17}$-10$^{18}$ cm$^{-3}$ [47]. Hence the presence of oxygen in CZ crystals has a greater significance as it can affect the electrical, mechanical, chemical, and physical properties of single crystal silicon. The main source for oxygen is the quartz or vitreous crucible used for the CZ crystal growth. The surface of the crucible in contact with the silicon melts gradually and dissolves into the melt at high temperature [111] due to the reaction

$$\text{SiO}_2 + \text{Si} \rightarrow 2\text{SiO}$$

Due to this reaction the silicon melt is enriched with oxygen, but most of the oxygen escapes the melt as volatile silicon monoxide (SiO) (~99%) but around (~1%) oxygen gets into the melt and then into the ingot through the crystal-melt interface [112]. At steady state oxygen in the CZ melt = Oxygen from crucible – Oxygen evaporated – Oxygen incorporated. Fuller et al. in 1954 first showed the resistivity changes in CZ silicon crystals subjected to heat treatment at 450ºC and subsequent reversal of the effect beyond 500ºC. These observations were later related to the presence of oxygen in silicon [8, 113]. Later, by using infrared absorption spectroscopy Kaiser et al. confirmed that the oxygen concentration as an impurity in Si is of the same order or higher than that of the intended dopants [114]. The oxygen concentration in silicon is not uniform; it depends on the interaction of various factors, such as, crucible dissolution rate and the nature of fluid flow.
Depending on its concentration in CZ crystals, oxygen has both desirable and undesirable properties, such as internal gettering ability, mechanical strength, and creation of thermal donors that affect the electrical properties mainly in the HRS wafers. Rozgonyi et al. in 1976 reported for the first time that the interior defects caused by oxygen can effectively suppress stacking faults or their origin in CZ wafers, which was later termed as internal gettering and found to be the beneficial property of oxygen in silicon [115]. Due to very low doping of HRS wafers (≈ 10^{12} – 10^{13} cm^{-3}) the oxygen concentration in this type of wafer plays a major role in their electrical properties.

2.6.1. Atomic Configuration of Oxygen in Silicon

The great affinity of oxygen for silicon as evident from its very high concentration in CZ crystals (≈10^{18} cm^{-3}) can be attributed to the stronger bond strength of Si-O bonds (≈5.6 eV in HOSi(CH_3)_3) compared to Si-Si bonds (≈2.3 eV in silicon). At room temperature, most of the oxygen in the as-grown CZ crystal is in a dispersed form called interstitial (O_i) form as shown by the infrared absorption measurements by Jastrebski et al. in 1982 [116] and Pajot et al. in 1985 [117]. The oxygen solubility in silicon is 2.1 x 10^{18} atoms/cm^3 at 1414°C, the melting point of silicon [118], and hence the equilibrium solubility of oxygen in silicon at room temperature is many orders lower than the interstitial oxygen concentration in the as-grown CZ crystals. This implies that the as-grown CZ silicon crystals are super-saturated with oxygen which can precipitate into various forms of silica (SiO_2) at different annealing temperatures. Hence oxygen can transform from the initial interstitial state to the new precipitate forms depending
on the annealing temperature. But this process is also reversible, oxygen can again return to the interstitial state by annealing at very high temperatures (~1300-1350°C) and quenching at room temperature. Also, at such high temperatures, oxygen can out-diffuse from the near surface region of silicon and then the total $O_i$ concentration is mainly the bulk concentration.

The presence of interstitial oxygen in silicon increases the average lattice spacing of silicon depending on the oxygen concentration, as measured by Takano and Maki using high resolution X-rays diffraction measurements [119]. This increase in the lattice spacing leads to expansion of silicon and built-in stresses. In case of large precipitates the stresses are relieved by growth of dislocations. The interstitial oxygen configuration can be explained by a Si-O-Si pseudo-molecule model as shown by the infrared studies of Hrostowski and Kaiser in 1957 [120]. In this pseudo-molecule the Si atoms were assumed to be the nearest neighbors atoms of the crystal, and bridging with the O atom resulted in breaking the Si-Si bond. In this configuration the interstitial O atom is located in a (111) plane equidistant from the two Si atoms; and its exact position depends on the Si-O-Si angle, as shown in Fig. 2.16. This structure is also influenced by different O isotopes. O’Mara et al. [121] proposed, on the basis of the IR data by Bosomworth et al. [122], that oxygen can be present simultaneously at interstitial and substitutional sites. However, there is no general agreement on the existence of oxygen on substitutional sites. IR spectroscopy is the only technique that can discriminate between interstitially dissolved oxygen and oxygen in complexes or precipitates [123].
Interstitial Oxygen transforms to precipitates after heat treatment. Oxygen precipitation in silicon is a phenomenon of aggregation of oxygen atoms, normally uniformly distributed within the Si crystal. As a consequence, small particles of SiO\(_x\), \(1\leq x\leq 2\), form within the silicon crystal. It is widely accepted that precipitation is driven, in a wide temperature range, by the diffusion kinetics. In 1958 Ham [124] proposed a general theory to explain the kinetics of precipitation. The first stage of oxygen precipitation in silicon is nucleation, a process leading to the formation of aggregates of a few O atoms, the so-called nuclei or precipitate embryos, within the silicon lattice. Once formed, precipitation nuclei can either further grow and form oxide precipitates or dissolve, depending on the characteristics of silicon crystals and on the thermal treatments performed. The fundamental parameter for nucleation (and, therefore, precipitation) is the degree of super-saturation of the solid solution constituted by the Si crystal (solvent) and the interstitial oxygen (solute), i.e., the ratio between...
the concentration of oxygen in the Si crystal, and its solubility limit (which is a function of temperature) [123].

2.6.2. Electrical Characteristics of Oxygen in Silicon - Thermal Donors

Oxygen in interstitial form is electrically neutral but when subjected to heat treatment it can affect the electrical properties of CZ silicon by forming thermal donors and can convert a p-type CZ crystal to n-type depending on the background doping concentration and the annealing temperature during various processing steps. Fuller et al. in 1954 discovered that upon annealing in the temperature range of 300-550ºC electrically active centers were formed in oxygen-rich silicon ([O] ~ 10^{18} \text{ cm}^{-3}) [113]. Kaiser et al. determined these centers to be donors [9]. And because these donors are generated under thermal treatment they are called Thermal Donors (TD). A second electrically active center associated with oxygen was later identified in silicon in 1977 by Liaw et al. These are called New Donors and are formed in the temperature range of 650-850ºC. Thermal Donors can be annihilated in the temperature range of 540-560ºC [125, 126].

Thermal Donors are formed upon heat treatment of oxygen rich CZ crystal at near 450ºC. The formation rate and maximum concentration of TDs depend on the fourth and third power of the oxygen concentration, respectively [9]. Anneal temperature and the anneal time are the two important factors that control the formation of TDs and studies by Oehrlein et al. showed that the maximum concentration and the anneal temperature at which it occurs depends on the anneal time as shown in Fig. 2.17 [126]. There can be several species of TDs
which can behave as double donors as discovered by Hall effect and IR absorption measurements by Wruck *et al.* [127]. Wagner *et al.* [128] and Pajot *et al.* [129] identified up to 9 different TD species formed sequentially with different binding energies. The sequential formation and annihilation of the TDs with annealing time suggests successive generation of each species by addition of oxygen impurities, leading to larger and larger centers. *Hydrogen plasma annealed samples* (350-450°C) showed a significant increase in TD concentration which indicates that hydrogen accelerates the diffusion of oxygen.

![Fig. 2.17. Thermal donor concentration as a function of inverse annealing temperature for various anneal times [126].](image)
The diffusivity of oxygen at elevated temperature plays a major role in Thermal Donor formation. Various models have been proposed to describe the TD formation. Bourret in 1985 [130] summarized the various TD formation models: (a) the formation and diffusion of di-oxygen molecules, (b) oxygen-vacancy interactions leading to the switching of oxygen to substitutional sites, or (c) interactions between self-interstitials and interstitial oxygen. Features common to all the models are (i) that enhanced diffusion occurs by some means, and (ii) that oxygen clusters consisting of four or more atoms are formed and that it is these clusters that act as the donors. Newman et al. [131] challenged this model and proposed: oxygen atoms diffuse at their normal rate to form di-oxygen molecules. Self-interstitials generated during this process are found to be mobile and they form clusters which grow during the heat treatment. And these self-interstitials clusters should be identified with thermal donor centers.

2.7. Conclusion

High-resistivity silicon plays a crucial role in the modern era of mobile technology with its ability to suppress coupling between devices and reduce the losses. The need for high-resistivity silicon, its applications, and the characteristics of HRS wafers to be industrially competitive were discussed. HRS wafers are available in both bulk silicon and SOI form. SOI wafers have greater coupling prevention ability than bulk silicon of similar resistivity due to its inherent construction. Various manufacturing processes for both bulk and SOI wafers were also covered. Bulk silicon crystal is grown by two basic growth processes: Czochralski and Float Zone. CZ crystals have lower resistivity
(maximum up to few thousands ohm.cm) than FZ (nearly 10,000 ohm.cm) but are mechanically stronger and have internal gettering capability due to higher oxygen concentrations. CZ crystals are the most commonly used crystals in IC fabrication but FZ is used in high-resistivity application such as mobile communication and power devices. CZ uses a crucible-based pulling technology invented by J. Czochralski and FZ uses a crucible free hot-zone based growth technology invented by Theuerer. In CZ, the dopants are added to the polysilicon melt from which the crystal is pulled and in FZ, the dopants are in gas phase. Magnetic CZ method is used to control the oxygen and dopant concentration in CZ crystal to grow low-oxygen high-resistivity CZ crystals. The double crucible CZ method is used to grow large diameter longer CZ ingot and can also control the oxygen concentration in the crystals. Neutron transmutation doping (NTD) method is used to minimize dopant non-uniformities in FZ crystals and to grow very high-resistivity n-type FZ crystals; it cannot be used for p-type FZ crystals. FZ crystals are doped with oxygen or nitrogen to increase the mechanical strength and make them suitable for IC fabrication which involves integration of both digital and microwave technology.

High-resistivity SOI wafers use a high-resistivity substrate grown by CZ or FZ. SOI wafer manufacturing has advanced from the initial days of SIMOX and Bonded SOI to the current Smart Cut™ technology which has the major market share. The defect rate has decreased significantly and it is possible to fabricate a very thin uniform single crystal silicon film on top of the buried oxide. The challenge still remains to create thinner uniform films on larger wafers.
CHAPTER 3. DEVICE MODELING

3.1. Introduction

The exponential growth of device miniaturization and manufacturing complexities has rendered the testing and accurate prediction of all device characteristics a very complex, expensive and time consuming process. Today’s industry with growing competition, increased R&D cost, and shorter technology lifecycles needs means to accurately predict the device behavior and understand its mechanism prior to the actual fabrication process with fast turnaround time. Numerical solution and device modeling help achieve these objectives.

Technology Modeling and Simulation covers the region of the semiconductor modeling world called extended TCAD (Technology for Computer Aided Design), and it is one of the few enabling methodologies that can reduce development cycle times and costs. Extended TCAD covers the following topical areas, as shown in Fig. 3.1.
The advantages of TCAD are [133]:

- Evaluating “what-if scenarios” rapidly
- Providing problem diagnostics
- Providing full-field, in-depth understanding
- Providing insight into extremely complex problems/phenomena/product sets
- Decreasing design cycle time (savings on hardware build lead-time, gain insight for next product/process)
- Shortening time to market
3.2. Device Modeling Approach

Physically based device simulators predict the electrical characteristics associated with specified physical structures and bias conditions. This is achieved by approximating the operation of a device onto a two- or three-dimensional grid, consisting of a number of grid points called nodes. By applying a set of differential equations, derived from Maxwell’s laws, onto this grid it is possible to simulate the transport of carriers through a structure so that the electrical performance of a device can now be modeled in DC, AC, or transient modes of operation [134].

The main advantages of physically based simulation are [134]:

- It is predictive
- It provides insight
- It conveniently captures and visualizes theoretical knowledge
- It is cheaper and quicker than experimental measurements
- It provides information that is difficult or impossible to measure

The drawbacks of physically based simulations are

- All the relevant physics must be incorporated into a simulator
- Numerical procedures must be implemented to solve the associated equations

In the sequence of predicting the impact of process variables on circuit performance, device simulation fits between process simulation and SPICE model extraction. The main components of semiconductor device simulation at any level
are illustrated in Fig 3.2. There are two main kernels, which must be solved self-consistently with one another, the transport equations governing the charge flow, and the fields driving the charge flow. Both are coupled strongly to one another, and hence must be solved simultaneously. The fields arise from external sources, as well as the charge and current densities which act as sources for the time varying electric and magnetic fields obtained from the solution of Maxwell’s equations. Under appropriate conditions, only the quasi-static electric fields arising from the solution of Poisson’s equation are necessary [133].

![Diagram of device simulation sequence](image)

**Fig. 3.2.** Process flow of device simulation sequence [133].

Device modeling refers in general to a suite of models and methods describing carrier transport in materials. Models range from the simple drift diffusion, which solves Poisson and continuity equations, to more complex and CPU intensive ones as the energy balance, which solve some higher moment simplification of the Boltzmann equation. In addition, the complex physics of today’s devices
mandates at times the usage of Monte Carlo codes, which stochastically solve the Boltzmann equation, and the use of Schrödinger’s equation solvers that account for quantum effects. Despite the significant advances of recent years in both numerics and physics, continuing development is required to meet the increasingly challenging industry needs for device exploration and optimization [132]. The classification of the commercially available device simulators based on the capability to simulate a particular device technology is shown in Table 3.1.

<table>
<thead>
<tr>
<th>Device Technology</th>
<th>Simulator</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D MOS</td>
<td>MINIMOS, GEMINI, PISCES, CADDET, HFIELDS, CURRY</td>
</tr>
<tr>
<td>3D MOS</td>
<td>WATMOS, FIELDAY, MINIMOS3D</td>
</tr>
<tr>
<td>1D BJT</td>
<td>SEDAN, BIPOLE, LUSTRE</td>
</tr>
<tr>
<td>2D BJT</td>
<td>BAMBI, CURRY</td>
</tr>
<tr>
<td>MESFETs</td>
<td>CUPID</td>
</tr>
</tbody>
</table>

As the device size approaches the nanoscale regime, new physical phenomena such as quantum effects appear and the simulator based on semi-classical physics such as drift diffusion model and even energy balance model fail to fully model all the device behaviors. New advanced simulators that rely on direct solution of the Boltzmann’s transport equation e.g. DAMOCLES simulator developed by Fischetti and Laux at IBM Research Labs or simulators based on the solution of a fully quantum mechanical recursive Green’s function method are developed to
model the submicron and nano scale devices. Figure 3.3 describes the advantages and limitation of various simulation models of modern simulators.

Fig. 3.3. Advantages and limitations of different simulation models [133].

3.3. Introduction to the SILVACO ATLAS Simulation Tool

3.3.1. ATLAS Overview

ATLAS is a device simulation tool from SILVACO Corp. designed to provide capabilities for physically-based two- and three-dimensional simulation of semiconductor devices. ATLAS can be used standalone or as a core tool in Silvaco’s VIRTUAL WAFER FAB (VWF) simulation environment [134]. VWF includes DECKBUILD, TONYPLOT, DEVEDIT, MASKVIEWS, and OPTIMIZER. DECKBUILD provides an interactive run time environment. TONYPLOT supplies scientific visualization capabilities. DEVEDIT is an
interactive tool for structure and mesh specification and refinement. MASKVIEWS is an IC layout editor. The OPTIMIZER supports black box optimization across multiple simulators [134].

ATLAS, however, is often used with the ATHENA process simulator. ATHENA predicts the physical structures that result from processing steps. The resulting physical structures are used as input by ATLAS, which then predicts the electrical characteristics associated with specified bias conditions. The combination of ATHENA and ATLAS makes it possible to determine the impact of process parameters on device characteristics [134].

3.3.2. ATLAS Process Flow

The process flow in ATLAS is illustrated in Fig. 3.4. Most ATLAS simulations use two input files. The first input file is a text file that contains commands for ATLAS to execute. The second input file is a structure file that defines the structure to be simulated. ATLAS produces three types of output files. The first type of output file is the run-time output, which gives the progress and the error and warning messages as the simulation proceeds. The second type of output file is the log file, which stores all terminal voltages and currents from the device analysis. The third type of output file is the solution file, which stores 2D and 3D data relating to the values of solution variables within the device at a given bias point [134].
3.3.3. The Order of ATLAS Commands

In ATLAS, the device simulation problems are specified by defining:

- The physical structure to be simulated
- The physical models to be used
- The bias conditions for which electrical characteristics are to be simulated

The order in which statements required to perform a proper device simulation occur in an ATLAS input file is important. There are five groups of statements that must occur in the correct order (Fig. 3.5). Otherwise, an error message appears which may cause incorrect operation or termination of the program. For example, if the material parameters or models are set in the wrong order, then they may not be used in the calculations. The order of statements within the mesh...
definition, structural definition, and solution groups is also important. Otherwise, it may also cause incorrect operation or termination of the program [134].

<table>
<thead>
<tr>
<th>Group</th>
<th>Statements</th>
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<tbody>
<tr>
<td>1. Structure Specification</td>
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<td>REGION</td>
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<td>ELECTRODE</td>
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<td>2. Material Models Specification</td>
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<td>MODELS</td>
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<td>CONTACT</td>
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<td></td>
<td>INTERFACE</td>
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<tr>
<td>3. Numerical Method Selection</td>
<td>METHOD</td>
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<td>4. Solution Specification</td>
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<td>SAVE</td>
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<td>5. Results Analysis</td>
<td>EXTRACT</td>
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<td>TONYPLOT</td>
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Fig. 3.5. ATLAS command groups with the primary statements in each group [134].

3.4. Simulation Approach in this Research

2D device simulation was used to understand the effect of material parameters such as film and substrate doping, interface charges, film and oxide thickness, type of contacts etc. The device structure was defined using ATLAS command statements, such as: MESH, DOPING, REGION, ELECTRODE, and CONTACT. The simulation results qualitatively matched the experimental results.
3.4.1. Numerical Methods Used

Several different numerical methods can be used for calculating the solutions of semiconductor device problems. Different solution methods are optimum in different situations. There are basically three types of solution techniques: (a) decoupled (GUMMEL), (b) fully coupled (NEWTON), and (c) BLOCK. In simple terms, a decoupled technique like the Gummel method solves for each unknown in turn, keeping the other variables constant, repeating the process until a stable solution is achieved. Fully coupled techniques, such as the Newton method, solve the total system of unknowns together. The combined or Block methods will solve some equations fully coupled, while others are decoupled [133].

Isothermal Drift Diffusion (DD) model was used for device modeling. Isothermal DD model requires the solution of three equations for the potential, the electron concentration, and the hole concentration. Specifying GUMMEL or NEWTON alone will produce simple Gummel or Newton solutions. For almost all cases the Newton method is preferred and it is the default. Specifying: METHOD GUMMEL NEWTON will cause the solver to start with Gummel iterations and then switch to Newton, if convergence is not achieved. This approach is a very robust, although more time consuming to obtain solutions for any device. However, this method is highly recommended for all simulations with floating regions such as Silicon-on-Insulator (SOI) transistors [133].

*Both GUMMEL and NEWTON method are used* in simulations performed in this research for the reasons mentioned above.
3.4.2. Physical Models Used

The following models were used for device simulation in ATLAS:

- Mobility: CONMOB, FLDMOB, KLA, SHI
- Interface charge: INTERFACE statement used for both interfaces
- Recombination: SRH
- Band-gap narrowing: BGN
- Carrier generation: IMPACT
- Lattice heating: LAT.TEMP on MODELS statement

MODELS statement in ATLAS specifies the model flags to indicate the inclusion of various physical mechanisms, models, and other parameters such as the global temperature for the simulation.

CONMOB represents the concentration-dependant low-field mobility model for silicon, valid at 300 K for Si and GaAs only. This look-up table provided by ATLAS for the doping-dependent low-field mobilities of electrons and holes in silicon at 300K only. It uses simple power law temperature dependence and relates the low field mobility at 300K to the impurity concentration.

FLDMOB represents field-dependant mobility model for Si and GaAs. It models the change in mobility due to electric filed, required to model any velocity saturation effects.

KLA represents Klaassen mobility model. KLA provides a unified description of majority and minority carrier mobilities. It includes the effects of lattice scattering, impurity scattering (with screening from charged carriers), carrier-
carrier scattering, and impurity clustering effects at high concentration. It applies separate mobility to majority and minority carriers.

SHI represents the Shirahata mobility model to take into account surface scattering effects at the silicon/oxide interface, which is a function of the transverse electric field.

AUGER is a recombination model that adds a dependence of recombination lifetime on carrier concentration, and is significant at high carrier densities.

In SOI transistors, there exist two active silicon/oxide interfaces on the wafer. The top interface, under the top gate, is similar to conventional MOS technology. The bottom interface is quite different and typically contains significantly more charge. Different interface charges can be set using the INTERFACE statement with region specific parameters.

SRH activates the Shockley-Read-Hall recombination model which uses fixed minority carrier lifetimes. This simulates the leakage currents that exist due to thermal generation.

BGN stands for band gap narrowing. This model (BGN) is necessary to correctly model the bipolar current gain when the SOI MOSFET behaves like a bipolar transistor.

3.5. Conclusion

With shrinking of semiconductor feature sizes into the nanometer scale regime, even conventional device behavior becomes increasingly complicated as new physical phenomena at short dimensions occur. In addition to the problems related to the understanding of actual operation of ultra-small devices, the reduced feature
sizes require more complicated and time-consuming manufacturing processes. This fact signifies that a pure trial-and-error approach to device optimization will become impossible since it is both too time consuming and too expensive. Since computers are considerably cheaper resources, simulation is becoming an indispensable tool for the device engineer. Besides offering the possibility to test hypothetical devices which have not (or could not) yet been manufactured, simulation offers unique insight into device behavior by allowing the observation of phenomena that cannot be measured on real devices.
CHAPTER 4. C-V CHARACTERISTICS OF HIGH-RESISTIVITY SOI

4.1. Introduction

Capacitance-Voltage (C-V) is a widely used popular technique to characterize bulk silicon wafers to measure carrier concentration, doping profile, carrier lifetimes, oxide thickness, oxide quality, etc [11]. This technique has also been used to characterize the oxide and film thickness of SOI wafers [12]. C-V characterization is performed using various types of devices such as MOS capacitors, \textit{pn} diodes, and Schottky diodes [11]. In most of the reported C-V characteristics of SOI wafers using a gate oxide, the maximum capacitance was proportional to the gate area [12-16]. During capacitance-voltage measurements using an aluminum contact directly on the SOI film without a gate oxide, very different behavior for such devices is observed compared to devices with gate oxides, under certain bias conditions. The device in Fig. 4.1(a), consisting of a substrate which may be depleted, accumulated or inverted (space-charge region width \(W\)), a buried oxide (\(t_{\text{BOX}}\)), a Si film (\(t_{\text{film}}\)) and a gate oxide (\(t_{\text{ox}}\)), shows conventional C-V behavior, i.e., the capacitance depends on the gate area, indicated by the vertical dashed lines in Fig. 4.1(a). However, for device in Fig. 4.1(b) with a metal contact directly to the Si film without a gate oxide, the capacitance can be governed by an area significantly larger than the gate area, indicated by the vertical dashed lines in Fig. 4.1(b). How can this be?

Simulations and measurements in this research show that if the film is completely accumulated or inverted, the effective area can extend beyond the gate area. This effective area depends mainly on the frequency of the ac signal during
the capacitance measurements, the type of contact and also the film thickness. Figure 4.1(c) shows such a case, where the film is represented by resistance R and the BOX and underlying substrate by capacitance C. This is a distributed transmission line and the distance for the ac signal to propagate laterally depends on the frequency, and R and C. It is this lateral distance, indicated by the vertical dashed lines in Fig 4.1(c), that determines the effective gate area which varies with frequency and depends on whether the film is accumulated, depleted or inverted. Bulk substrates do not exhibit this unusual behavior.

![Cross sections of SOI wafers](image)

**Fig. 4.1.** Cross sections of SOI wafers (a) with and (b, c) without gate oxide; (c) shows an accumulated film and its representation by the distributed RC circuit.

C-V characterization carried out in this research focuses mainly on high-resistivity SOI wafers. Before going into the details, it should be mentioned that MOS capacitors on high-resistivity substrates do not behave the same as on low-resistivity substrates due to the substrate potential drop and the longer Debye length [135]. Furthermore, low-frequency MOS-C behavior is observed at higher frequencies due to the shorter response time $t_r = (N_A/n_i) \tau_g$, since $N_A$ is very low.
Minority inversion carriers follow the ac signal provided the period of the ac signal is much longer than the response time. For example, $N_A = 10^{16} \text{ cm}^{-3}$, $n_i = 10^{10} \text{ cm}^{-3}$, and $\tau_g = 1 \text{ ms} \Rightarrow t_r = 1000 \text{ s}$, while $N_A = 10^{12} \text{ cm}^{-3} \Rightarrow t_r = 0.1 \text{ s}$. The MOS-C frequency response is proportional to $1/t_r$ leading to low-frequency behavior for frequencies as high as 1 kHz.

The objective of this chapter is to highlight the challenges in C-V characterization of an SOI wafer using a Schottky contact directly on the film, the phenomenon of associated bias spreading, understand why this happens and discuss the effects of various factors, such as: frequency, contact and substrate sizes, gate oxide, SOI film thickness, film and substrate doping, carrier lifetime, contact work-function, temperature, light, annealing and radiation on the C-V behavior.

4.2. C-V Characterization Technique

The C-V technique is a simple, accurate and quick method to measure the carrier concentration, doping profile, interface traps, oxide charges, oxide thickness, oxide quality etc. The method is based on the concept of dependence of the width of the space-charge-region (scr) of a semiconductor junction on the applied bias [11]. The depletion region capacitance is part of the total device capacitance and the depletion capacitance depends on the width of the depletion region ($t_{dep}$) for a constant depletion area ($A_{dep}$) and hence on the applied bias by the equation $C_{dep} = \varepsilon_0\varepsilon_{ox}A_{dep}/t_{dep}$. The differential capacitance given by $C = dQ/dV$ was used for C-V measurements.
There are two types of C-V measurement techniques depending on how the C-V instrument considers the device under test, namely: Series C-V and parallel C-V method. Figure 4.2 shows an equivalent circuit of a MOS capacitor with oxide capacitance $C_{ox}$, semiconductor capacitance $C_{sc}$, substrate capacitance $C_{sub}$, and substrate resistance $R_{sub}$. The series and parallel equivalent circuits are shown next to it. In the series measurement mode $C_S$ is the equivalent series capacitance and $R_S$ is the equivalent series resistance of the MOS capacitor circuit. Similarly, in the parallel measurement mode, $C_P$ is the equivalent parallel capacitance and $R_P$ is the equivalent parallel resistance of the MOS Capacitor. The values of $C_S$, $R_S$, $C_P$ and $G_P$ in terms of MOS Capacitor circuit parameters ($C_{ox}$, $C_{sc}$, $C_{sub}$ and $R_{sub}$) are given in Eqn. 4.1 and 4.2.

Fig. 4.2. Equivalent circuit representation of a MOS-Capacitor, and the corresponding series and parallel configuration for series and parallel C-V measurement respectively.
\[ C_s = \frac{C(1 + \omega^2 \tau_{sub}^2)}{1 + \omega^2 \tau_{sub}(\tau_{sub} + \tau)} \quad R_s = \frac{R_{sub}}{1 + \omega^2 \tau_{sub}^2} \] (4.1)

\[ C_p = \frac{C[1 + \omega^2 \tau_{sub}(\tau_{sub} + \tau)]}{1 + \omega^2(\tau_{sub} + \tau)^2} \quad G_p = \frac{\omega^2 C \tau}{1 + \omega^2(\tau_{sub} + \tau)^2} \] (4.2)

Where, \( \tau_{sub} = R_{sub} C_{sub} \); \( \tau = R_{sub} C \) (4.3)

4.2.1. Which C-V Method to Choose for High-resistivity Silicon?

Figure 4.3 shows the C-V characteristics plotted using Eqn. 4.1 and 4.2 for various substrate doping concentrations. Fig. 4.3 shows that during parallel C-V measurement, for higher substrate resistivity, i.e. lower substrate doping concentration, the accumulation capacitance is lower than the inversion capacitance, which is not correct. But the series C-V does not show any such anomalies. In parallel mode as the substrate doping concentration reduces, the substrate resistivity \( R_{sub} \) term begins to dominate causing the calculated \( C_p \) to be much lower than the actual \( C_{OX} \) in accumulation. Hence series C-V measurement were used for HRS substrates because they are more accurate.
Fig. 4.3. Calculated C-V plots of a MOS-Capacitor for series (a) and parallel (b) equivalent circuits using eqn. 4.1 and 4.2 respectively. Series C-V is the preferred method for HRS substrates as in the parallel method, for very low doping concentration (i.e. high resistivity), the accumulation capacitance becomes lower than the inversion capacitance due to dominance of series resistance.

4.2.2. Where to Apply the DC Bias During C-V Measurements?

It was determined from measurements that applying the bias to the top contact on the film gives a very noisy output and the sensitivity is poor, i.e., one cannot measure very low capacitances in the pico-faraday range but applying the DC bias to the substrate reduces the noise and improves the instrument sensitivity, as shown in Fig. 4.4.
Fig. 4.4. Comparison of C-V plots between biases applied to the top-contact and to the substrate. Clearly the measurement with substrate bias is less noisy and more sensitive.

4.3. Schottky Barrier Height

Schottky contacts play an important role during C-V characterization using a metal contact directly on the silicon film of an SOI wafer. A short analysis of Schottky barrier heights is presented in this section for better understanding of the observed C-V characteristics.

When a metal is placed in close contact with a semiconductor then they form the metal-semiconductor device, discovered by Braun in 1874 [136]. The first acceptable theory was proposed by Schottky in 1930s [137] and in his honor these devices are called Schottky barrier devices. Depending on the doping concentration of the semiconductor, the metal-semiconductor devices can exhibit either non-linear characteristics (Schottky diode), much like a $pn$ diode, or linear characteristics (Ohmic contact).
The **Schottky model** of the metal semiconductor barrier is shown in Fig. 4.5(a, b, c). The energy band diagrams are shown: before contact in the upper part of the figure and after contact in the lower part. Intimate contact between metal and semiconductor is assumed. The work function of a solid is defined as the energy difference between the vacuum level and the Fermi level. The work function is given as the energy $\Phi_M$ related to the potential $\phi_M$ by $\Phi_M = \phi_M \gamma$. In Fig. 4.5(a) $\phi_M < \phi_S$ and creates an accumulation type contact, in Fig. 4.5(b) $\phi_M = \phi_S$ and creates a neutral contact, and in Fig. 4.5(c) $\phi_M > \phi_S$ and creates a depletion type contact [11].

The ideal electron ($\phi_{bn}$) and hole ($\phi_{bp}$) barrier heights for a contact are given by:

$$\phi_{bn} = \Phi_M - \chi; \quad \phi_{bp} = E_G - \phi_{bn} = E_G - \Phi_M + \chi \quad (4.4)$$

where $E_G$ is the band gap, $\Phi_M$ the work function and $\chi$ the electron affinity.

According to the Schottky theory the barrier height depends only on the metal work function and is independent of the semiconductor doping concentration. The barrier height can be varied by using metals of the appropriate work function to implement any one of the three barrier types Fig. 4.5(a, b, c). They are named as accumulation, neutral and depletion contacts because majority carriers are accumulated, unchanged (neutral), or depleted compared to their density in the neutral substrate [11].

Figure 4.5(d) represents the Schottky barrier height for a p-type silicon for different metal contacts. $E_{Vac}$, $E_C$, $E_V$, $E_i$ and $E_F$ represent the vacuum energy,
conduction band energy, valence band energy, intrinsic energy, and Fermi energy level respectively. As $\phi_M$ increases, $\phi_{bn}$ increases and $\phi_{bp}$ decreases. The lower the hole barrier height the easier it is for the holes to cross over the barrier by thermionic emission. This is one of the main controlling mechanisms for the shape of HRSOI C-V characteristics using a Schottky contact on the silicon film as discussed in the subsequent experiments and simulations.

The current voltage behavior of an ideal Schottky diode of area $A$ is given by the thermionic-emission equation originally derived by Bethe [138]:

$$I = AA^* T^2 e^{-q \phi_b / kT} e^{qV / nkT} = I_s e^{qV / nkT}$$  \hspace{1cm} (4.5)

where $I_s$ is the saturation current given by:

$$I_s = AA^* T^2 e^{-q \phi_b / kT}$$  \hspace{1cm} (4.6)

where $A^*$ is the Richardson constant, $n$ the ideality factor and $\phi_b$ the barrier height. It can also be described by the diffusion theory derived by Schottky [137], and the combination of thermionic emission-diffusion theory developed by Crowell and Sze [139]. However, thermionic emission theory is generally considered valid when a semiconductor has a reasonable mobility and modest doping concentration [140], which is the present case.
Fig. 4.5. (a, b, c) Metal-semiconductor contacts according to the simple Schottky model. The upper and lower parts of the figure show the metal-semiconductor system before and after contact respectively [11]. (d) Schottky barrier heights for a p-type silicon, $\phi_{BpH}$ – High hole barrier height and $\phi_{BpL}$ – Low hole barrier height.
4.4. Device Fabrication

Both MOS-C and Schottky contacts of various sizes were fabricated on SOI wafers with different substrate resistivities (i.e., doping concentrations), buried oxide thickness, and film thicknesses. Schottky contacts were fabricated by evaporating aluminum on the silicon film using a shadow mask or by photolithography and annealing the contacts at 400°C for 30 mins in forming gas to form better contacts. The MOS-Cs were fabricated by growing a 100 nm thick thermal oxide and evaporating 300 nm thick aluminum on the oxide layer using a shadow mask and subsequent annealing as mentioned above. The contacts were circular with 900 \( \mu \text{m} \) diameter. The wafers were cleaned using RCA1 (5:1:1 ratio of water, ammonium hydroxide (NH\(_4\)OH), and hydrogen peroxide (H\(_2\)O\(_2\))) and RCA2 (6:1:1 ratio of water, hydrochloric acid (HCl), and hydrogen peroxide (H\(_2\)O\(_2\))) cleaning method. Figure 4.6 and 4.7 describe the fabrication steps for Schottky contacts/MOS-C using shadow mask and photolithography respectively.

Processing Steps to fabricate Schottky Contacts/MOS-Cap (Shadow Mask Process)

1. Tools – Torr-Vac/Lesker 3 (metal deposition), Furnace (anneal), Trystar Horizontal Oxidation Furnace.
2. Chemicals BOE (20:1), RCA etch - Ammonium Hydroxide (NH\(_4\)OH), Hydrogen Peroxide (H\(_2\)O\(_2\)), Hydrochloric Acid (HCl), Hydrofluoric Acid (HF)
3. Break the wafer into the required size and then clean both sides using RCA etch (refer to appendix for RCA etch procedure). Clean in DI water and dry thoroughly.
4. For MOS-Cap – Grow 100 nm thick dry oxide in Trystar Horizontal Oxidation Furnace, with HCl mixture at 1000°C, 6 hr (2hr of actual growth time)
5. Soft bake (only when ready for Metal) at 85°C/30 min.
6. ONLY for Schottky contacts - Etch native oxide by first putting the wafer in BOE for 15 sec, then put it in the water container for 1 min and then rinse thoroughly in DI water and dry.
7. Deposit metal. AL - 3,000 A\(^\circ\) using a Shadow Mask in Lesker 3 evaporator.
8. Anneal the devices in a furnace at 400°C/30 min to make better contacts.

Fig. 4.6. Processing steps for Schottky contacts/MOS-Cap using shadow mask.
Processing Steps to fabricate Schottky Contacts  
(Lift Off Process – Dark field Mask)

1. Tools – Spinner, EVG620 (Photo-lithography), Torr-Vac/Lesker 3 (metal deposition), Furnace (anneal).
2. Chemicals BOE (20:1), AZ400T, MIF300 (developer), AZ4620 (Photo-resist)
3. Break the wafer into the required size and then clean both sides by putting in AZ400T for 10 mins heated at 160°C. Rinse thoroughly in DI water and dry completely.
4. Dehydration bake at 120°C for 15 min (to remove moisture).
5. Spin coat HMDS (transparent liquid) at 4000 rpm for 50 sec.
6. Put AZ4620 and spin at 3000 rpm for 40 sec (7µm thick PR coating).
7. Soft bake (only when ready for Metal) at 85°C/30 min slowly to have 90 deg step coverage else edges will be slanted.
8. Using EVG620 expose for a dose ~ 500mj/cm².
9. Develop using MIF 300 for ~ 5 - 6 min.
10. Rinse with DI water. Dry and inspect under the microscope to check the sharpness of the edges. If not sharp then repeat steps 3 to 6.
11. Bake at 85°C for 30 min, makes smooth profile, removes solvent and makes the resist stick to the surface thoroughly so that acid won’t etch it.
12. Etch native oxide by first putting the wafer in BOE for 15 sec, then put it in DI water for 1 min and then rinse thoroughly in DI water and dry.
13. Deposit metal, Al- 10,000 Å using Lesker 3 evaporator.
14. Liftoff the unexposed layer (to bring out the contacts) using AZ400T (at 200°C, set heater temp to 200°C). Heat the hot plate to 200°C – Put the Beaker with 400T – Put the wafer in 400T – Keep it on the hot plate for 10 min – put in the ultrasonic vibrator for 5 min – check for metal coming out. Make sure no water mixes with AZ400T. Removal takes around 10 to 15 mins.
15. Rinse thoroughly in DI water and dry.
16. Check under microscope for sharpness of edges.
17. Anneal the devices in a furnace at 400°C/30 min to make better contacts.

Fig. 4.7. Processing steps to fabricate Schottky contacts using photolithography.

4.5. Experimental Setup

C-V measurements were made using HP4284 and microprobe station on various high-resistivity SOI wafers with different sizes of aluminum contacts placed directly on the Si film and also with a gate oxide on top of the film for comparison. The measurements were made using the series C-V setting of HP4284, 100 kHz ac signal as default and applying the DC bias to the substrate to suppress noise and increase the measurement sensitivity. The experimental graphs were plotted by converting the bias to the top contact. The default device configuration for measurements is: circular aluminum contacts with 0.9 mm
diameter placed directly on the silicon film of an SOI wafer with 145 nm thick film, 1 µm thick oxide, and 725 µm thick substrate. The substrate area is 8 cm x 4 cm. The experimental device cross section is shown in Fig 4.8(a).

4.6. Simulation Setup

The C-V characteristics were simulated using 2D ATLAS/SILVACO (2007) device simulator. The simulated device dimensions are: SOI wafer with 145 nm thick p-type film $N_A = 10^{14} \text{ cm}^{-3}$, 1 µm thick oxide, 350 µm wide and 100 µm thick n-type substrate with $7 \times 10^{11} \text{ cm}^{-3}$ substrate doping concentration, the doping concentration and polarities were chosen to match the simulated and the experimental results; described in subsequent sections. The top film contact is 50 µm diameter and the back contact is the entire substrate width of 350 µm. These are the default simulation specifications for the rest of the chapter unless otherwise specified. The default temperature is 300 K for all simulations. The simulated device cross section is shown in Fig. 4.8(b). Concentration-dependent mobility, field-dependent mobility, Klaassen mobility model, Shirahata mobility models and Shockley-Read-Hall recombination model were used as model parameters in the simulator.
4.7. Analysis of C-V Characteristics of HRSOI using Schottky Contact

4.7.1. A New Effect of Bias Spreading

Figure 4.10 shows the experimental and simulated C-V curves of HRSOI using aluminum contact directly on the silicon film. Figure 4.10 (b) shows the comparison between simulated C-V plots with and without gate oxide on an HRSOI wafer, and it clearly shows that with gate oxide (100 nm) the maximum capacitance in accumulation is proportional to the gate area (0.9 mm diameter) and without gate oxide the capacitance is around 5 times greater for the same contact size. The samples were fabricated with lightly-doped p-type substrates, with doping concentrations less than $5 \times 10^{12}$ cm$^{-3}$ and film doping $N_A > 10^{14}$ cm$^{-3}$. At such low doping concentrations, after 30 min annealing at 400ºC the oxygen thermal donors have converted the p-type substrate into n-type [8-10] but not the higher doped film, shown by simulations comparing different combinations of film and substrate doping types (p- and n-type). Clearly, only when the substrate is lightly-doped n-type and the film is p-type, do the simulation results match the
experimental results, as shown in Figs. 4.9 and 4.10.

Fig. 4.9. Simulated C-V plots for different combinations of film and substrate doping polarities (p- and n-type).

Fig. 4.10. (a) Experimental and (b) simulated C-V plots with and without gate oxide for HRSOI. Capacitance after 10 V is much higher than that due to the contact area at point D indicating bias spreading. With gate oxide ($t_{\text{Gate-Ox}} = 112$ nm) the maximum capacitance corresponds to that of the contact area (no spreading).
The work function difference between the aluminum contact ($\Phi_M = 4.08\text{eV}$) and the p-type silicon film ($\Phi_S = \chi + E_G/2 - \phi_{Si} = 4.05 + 1.12/2 - 0.24 = 4.85 \text{eV}$ for $N_A = 10^{14} \text{ cm}^{-3}$) is $\Phi_{MS} = -0.77\text{eV}$ and the work function difference between the n-type silicon substrate and the aluminum contact is $\Phi_{MS} = -0.42\text{eV}$ ($\Phi_S = 4.05 + 1.12/2 - 0.11 = 4.5 \text{eV}$ for $N_D = 7 \times 10^{11} \text{ cm}^{-3}$). This creates a high hole barrier height ($\phi_{bp} = E_G - (\Phi_M - \chi) = 1.12 - (4.08 - 4.05) = 1.09\text{eV}$) or a very low electron barrier height ($\phi_{bp} = \Phi_M - \chi = 4.08 - 4.05 = 0.03\text{eV}$) at the film Schottky contact; as a result there is minority carrier (electron) injection into the film causing the film below the contact to invert and the region away from the contact to deplete. The film below the contact acts as a source of minority carriers which affects the C-V at higher frequencies and biases.

To explain the behavior of the C-V plots some of the critical bias points are marked in the experimental/simulation results in Fig. 4.10. With the aluminum contact directly on the film, the bias is no longer confined to the contact area but spreads to a larger area in the film due to direct coupling between the film and the contact. At higher positive bias the entire p-type film, including the film/BOX interface is accumulated with holes and the n-type substrate/BOX interface is accumulated with electrons (see point A in Fig. 4.10 and Fig. 4.11). As the film is completely accumulated, there is no minority carrier injection. The continuous sheet of holes in the film provides a conducting path to the ac signal which spreads through this layer limited by the layer sheet resistance. Due to this spreading, the measured capacitance is the total capacitance spread along the
BOX area which is much larger than the contact area. The spreading is frequency and bias dependent and is controlled by the *low pass filter* behavior of the RC network of film/BOX/substrate in Fig. 4.11(a). The corresponding carrier concentration in the film at 15 nm above the film/BOX interface is shown in Fig. 4.11(b, c).

Fig. 4.11. Bias = +22 V, point A in Fig. 4.10, (a) device cross section, entire film is completely accumulated with holes and the substrate is accumulated with electrons (charge spreading), (b) carrier concentration, and (c) energy band diagram in the film at 15 nm above the film BOX interface.

This spreading effect is also confirmed by calculating the effective area from the measured capacitance. The capacitance at point A (22 V) at 110 pF is much higher than that for a contact diameter of 0.9 mm. The area from the measured capacitance at “A” is more than 5 times larger than the contact area. A similar increment is observed in simulation. The extent of spreading also depends on the contact size and the frequency of the ac signal for a particular dc bias. In
simulation, the capacitance saturates at higher positive bias whereas in the experiments it has a shallow rising slope, mainly due to the fixed substrate width of 350 µm in simulation. The charges tend to saturate within this area after a certain bias whereas in experiment the sample size is much larger than the contact size and therefore the spreading continues to increase with bias.

When the bias is reduced, the holes try to leave the film but they encounter a high hole barrier Schottky contact. This effect is predominant at lower positive biases. At around 12 V (see point B, in Fig. 4.10) the film below the contact begins to deplete/invert due to the Schottky contact, Fig. 4.12(a, b, c) and the inverted region below the contact is separated from the accumulated region of the film by a depletion region. Figures 4.12(b and c) show carrier concentration, and energy band diagram respectively in the film 15 nm above the film BOX interface. A split in the Fermi level indicates minority carrier injection from the Schottky contact. Fig 4.12(d) shows the simulated film cross section showing electron concentration at \( V_{\text{contact}} = 3 \) V. The region below the contact is inverted (film doping concentration \( N_A = 10^{14} \) cm\(^{-3}\)); electron concentration decreases gradually into the film on both sides of the contact. This depletion region at the contact acts as a large resistor \( R_f \) connecting the contact region of the film to the lateral region, as shown in Fig. 4.12(a). \( R_f \) increases as positive bias reduces, the coupling to the lateral region is reduced and the ac signal is confined closer to the contact, hence the spreading reduces and the measured capacitance gradually reduces to the contact area capacitance. More and more carriers below the contact area begin to respond (the film below the Schottky contact acts as a source of
minority carriers, electrons) compared to other parts of the still accumulated film. This behavior results in capacitance change from a high (~spread area) to a low value (~contact area) along the “S” shape (point B to C in Fig. 4.10). At bias < 5 V the capacitance corresponds to that due to the contact area, as in point D in Fig. 4.10.
Fig. 4.12. Bias = +3 V, point D in Fig. 4.10. (a) Device cross section, only the film below the contact is inverted and the rest partially accumulated with holes and the substrate is accumulated with electrons, (b) carrier concentration, and (c) energy band diagram in the film 15 nm above the film BOX interface. Fermi level splits due to minority carrier injection from the Schottky contact. (d) Film cross section showing electron concentrations at $V_{\text{Contact}} = 3$ V. The region below the contact is inverted (film doping $N_A = 10^{14}$ cm$^{-3}$); electron concentration decreases gradually into the film on both sides of the contact.
At a negative bias close to zero, the substrate is completely depleted. The depletion region is much wider than the BOX thickness and the capacitance reaches its minimum value (see point F, Fig. 4.10). With further negative bias the film inverts within a few 100 mV after the minimum capacitance (see point G, Fig. 4.10). Unlike accumulation with a discontinuity of charges under and away from the contact, in inversion there is a continuous layer of electrons in the film all along due to the negative bias and the Schottky contact, Fig. 4.13. Simultaneously the substrate/BOX interface is also inverted with holes. This gives a continuous path to the ac signal to flow along the film/box interface and the capacitance measured should be same as the accumulation capacitance but it is lower. Because, even though the minority electrons in the film can be easily supplied by the contact, the minority holes in the substrate have to be thermally generated and the substrate inversion layer cannot respond to the higher frequency and the capacitance saturates at a value corresponding to the spread substrate depletion capacitance. The inversion layer spreads all along the BOX interface in the film and the substrate. Due to this spreading, the area through which the ac signal flows is larger, and as a result the inversion capacitance is larger than the minimum depletion capacitance at point F, but smaller than the accumulation capacitance due to the inability of the substrate inversion charge to respond to the 100 kHz ac signal.
Fig. 4.13. Bias = -2 V, point G in Fig 4.10. (a) Device cross section, entire film is completely inverted with electrons and substrate is inverted with holes (charge spreading), (b) carrier concentration, and (c) energy band diagram in the film at 15 nm above the film BOX interface. Fermi level does not split.

Figure 4.14 shows the vertical distribution of charges in the device from the top contact to the bottom substrate contact through the center of the device at different gate biases. Figure 4.14 along with Figs. 4.11(b), 4.12(b), and 4.13(b) shows how the entire film (spread) not just the contact region goes from accumulation to inversion as $V_{contact}$ changes from high positive to high negative bias. They also show that at low positive bias the contact work-function dominates and creates a localized inversion and depletion region just below the contact with other part of the film still in accumulation, giving rise to the “S” shape.
Fig. 4.14. Carrier concentration through the center of the device (a) in the film below the contact, (b) in substrate. The film changes from accumulation at A (22 V) to depletion at C (6 V) and then becomes inverted for bias below 3 V (D,F,G).

Correspondingly the substrate remains accumulated for all positive biases, at point F (-0.25 V) the substrate is depleted and capacitance is the minimum in the C-V plot; then the substrate inverts, point G (-2 V).

For the positive to negative sweep direction (see Fig. 4.10(a, b) bold line), when the bias becomes less positive, holes accumulated in the film during the initial high positive bias cannot move out of the film easily due to the high hole barrier at the Schottky contact. The accumulated holes create a higher positive potential in the film and prevent the film potential from reducing in response to the reduction in applied bias; lower positive bias is required to drain the holes and reduce the capacitance accordingly. In the negative to positive sweep direction
(see Fig. 4.10(a, b) dotted line), there are no accumulated holes in the film as the film is inverted. So it takes a higher positive bias compared to the previous sweep direction to build up enough holes along the BOX/film interface leading to a hysteresis-like behavior.

4.7.2. Effect of Frequency

The film, BOX, and the substrate behave as an RC circuit of a transmission line as shown in fig 4.11(a). The resistance “R” of the film is controlled by the concentration of the accumulated holes or inverted electrons and hence on the applied bias. This RC circuit when subjected to an ac signal behaves as a low pass filter. So the frequency response of this low-pass filter controls how far the ac signal can spread at different frequencies and hence the C-V characteristics. At low frequencies for all positive and negative bias the ac signal can spread further due to the low-pass nature of the RC circuit, so the charges in the film under and away from the contact and the corresponding substrate charges can respond. Hence, a higher low-frequency capacitance than that at high frequency is observed at all biases Figs. 4.15(a, b) and 4.11(a). With increasing frequency, the ac signal flows closer to the contact due to lower capacitive reactances. It spreads less into the film leading to lower measured capacitances, Fig 4.15(c). The ‘S’ shape remains during positive bias. In simulation, for f < 1 kHz both inversion and accumulation capacitances are the same and are the spread values, Fig. 4.15(b).

At very high frequencies the “S” shape in the positive bias vanishes as almost all of the ac signal flows very close to the contact area, beyond 2 MHz in Fig.
4.15(b). With further increase in frequency, the capacitances at all biases (including the minimum capacitance) reduce as the substrate resistance of an HRS wafer becomes more dominant. Nicollian et al. [141] observed bias spreading and focused on the RC behavior in the inversion region and the spreading was controlled by the oxide charges; in our case the RC behavior and its effect on the measured capacitance is in both accumulation and inversion regions with no lateral source of minority carriers.
4.7.3. Effect of Contact and Substrate Size

Figure 4.16(a) shows the experimental results for change in contact size and its effect on C-V plots. The capacitances mentioned in Fig. 4.16(a) are calculated...
using \[ C_{\text{box}} = \frac{K_{\text{ox}} \varepsilon_0 (A_{\text{contact}})}{t_{\text{ox}}} \times 10^{15} \text{ fF} ,\]
\[ K_{\text{ox}} = 3.9,\ v_0 = 8.854 \times 10^{-14} \text{ F/cm} \]
for the contact area mentioned, for simplicity only the BOX thickness was considered to calculate the accumulation capacitance. Figure 4.16(b) shows the corresponding simulation results. In both cases, with the increase in the contact size an increase in the capacitance is observed at all biases. The capacitances at the lower portion of the “S” match the oxide capacitance for the corresponding contact sizes and at higher positive bias it is many times higher, observed in both experiment and simulation, as shown in Fig. 4.16(a, b), confirming the spreading theory that at lower positive bias the Schottky effect dominates and the capacitance is confined to the contact area and at higher bias the entire film is accumulated and the ac signal spreads resulting in higher capacitance.

As the contact size increases the oxide capacitance increases due to the larger area and hence the lower portion of “S” also increases. The spreading area increases with increase in contact area which in turn increases all other capacitances (accumulation and inversion). But the increase in the spreading area is not always proportional to the increase in the contact area. Figure 4.17 is the same plot as in Fig. 4.16 but the capacitances are normalized w.r.t. to \( C_{\text{box}} \) for the corresponding contact areas. In both simulation and experiment, as the contact area increases the percentage of spreading reduces, i.e., for smaller contact area the spreading area is much larger than the actual contact area compared to that for larger contacts, Figs. 4.17(a, b).
Next, we will discuss the relation between the substrate area and the contact area and its effect on bias spreading using simulation (see Fig. 4.18). If the
substrate length is reduced from 350 µm to 150 µm for the same contact length (50 µm) then the accumulation and the inversion capacitances are also reduced, which points to reduction in bias spreading with decrease in substrate area across the film/BOX and substrate/BOX interface. And at lower positive biases ($0V < V_{\text{contact}} < 5V$) the capacitance is the same for both substrate sizes. Because at these biases the depletion layer due to the Schottky contact separates the contact area from the other parts of the film, so the ac signal cannot spread farther and is confined to the contact area only, and as both the experiments have the same contact sizes they have the same capacitances. So this again validates the spreading theory. In another experiment the substrate length was kept constant at 350 µm and the contact length was changed from 50 µm to 10 µm and the capacitance for 10 µm contact is less than 50 µm. This implies the spreading area for smaller contact is less than that for larger contacts, i.e., the spreading depends on the gate area (simulation and experiment), as explained in the preceding section. It is also observed that the accumulation capacitance at higher biases is greater for the sample with the smaller contact (10 µm) and larger substrate width (350 µm) than that for the sample with a larger contact (50 µm) and smaller (150 µm) substrate width, again confirming the spreading effect.
4.7.4. Effect of Gate Oxide

Comparing the C-V characteristics of a sample without a gate oxide (i.e., Schottky contact on the film) with another sample of similar dimensions but with 100 nm gate oxide on the Si film (both experiment and simulation), the spreading effect was not observed with a gate oxide. The maximum capacitance with a gate oxide in accumulation was proportional to the contact area as shown in Fig. 4.19(b). This is consistent with previous experimental results which did not show any spreading effect with a gate oxide on SOI samples either [7]. The inversion capacitance with a gate oxide was close to the depletion capacitance at 100 kHz without any rise, as observed in the Schottky contact case. Also, in simulation, the “S” shape was not observed for the sample with a gate oxide.
The experimental results for a thin film SOI with a 100 nm gate oxide was not measureable and was not conclusive as shown in Fig. 4.19(a). Dry oxidation was carried out at 1000°C and the sample was pulled out of the chamber at 700°C. The measurement abnormalities are most probably due to the following reasons: (a) oxygen vacancies being neutralized at such high temperature, resulting in part of the sample turning back to p-type (one curve shows a p-type result), (b) some part may be intrinsic hence a flat C-V plot is observed, and (c) the vacancies may be present in patches which causes local variation of C-V between different contacts. The dotted line in Fig. 4.19(a) is for the total calculated maximum accumulated capacitance for series combination of $C_{\text{BOX}}$ and $C_{\text{Gate-Ox}}$ for 1 µm thick BOX and 100 nm thick gate oxide respectively.

$Experimental \ C_{\text{TOTAL}} = \frac{1}{\frac{1}{C_{\text{OX}}} + \frac{1}{C_{\text{BOX}}}} = \frac{1}{\frac{1}{219.56} + \frac{1}{21.96}} = 20 \ pF$

Calculate value for dia $= 0.9 \ mm$

**SIMULATION:** (see Fig 4.19 (b) simulation plot with gate oxide)

For $t_{\text{OX}} = 100 \ \text{nm}$ and $L = 50 \ \mu m$ $\Rightarrow C_{\text{OX}} = 17.27 \ \text{fF}$

For $t_{\text{BOX}} = 1 \ \mu m$ and $L = 50 \ \mu m$ $\Rightarrow C_{\text{BOX}} = 1.73 \ \text{fF}$

So $C_{\text{TOTAL}} = \frac{1}{\frac{1}{C_{\text{OX}}} + \frac{1}{C_{\text{BOX}}}} = \frac{1}{\frac{1}{17.27} + \frac{1}{1.73}} = 1.57 \ \text{fF} \ Calculated \ value \ for \ simulation$

$C_{\text{TOTAL}} \ from \ simulation = 1.24 \ \text{fF} \ (3.7 \ \text{V to 20 \ V}) \ (see \ Fig. \ 4.19(b) \ simulation \ plot \ with \ gate \ oxide)$
The simulated value of the total capacitance (accumulation) with gate oxide is close to the calculated value. It is slightly less due to smearing of accumulation layer. There is no spreading effect with gate oxide.

Fig. 4.19. SOI C-V - effect of gate oxide for thin film SOI ($t_{\text{film}} = 145$ nm and $t_{\text{BOX}} = 1 \mu$m). (a) Experimental results are inconclusive, (b) simulation results - no spreading.

4.7.5. Effect of Film Thickness

Spreading was observed for thin ($t_{\text{film}} = 145$ nm) and thick ($t_{\text{film}} = 1.25$ $\mu$m) film SOI in both simulation and experiments, as shown in Fig. 4.20, but the “S” shape was absent in thick film SOI. For the p-type film and n-type substrate combination with the Al contact directly on the film an n-type C-V curve is observed for both thick film and thin film SOI in both simulation and experiment. But when the Al contact is placed over a gate oxide then for the same combination of film and substrate doping the thin film SOI shows an n-type C-V
whereas the thick film SOI shows a p-type C-V in both simulation and experiment. In thick films the film depletion layer may not touch the interface thereby dominating the C-V behavior; as a result, a p-type C-V is observed with gate oxide as the film is p-type. And for the same reason, the “S” shape is not observed in thick film SOI samples.

The key to the “S” shape in thin film SOI is the complete inversion of the film below the contact region due to the contact work function difference and the creation of a discontinuity in the accumulated region by the depletion region at low positive bias. In thick film SOI, the entire film, from the contact to the BOX interface is not inverted, but only partially inverted by the contact work function difference. As a result, in the positive bias region, the film/BOX interface in thick film SOI wafer remains completely accumulated. This continuous sheet of holes at the film/BOX interface allows the ac signal to spread at all positive biases and the capacitance becomes instantly higher. For thick films the hysteresis effect is also not observed (see Fig. 4.21).
Fig. 4.20. Effect of film thickness (thick => film/BOX = 1.25/0.145 µm vs. thin => film/BOX = 0.145/1 µm) (a) simulation, (b) experiment. “S” shape is absent in thick film SOI. In thin film SOI, n-type C-V for both with and without gate oxide. But in thick film SOI, “without gate oxide” → n-type and “with gate oxide” → p-type C-V.
4.7.6. Effect of Film Doping Concentration

To check the effect of film doping concentration on C-V characteristics of HRSOI the substrate doping concentration was kept constant at $N_D = 10^{14} \text{ cm}^{-3}$ and the film doping concentration was changed from $N_A = 5 \times 10^{12} \text{ cm}^{-3}$ to $5 \times 10^{15} \text{ cm}^{-3}$. Increasing the film doping concentration shifts the curve to the left with the same slope, Fig. 4.22. An upward kink is observed near 0 V for very low film doping concentration, for $N_A = 5 \times 10^{12} \text{ cm}^{-3}$. With increase in the film doping concentration the region below the contact can no longer be easily inverted by the Schottky contact as the hole barrier height is reduced, so even at lower positive bias the film/box interface below the contact can easily go into accumulation creating a continuous accumulation layer compared to lightly-doped films and
hence the “S” shape begins to shift towards left and the capacitance reaches the spread value at lower positive bias and ultimately it vanishes.

![Graph showing simulated SOI C-V using Schottky contact](image)

**Fig. 4.22. Simulated SOI C-V using Schottky contact – effect of change in film doping concentration, \( t_{\text{film}}=145 \text{ nm}, t_{\text{BOX}} = 1 \mu\text{m} \).**

### 4.7.7. Effect of Substrate Doping Concentration

To check the effect of substrate doping concentration on C-V characteristics of HRSOI the film doping concentration was kept constant at \( N_A = 10^{14} \text{ cm}^{-3} \) and the substrate doping concentration was changed from \( N_D = 3 \times 10^{11} \text{ cm}^{-3} \) to \( 10^{12} \text{ cm}^{-3} \). When the substrate doping concentration reduces, the inversion capacitance reduces, as the inversion layer becomes thicker and the depletion layer becomes wider. The “S” shape is not affected as the film doping is kept constant but the accumulation capacitance decreases with reduction in substrate doping concentration due to smearing of the accumulation layer at low doping concentration [135], as shown in Fig. 4.23.
4.7.8. Effect of Carrier Lifetime

The film lifetime affects the C-V characteristic of HRSOI in the accumulation region, increasing the film electron and hole carrier lifetimes from $\tau_{n/p} = 10^{-7}$ s to $\tau_{n/p} = 10^{-4}$ s increases the capacitance at a particular positive bias. But changing the substrate carrier lifetimes does not have any significant impact on the C-V plots, as shown in Fig. 4.24. The film carrier lifetime affects the lateral minority carrier injection and recombination in the film. As the lifetime increases the recombination rate decreases and the holes in the film cannot be neutralized faster and the capacitance remains high for a particular bias. The carriers can spread to greater distances compared to that at lower lifetimes ($10^{-7}$ s).
Fig. 4.24. Simulated SOI C-V using Schottky contact – effect of change in carrier lifetime, \( t_{\text{film}} = 145 \text{ nm}, t_{\text{BOX}} = 1 \mu\text{m}, N_{A,\text{film}} = 10^{14} \text{ cm}^{-3}, N_{D,\text{sub}} = 7 \times 10^{11} \text{ cm}^{-3}. \)

### 4.7.9. Effect of Contact Work-function

The work-function of the source and substrate contacts affects the “S” shape in the accumulation region during positive bias. In simulation, samples with high hole barrier height contacts (WF = 3.4, 3.9, 4.08 eV) have the “S” shape and all of them have almost the same C-V plot but for low hole barrier height contacts (WF = 4.2, 4.8 eV) the “S” shape is not observed, it has a constant accumulation capacitance and then falls to depletion capacitance near 0 V and then enters inversion with a step, Fig. 4.25(a). The high hole barrier causes complete inversion of the film below a certain positive bias and subsequent minority carrier injection into the film. Due to the higher hole barrier height it is difficult for the holes present in the other part of the film to leave causing hole accumulation and the “S” shape in C-V as explained earlier. But for low hole barrier heights, the film region below the contact cannot be completely inverted during positive bias.
and does not create any interruption in the accumulation layer in the film. Hence
the ac signal can spread easily and the “S” shape is not observed.

The nature of the top film contact (Ohmic or Schottky) has a significant
impact on the C-V curve compared to the substrate contact. Similar “S” shaped
curves are observed when the substrate contact is Ohmic and the film contact is
Schottky, and when both substrate and the film contacts are Schottky (WF = 4.08
eV), Fig. 4.25(b). But when both the film and the substrate contacts are Ohmic
then the “S” shape is not observed in the positive bias region of the film contact,
but a constant accumulation capacitance is observed followed by the depletion
capacitance. The Ohmic contact prevents minority carrier injection and also it
does not create the inverted/depleted region below the contact interrupting the
film accumulation layer, as explained earlier. Now the entire film is accumulated
during all positive bias, the ac signal can spread easily immediately after 0V (in
accumulation) and the majority carries respond equally all along the film/BOX
interface leading to a higher capacitance (spread).
4.7.10. Effect of Radiation (Interface Charges and Interface Traps)

Figure 4.25. Simulated HRSOI C-V - Effect of contact type (Ohmic/Schottky).

Interface traps change the slope of C-V plots and oxide charges shift the C-V plots [11]. Radiation creates interface traps and oxide charges in an oxide and at the oxide-silicon interface. Previous studies on radiation effect on MOS oxide have shown that after radiation, if the sample is left as it is, the oxide automatically heals due to room temperature annealing that heals the interface traps and oxide charges [142, 143]. Annealing a sample at moderately high temperature after radiation completely removes the interface traps and oxide charges and the pre-radiation C-V curve is obtained [142, 143]. We tried to find out how radiation affects the HRSOI C-V characteristics using a Schottky contact when the film is p-type and the substrate is n-type. The samples were radiated with different doses of Cobalt-60 radiation, such as, 25 krads and 100 krads. The experimental results in Fig. 4.26(a) show the effect of radiation dose (0 rad, 25
krads, and 100 krads) on the C-V plot. Figure 4.26(b) shows the effect of room temperature annealing on C-V plots for a particular radiation dose (100 krad). And figure 4.26(c) shows the effect of annealing the sample at 400°C for 30 min in forming gas ambient. The simulation results for various densities of interface traps and oxide charges are shown in Fig. 4.26(d).

The concentration of interface traps and oxide charges increases with the increase in radiation dose and they create both shift and change in the slope of C-V plots [11]; similar effects are also observed but in a different manner as shown in Fig. 4.26(a). As the radiation dose increases the slope of the C-V plot in the accumulation region including the “S” shape becomes shallower indicating an increase in interface traps, also a new phenomenon of a rising peak is observed at $V_G \rightarrow 0V$ in the positive bias region, as shown in Fig. 4.26(a). Comparing with the simulation results in Fig. 4.26(d) this rise is mostly due to an increase in interface trap densities. The effect of oxide charges can be seen by the left shift of the depletion portion of the C-V plot in the negative bias region. Though this effect could not be replicated in the 2D simulation, positive oxide charges are the likely cause for the left shift, similar to the effect in a MOS capacitor. At higher radiation dose (100 krad) the low frequency portion of the C-V plot is completely flat. Also higher radiation dose widens the depletion portion compared to the pre radiation case, most likely due to interface traps, which reduce the slope of the C-V curve, hence the curve looks widened during depletion.

Room temperature annealing causes the interface traps to heal gradually with time. Multiple measurements were taken at different time intervals such as 4, 29,
46 and 99 hours after radiating the sample at 100 krad. Figure 4.26(b) shows the room temperature annealing effect in action. With time, the slope in the accumulation region i.e., in positive gate bias, becomes steeper, the peak observed near \( V_{\text{contact}} = 0 \text{V} \) gradually reduces, and the depletion portion, which had shifted left, starts shifting towards right, i.e., the radiated C-V plot begins to approach the pre radiation plot. The sample was annealed at 400°C for 30 min in forming gas to see if the interface tarps and oxide charges are completely removed; and as expected, the C-V measurement after annealing showed a plot very close to the original pre-radiation case, Fig. 4.26(c).
Fig. 4.26. HRSOI C–V - effect of radiation due to interface charges and interface traps. Experimental C–V after Cobalt-60 radiation (a) effect of radiation dose, the curves shift left and depletion region widens, (b) effect of room temperature annealing, curve shifts towards the no radiation plot as the interface traps and charges heal, (c) effect of annealing after radiation, and (d) simulation of interface and oxide charges: substrate $N_D = 7 \times 10^{11}$ cm$^{-3}$, film $N_A = 10^{14}$ cm$^{-3}$, substrate and film (gate) contacts Schottky (WF = 4.08 eV), $L_{Gate} = 50 \mu$m, $L_{Substrate} = 350 \mu$m,

$t_{Film} = 145$ nm, $t_{BOX} = 1$ μm, $t_{Sub} = 100$ μm.
4.7.11. Effect of Light, Temperature, and Annealing

Figure 4.27(a) and (b) show the effect of light and temperature respectively, as the light intensity increases or the temperature increases (24°C to 300°C) the spreading increases mainly due to more carrier generation and reduction in sheet resistance. At very high temperatures it tends to act like a parallel plate capacitor. Figure 4.27(c) shows the effect of annealing in forming gas at 450°C, 525°C and 550°C. Annealing temperature could not be increased beyond 560°C as it can form aluminum-silicon eutectic. Spreading reduces with annealing.

Fig. 4.27. Effect of light, temperature and annealing.
4.8. Conclusion

The C-V characteristics of HRSOI were studied in detail by experiments and simulation with a metal contact directly on the film. Various factors affecting the C-V characteristics were also studied, they are: frequency, size of the top film contact, effect of the contact size and the substrate size, film thickness, film and substrate doping concentrations, carrier lifetimes, contact work-function, and type of film contact i.e. Schottky or Ohmic, radiation, temperature, light, and annealing. Series C-V method with the bias applied to the substrate is preferable for HRSOI for lower noise and more accurate measurement. The substrate HRSOI doping type can undergo a reversal from p- to n-type at low substrate doping concentration due to formation of oxygen thermal donors after annealing. Samples with p-type films and n-type substrates with very low doping concentrations \( (7 \times 10^{11} \text{ cm}^{-3} \text{ to } 10^{12} \text{ cm}^{-3}) \) were studied.

The C-V plots showed spreading of capacitance following an “S” shape at high frequency where the capacitance changes from a value proportional to the contact area to a value 5 to 10 times larger. The spreading is mostly due to the floating body and the contact being directly on the film and due to the RC transmission line behavior of the film/BOX/substrate interface. The capacitance spreading is not observed when there is a gate oxide. This shape is mainly due to the Schottky contact and its work-function. The “S” shape was not observed for Ohmic contacts and Schottky contacts with low hole barrier heights. It occurs due to the depletion and inversion of the film below the contact at a particular positive gate bias due to the large work-function difference between the p-type film and
the aluminum contact. The Schottky contact can supply minority carriers (electrons) which respond to the ac signal and the capacitance is confined to the contact area. The “S” shape does not occur for thick film SOI as the inversion layer does not touch the film/BOX interface allowing a continuous accumulation layer to be formed in the positive gate bias all along the BOX interface.

The RC transmission line behavior of the film and the substrate plays a significant role in the bias spreading and the shape of the C-V characteristic. At higher frequencies the ac signal flows very close to the contact due to the low-pass filter nature of the RC circuit and spreads less into the other part of the film giving smaller capacitances than at a lower frequency.

Radiation effects on the C-V plots were also studied. The C-V plot shifted to more positive voltages at higher radiation doses and had shallower slopes due to radiation induced interface traps and oxide charges. The radiated samples also had an upward peak near zero bias, which is not observed in any other C-V plots; most probably due to interface traps. Due to the room temperature annealing effect a gradual change in the slope, reduction in the peak near zero bias, and shift of the C-V plot towards the pre-radiation plot indicating healing of interface traps were observed with time. When the sample was annealed at 400°C for 30 mins in forming gas ambient the radiation induced damages were healed.
CHAPTER 5. CROSSTALK IN HIGH-RESISTIVITY SILICON WAFERS
– BULK AND SILICON-ON-INSULATOR

5.1. Introduction

Today’s IC chips are operating at ever higher speeds in the GHz range and becoming smaller and more powerful with multiple functionalities being integrated in a single chip. This integration of different circuits or systems such as analog, digital and microwave on a single chip is called the System-on-Chip (SOC) configuration, as shown in Fig. 5.1. The first true SOC appeared in a Microma watch in 1974 when Peter Stoll integrated the LCD driver transistors as well as the timing functions onto a single Intel 5810 CMOS chip [144, 145]. Ever since, the SOC chips have become denser, faster and more powerful [146]. But this complex integration of analog, digital and microwave systems and higher operating frequency gave rise to another problem called crosstalk. While the digital circuits run at a very high speed in the GHz range, the analog circuits are very sensitive to any noise. At high frequencies some spurious signals from the digital node can pass through the substrate and couple to the analog side and disrupt the analog operation [17-19]. This is termed as crosstalk through the substrate. Figure 5.2(a) illustrates an example of coupling mechanism between a digital and an analog circuit present on the same substrate [147]. The digital inverter generates noise which couples into the analog NMOS transistor.

SOI substrates were found to have lower substrate crosstalk than bulk substrates of similar resistivity [20, 21]. High-resistivity silicon (HRS) wafers minimize this coupling compared to low-resistivity substrates (LRS) and
specifically high-resistivity SOI wafers are found to have better cross talk prevention capabilities than bulk Si of similar resistivity [22, 23]. This chapter will focus on substrate coupling in HRSOI and effects of various factors, such as: substrate resistivity, separation between devices, buried oxide (BOX) thickness, radiation, temperature, annealing, light, and device types. And also various ways to minimize substrate crosstalk will be discussed.

Fig. 5.1. Block diagram of a typical System-on-Chip configuration integrating digital, analog, and RF systems in one chip [148].

5.2. What is Substrate Crosstalk – Mechanism and Factors Affecting It?

Substrate crosstalk can be defined as coupling of signal or noise through the substrate between two devices or systems residing on the same substrate. When we have both high speed digital circuit and sensitive analog circuits on the same chip sharing the same substrate then during high frequency operation the
switching transients can couple from digital to analog circuit through the substrate [149]. Substrate cross talk mechanism can be segregated into three parts: generation, transmission and detection of substrate noise; and can be explained with the help of Fig. 5.2(b).

![Diagram of substrate cross talk mechanism](image)

**Fig. 5.2.** (a) An example of coupling mechanisms between a digital (noise source) and analog (affected) circuit on the same substrate [147]. (b) Schematic of noise injection, reception and substrate paths in CMOS technology [150].
There are different mechanisms by which noise can be injected into the substrate [149]:

1. Capacitive coupling of voltage fluctuation at the drain and at metal layers to the substrate through the source/substrate or drain/substrate junction capacitors, in SOI it can couple through the BOX capacitor.

2. Another mechanism is by the impact ionization induced substrate current. Impact ionization at the drain end of an NMOS creates hole current in the substrate, PMOS also creates a similar substrate current but it is much lower than NMOS and at the same time the capacitive shielding by the n-well junction reduces it further, making its contribution to the total substrate current insignificant. Hence the substrate current is mainly considered to be due to NMOS and this can couple to other devices through the substrate.

3. Noise injection by power supply lines connected to the substrate, e.g., digital ground.

The injected signal is transmitted through the substrate by its parallel RC circuit as shown in Figs. 5.2(a, b). The injected signals can again couple to other nodes (device drains and metal lines) by capacitive coupling.

The crosstalk is basically the transmission of a signal through an RC circuit and hence is dependant on the frequency of the coupled signal as shown in Fig. 5.3. Below a certain frequency the substrate can block the coupling and beyond a certain frequency, say $\omega$, dependant on R and C of the substrate, as shown in Fig 5.2(b), the substrate can gradually become transparent to the noise signal and
coupling increases. The frequency dependence of crosstalk (measured by $S_{21}$ parameter vs. frequency) in Fig. 5.3 indicates that at lower frequencies the crosstalk increases with increase in frequency as the capacitive coupling increases, at medium frequencies the substrate resistance begins to dominate as the crosstalk is lower for high resistive substrates, and at very high frequencies the capacitance of the silicon contributes [150].

Figure 5.4 shows the substrate coupling effect through various types of substrates: bulk silicon in Fig. 5.4(a), epitaxial silicon in Fig. 5.4(b), and high resistivity SOI in Fig. 5.4(c). In bulk silicon, the current lines indicating coupling are near the surface and through the substrate, this can be reduced by using guard rings. In epi silicon, substrate coupling increases as more current lines can pass through the low resistive path of the heavily-doped epi layer. High-resistivity SOI prevents substrate coupling to the maximum extent compared to all other substrate types due to the presence of the buried oxide layer that isolates the device layer from the substrate and the high resistivity of the substrate. SOI can prevent coupling better than bulk silicon of similar resistivity and HRSOI is better than LRSOI. The corresponding simulation results using Silvaco ATLAS Device simulator are shown in Fig. 5.3, modeled after Raskin et al. [23]. The device cross sections used in simulation are shown in Fig. 5.5. Two types of p-type substrates were used, one with HRS substrate, $\rho_{\text{substrate}} = 5000 \ \Omega \cdot \text{cm} \ (N_A = 3 \times 10^{12} \ \text{cm}^{-3})$ and the other with LRS substrate, $\rho_{\text{substrate}} = 20 \ \Omega \cdot \text{cm} \ (N_A = 7 \times 10^{14} \ \text{cm}^{-3})$. The two devices were $pn$ diodes with $n^+$ doping concentration of $N_D = 10^{19} \ \text{cm}^{-3}$; and the devices were 100 $\mu$m apart. For the epi substrate the $p^+$ epi layer doping
concentration was $N_A = 10^{19}$ cm$^{-3}$. The simulation results in Fig. 5.3 show that among various substrate types, HRSOI has the least crosstalk for the same device configuration.

It has been reported in prior studies that in SOI substrates crosstalk is affected by various factors, such as: spacing between the devices (the noise injecting source and the affected entity), the frequency of the signal, the buried oxide thickness, substrate resistivity and the nature of the substrate/BOX interface.

Fig. 5.3. Simulation - substrate coupling through various substrate types. High-resistivity SOI has the lowest substrate coupling.

Fig. 5.4. Substrate coupling through various substrate types. High-resistivity SOI has the lowest substrate coupling compared to other substrates.
5.3. Crosstalk Measurement Procedure

Substrate crosstalk measurement involves very high frequencies microwave measurements in the GHz frequency range. It is a two port measurement where the input port is the noise injecting node and the output port is the device being affected, and the main coupling medium is the substrate on which both the devices are present. Coplanar waveguides (CPW) with 50 ohm characteristic impedance ($Z_0 = 50 \, \Omega$) were used to transmit the high-frequency input signals to the device under test (DUT) and to measure the output i.e. the coupled signal to the output node. A Vector Network Analyzer (VNA) is the instrument to measure crosstalk. Crosstalk measurement like any microwave measurement is a two step process, first step is the calibration of the VNA and the second step is the actual measurement of the device S-parameters. A brief discussion of CPW and S-parameter are presented in the next subsections.

5.3.1. Coplanar Wave Guide (CPW)

The coplanar waveguide (CPW) was invented by C. P. Wen from RCA Laboratory in 1969 [151]. The basic coplanar waveguide consists of a center
signal line with two ground lines on both sides separated by a narrow gap in a GSG (Ground Signal Ground) configuration placed over a substrate which acts as the dielectric (see Fig. 5.6). The original design assumed the adjacent ground strip widths and the dielectric thickness to be infinite. In practice, the dielectric should be thick enough so that the electromagnetic waves die out before they leave the substrate, and the ground strips are of finite width. The dimensions of the center strip, the gap between the signal and the ground lines, the thickness and the permittivity of the substrate dielectric determine the effective dielectric constant ($\varepsilon_{eff}$) and the characteristic impedance ($Z_0$) of the CPW [152]. CPWs are most suitable for low-loss high-frequency signal transmission, it can be used to transmit signal with frequencies exceeding 100 GHz.

![Fig. 5.6. Coplanar waveguide (a) conventional (b) with finite conductor length.](image)

5.3.2. S-Parameter

A microwave circuit with an input and output node can be represented by the two-port network in Fig. 5.7(a). In this high frequency system a portion of the source power is delivered to the load by means of transmission lines. Voltage, current, and power can be considered to be in the form of waves traveling in both directions along this transmission line. Due to mismatch between the source
impedance \((Z_s)\), characteristic impedance of transmission line \((Z_0)\) and output impedances \((Z_L)\) a portion of the wave incident on the load will be reflected, it then becomes incident on the source, and in turn re-reflects from the source (if \(Z_s \neq Z_0\)), resulting in a standing wave on the line.

Scattering parameters, commonly called S-parameters, relate those waves scattered or reflected from the network to those waves incident upon the network [153]. S-parameters are important in microwave design because they are easier to measure and work with at high frequencies than other kinds of parameters. They are easier to understand because they are nothing but gains and reflection coefficients as described in eqns. 5.7 to 5.10. S-parameters and distributed models provide a means of measuring, describing, and characterizing circuit elements when traditional lumped equivalent circuit models cannot predict circuit behavior to the desired level of accuracy. They are used for the design of many products, such as cellular telephones.

S-parameters are measured by an instrument called Vector Network Analyzer (VNA). They are usually measured with the device embedded between a 50 Ω load and source, and there is very little chance for oscillations to occur. Generalized scattering parameters have been defined by Kurokawa [154]. The wave functions used to define S-parameters are shown in Fig. 5.7(a). The S-parameters describe the interrelationships between the normalized complex voltage waves incident on \((a_i)\) and reflected from \((b_i)\) the \(i^{th}\) port of the network. \(a_1\) and \(a_2\) are incident waves and \(b_1\) and \(b_2\) are reflected waves at port 1 and 2 respectively.
Fig. 5.7. (a) Two-port network with source impedance $Z_S$ and output load impedance $Z_L$ showing incident waves ($a_1, a_2$) and reflected waves ($b_1, b_2$) used in $S$-parameter definitions, (b) $S_{21}$ parameter of a two port network.

The independent variables $a_1$ and $a_2$, the normalized incident voltages, are expressed as [153, 155]:

\[
a_1 = \frac{V_1 + I_1 Z_0}{2 \sqrt{Z_0}} = \frac{\text{Voltage wave incident on port 1}}{\sqrt{Z_0}} = \frac{V_{i1}}{\sqrt{Z_0}} \quad (5.1)
\]

\[
a_2 = \frac{V_2 + I_2 Z_0}{2 \sqrt{Z_0}} = \frac{\text{Voltage wave incident on port 2}}{\sqrt{Z_0}} = \frac{V_{i2}}{\sqrt{Z_0}} \quad (5.2)
\]

The dependent variables $b_1$ and $b_2$, the normalized reflected voltages, are expressed as [153, 155]:

\[
b_1 = \frac{V_1 - I_1 Z_0}{2 \sqrt{Z_0}} = \frac{\text{Voltage wave incident from port 1}}{\sqrt{Z_0}} = \frac{V_{r1}}{\sqrt{Z_0}} \quad (5.3)
\]
\[ b_2 = \frac{V_2 - I_2 Z_0}{2\sqrt{Z_0}} = \frac{\text{Voltage wave reflected from port 2}}{\sqrt{Z_0}} = \frac{V_{r2}}{\sqrt{Z_0}} \] (5.4)

The linear equations describing the two-port network are [153, 155]:

\[ b_1 = S_{11} a_1 + S_{12} a_2 \] (5.5)

\[ b_2 = S_{21} a_1 + S_{22} a_2 \] (5.6)

The S-parameters \( S_{11}, S_{12}, S_{21}, \) and \( S_{22} \) are defined as [153, 155]:

\[ S_{11} = \frac{\text{Relected}}{\text{Incident}} \left| \begin{array}{c} b_1 \\ a_1 \end{array} \right|_{a_2 = 0} = \frac{b_1}{a_1} = \text{Input reflection coefficient with the output port terminated by a matched load } (Z_L = Z_0 \text{ sets } a_2 = 0) \] (5.7)

\[ S_{22} = \frac{\text{Relected}}{\text{Incident}} \left| \begin{array}{c} b_2 \\ a_2 \end{array} \right|_{a_1 = 0} = \frac{b_2}{a_2} = \text{Output reflection coefficient with the input port terminated by a matched load } (Z_S = Z_0 \text{ sets } V_S = 0) \] (5.8)

\[ S_{21} = \frac{\text{Transmitted}}{\text{Incident}} \left| \begin{array}{c} b_2 \\ a_1 \end{array} \right|_{a_2 = 0} = \frac{b_2}{a_1} = \text{Forward transmission (insertion) gain with the output port terminated in a matched load} \] (5.9)

\[ S_{12} = \frac{\text{Transmitted}}{\text{Incident}} \left| \begin{array}{c} b_1 \\ a_2 \end{array} \right|_{a_1 = 0} = \frac{b_1}{a_2} = \text{Reverse transmission (insertion) gain with the input port terminated in a matched load} \] (5.10)

\( S_{21} \) (forward transmission coefficient) as shown in Fig. 5.7(b) is used to measure the crosstalk. S-parameters are measured in dB, the lower the value of \( S_{21} \) i.e., the more negative \( S_{21} \) in dB is the lower is the crosstalk. Figure 5.8 illustrates the S-parameters along with the incident and reflected voltage waves.
5.4. VNA Calibration Techniques

Figure 5.9 shows the block diagram of a Vector Network Analyzer (VNA). The RF source at the top provides the required stimulus to the device-under-test (DUT). A forward/reverse switch directs the RF energy to either DUT port. The test set uses directional couplers or bridges to pick up the forward and reverse waves traveling to and from each port, and down-converts these signals to four “IF” sections. Each “IF” section filters, amplifies, and digitizes the signals for further digital processing and display [156].
A VNA measures vector ratios of reflected or transmitted energy to energy incident upon the DUT. As a stimulus-response measurement, a VNA measurement determines the properties of devices rather than the properties of signals [156]. A significant challenge in stimulus-response measurements is defining exactly where the measurement system ends and the DUT begins. In on-wafer VNA measurements this boundary is known as the “reference plane” of the measurement and is often located at the probe tips, as shown in Fig 5.10(a). Ideally the system will measure the characteristics of whatever is connected to the measurement reference plane.

VNA calibration is an essential step in the measurement process that removes the parasitic capacitances, inductances and resistances due to the VNA, cables, probe station, probes and the probe pads. Without calibration, the measurement
does not provide the correct S-parameters only due to the actual devices. Figure 5.10(b) illustrates the block diagram of Thru-Reflect-Line (TRL) calibration process. During calibration the VNA measures and stores the contribution due to the error boxes and removes these errors from the actual measurements to calculate the actual S-parameters due to the DUT only.

Fig. 5.10. Calibration removes the errors due to parasitic elements (VNA, probes, probe station, and cables) from the actual measurement and helps calculate the correct S-parameters due to the DUT only [155].

5.4.1. Calibration Options and Standards

The different calibration options such as un-corrected measurement, response calibration and full two port calibration methods are described in table 5.1.
Table 5.1 Calibration options [156].

<table>
<thead>
<tr>
<th>OPTION</th>
<th>ILLUSTRATION</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Un-corrected measurement:</strong></td>
<td></td>
</tr>
<tr>
<td>➢ A VNA will measure uncorrected S-parameters if not calibrated.</td>
<td>![DUT]</td>
</tr>
<tr>
<td>➢ Uncorrected measurements are rarely used.</td>
<td></td>
</tr>
<tr>
<td>➢ Poor accuracy but fast.</td>
<td></td>
</tr>
<tr>
<td><strong>Response calibration:</strong></td>
<td></td>
</tr>
<tr>
<td>➢ A “response” calibration is simply a vector magnitude and phase normalization of a transmission or reflection measurement.</td>
<td>![THRU] DUT</td>
</tr>
<tr>
<td>➢ Used only at low frequencies.</td>
<td></td>
</tr>
<tr>
<td>➢ Requires only one standard and low accuracy.</td>
<td></td>
</tr>
<tr>
<td><strong>Full two port calibration:</strong></td>
<td></td>
</tr>
<tr>
<td>➢ This method is typically a full calibration of all the error parameters; is used as a reference or to assure the highest accuracy.</td>
<td>![OPEN SHORT LOAD THRU] DUT</td>
</tr>
<tr>
<td>➢ Removes following errors</td>
<td></td>
</tr>
<tr>
<td>– Directivity</td>
<td></td>
</tr>
<tr>
<td>– Source/load match</td>
<td></td>
</tr>
<tr>
<td>– Reflection/transmission tracking</td>
<td></td>
</tr>
<tr>
<td>– Crosstalk</td>
<td></td>
</tr>
<tr>
<td>➢ Requires up to 7 standards.</td>
<td></td>
</tr>
</tbody>
</table>

There are two types of VNA calibration standards, they are: (a) On-wafer, and (b) Off-wafer VNA calibration. Off-wafer calibration standard uses an *Impedance Standard Substrate (ISS)* with predefined elements to calibrate the VNA. But as it is not done on the same substrate as the DUT there are errors in the calibration process which become significant during high frequency measurements.
On-wafer calibration standard uses the calibration structures fabricated on the same substrate as the DUT and hence are more accurate at high frequencies exceeding 20 GHz. On-wafer calibration standards most often are precision thin-film resistors, short-circuit connections, and 50 ohm transmission lines fabricated either on the wafer containing the DUT or on a separate Impedance Standard Substrate (ISS) [156]. Open circuit standards are normally implemented by raising the probe in air above the wafer by 250 µm or more. A true 'thru' standard does not exist for on-wafer measurements since probes cannot directly connect to each other and must instead use a very short transmission line as a thru standard.

A thru line standard may be referred to either with the label of thru or line.

The various VNA calibration techniques are:

- Thru-Reflect-Match (LRM)
- Thru-Reflect-Reflect-Match (LRRM)
- Thru-Reflect-Line (TRL or LRL)
- Short-Open-Load-Thru (SOLT)
- Short-Open-Load-Reciprocal (SOLR)

We will discuss two popular characterization techniques, SOLT and TRL techniques.

5.4.2. SOLT (SHORT-OPEN-LOAD-THRU) Calibration Technique

Traditional full two port calibration typically utilizes three impedance and one transmission standards to define the calibrated reference plane. These standards, typically a SHORT, OPEN, LOAD, and THRU make up the SOLT calibration kit. This is the most commonly used calibration technique available on every
commercially available VNA. SOLT calibration technique uses off-wafer calibration standard on an Impedance Standard Substrate (ISS) available in the calibration kit. This calibration is the combination of two one-port SHORT-OPEN-LOAD calibrations with additional measurements of a THRU standard to complete the two-port calibration. All of the standards must be fully known and specified [156].

The SOLT standards are reasonably well modeled with simple lumped elements: open-circuit has capacitance, short-circuit has inductance, load has inductance, and thru has delay (and loss). Often the open-circuit capacitance will have a negative value since the probe lifted in air has less tip loading than when it is in contact with a wafer. The SOLT calibration method is shown in Fig. 5.11.

Fig. 5.11. SOLT calibration using an Impedance Standard Substrate (ISS). The calibration steps are (a) SHORT, (b) OPEN, (c) LOAD, and (d) THRU.
Precautions and Source of errors in SOLT calibration [156]:

- Improper probe placement introduces error hence all standards must be *accurately contacted physically*, since the inductances are very dependent on probe placement on the standard.

- Calibration coefficients must be correctly entered into the VNA to be useful because improper cal-kit entry is one of the largest sources of error in Off-wafer VNA measurements.

- Another common source of error is to forget to enter the delay of the THRU line standard. A 1 ps THRU is normally used with the standard probe pitch ISS versions (PNs 101-190 and 103-726) while a 4 ps THRU is used with the wide probe pitch ISS versions (PNs 106-682 and 106-683). When using long THRU lines such as for Pyramid probes it is important to use an accurate delay value and to provide an accurate loss value.

### 5.4.3. TRL (THRU REFLECT LINE) Calibration Technique

TRL (THRU-REFLECT-LINE) calibration was proposed by Engen and Hoer in 1979 [157]. The TRL calibration method requires three standards, they are: a *THRU* connection, a high *Reflection* connected to each port, and a *LINE* connected between the test ports, as shown in Fig. 5.12. This technique is realized on the same wafer as the DUT using transmission line as the standard instead of any external prefabricated discrete impedance standards [158]. It results in the same 12 port error correction model as the other calibration methods. Only one well-defined standard is required in the TRL calibration process, compared to
minimum of three precisely-known standards required for the conventional FULL 2-PORT method.

The three basic steps in TRL calibration are [158]:

- **THRU** - connection of port 1 and port 2 directly or with a short length of transmission line.
- **REFLECT** - connect identical one-port high reflection coefficient devices to each port, either OPEN or SHORT can be used for this.
- **LINE** - insert a short length of transmission line between port 1 and 2 (different line lengths are required for the THRU and LINE). Different line lengths are used to calibrate for individual frequency ranges.

![THRU, Reflect (Short), Reflect (Open), Line](a) (b) (c) (d)

Fig. 5.12. On-wafer multi line TRL calibration technique using a CPW with $Z_0 = 50 \, \Omega$. The calibration steps are (a) THRU, (b) REFLECT (OPEN or SHORT), (c) LINEs (multiple lines of different lengths for corresponding frequency ranges).
For TRL calibration, the calibration standards need to be prepared meeting the following requirements [158, 159]:

- **THRU** (zero-length, or non-zero-length through)
  - Zero-length THRU
    - $S_{21}$ and $S_{12}$ are defined as equal to 1. *Typically used to set the reference plane.*
    - $S_{11}$ and $S_{22}$ are defined as equal to zero. A zero-length THRU has no loss and has no characteristic impedance.
  - Non-zero-length THRU
    - $Z_0$ of the THRU and LINEs must be the same. When the $Z_0$ of the THRU and LINE are not the same, the average impedance is used. $S_{11}$ and $S_{22}$ of the LINE are also defined to be zero. With this assumption, the system impedance is set to the characteristic impedance of the LINE. If the $Z_0$ is known but not the desired value, the impedance of the LINE can be specified when defining the calibration standards.
    - Attenuation need not be known.
    - Accurate electrical length must be known to set the reference plane.
    - Insertion phase or electrical length must be specified if the THRU is used to set the reference plane. If a non-zero-length THRU is used but specified to have zero
delay, the reference plane will be established in the middle of the THRU.

- **REFLECT** (SHORT, or OPEN termination)
  - Any unknown highly reflective termination may be used as the REFLECT (either OPEN or SHORT). Reflection coefficient magnitude (optimally 1.0) need not be known.
  - Phase of the reflection coefficient must be specified within 1/4 wavelength or +/-90 degrees.
  - Must be the same reflection coefficient on all ports.
  - May be used to set the reference plane if the phase response of the REFLECT is well-known and specified.

- **LINE** (transmission line)
  - \( Z_0 \) of the LINE establishes the reference impedance after error correction is applied.
  - Electrical length need only be specified within 1/4 wavelength.
  - *Cannot be the same length as the THRU*. Difference between the THRU and LINEs must be between 20 degrees and 160 degrees.
  - Optimal line length is 1/4 wavelength or 90 degrees relative to the THRU at the center frequency.
  - Usable bandwidth for a single LINE standard is 8:1 (frequency span : start frequency).
  - Attenuation need not be known.
Multiple THRU/LINE pairs ($Z_0$ assumed identical) can be used to extend the bandwidth to the extent transmission lines are realizable.

- **MATCH** (load termination, additional step for TRM/LRM method)
  - Must be the same $Z_0$ on all ports. $Z_0 = 50 \, \Omega$ is preferred.
  - $Z_0$ of the MATCH standard establishes the reference impedance of the measurement.

5.5. Design of 50 $\Omega$ CPW, TRL LINE Standards, and Mask

The design section is divided into three parts to design the calibration standards and the mask required for device fabrication. The design steps are:

- Design a CPW with 50 $\Omega$ characteristic impedance to transmit and measure microwave signals to and from the DUT.
- Design of various line lengths required for the “LINE” standard of the TRL calibration technique.
- Design of the photolithography mask needed for device fabrication.

5.5.1. Design of 50 $\Omega$ Characteristic Impedance CPW

The main goal of the overall design stage is to design a CPW with constant characteristic impedance of 50 $\Omega$ within 1 to 100 GHz frequency range in order to transmit microwave signal with minimal loss to the DUT and to measure the coupled signal. HFSS™, a 3D microwave design tool by Ansoft®, was chosen to design the CPW.
HFSS™ is an industry-standard simulation tool from Ansys Corporation for
3D full-wave electromagnetic field simulation [160]. The acronym HFSS stands
for High Frequency Structural Simulator. HFSS™ provides E- and H-fields,
currents, S-parameters and near and far radiated field results. It is a high-
performance interactive software package that uses finite element analysis (FEA)
to solve three-dimensional (3D) electric, magnetostatic, eddy current and transient
problems.

The CPW design was carried out using Design of Experiment (DOE)
techniques to achieve the required specification using scientific methods in
minimum number of simulation runs and least amount of time [161]. Latin
Hypercube model of Space Filling Design in JMP™ was used as a design tool.
The response variables (design output variables) are the average characteristic
impedance ($Z_0$) of the CPW and the standard deviation of $Z_0$ within the frequency
range 1 GHz to 100 GHz. The target value of $Z_0$ is 50 Ω with upper and lower
specification limits of $49.5 \, \Omega \leq Z_0 \leq 50 \, \Omega$; in the mentioned frequency range. The
characteristic impedance measured between two ports in HFSS™ should be the
same. $Z_0$ is the output of each successful HFSS™ simulation run; it is available
under “Results $\rightarrow$ Solution Data $\rightarrow$ $Z_0$” in HFSS™. Figure 5.13 shows the various
factors involved in CPW design on an SOI substrate.
Fig. 5.13. Coplanar waveguide structure used in HFSS™ simulation.

The actual design factors are length, width and thickness of the signal and ground lines, the gap between them, and the frequency of the applied TEM. Wave-port is only a HFSS™ simulation requirement, not a physical parameter. But the dimension (height and width) of the wave-port impacts the simulation result. Too small a size gives a low value of $Z_0$ and too large a size gives a large value due to various other modes. So this is a nuisance factor which is known and controllable. During the simulation the first step was to find out an optimal size of the wave-port and use that size to vary the actual design factors to achieve $Z_0 = 50 \, \Omega$. As a rule of thumb the height and width of the wave-port should be less than half the wavelength ($\lambda/2$) of the applied Transverse Electromagnetic wave (TEM). The wave-port size was fixed at height = 500 $\mu$m and width = 300 $\mu$m. The substrate width and length were held constant at 1 mm for all simulation. The thickness of ground and signal line was 1 $\mu$m. The simulations were carried out for ten frequency steps: $f$ (in GHz) = 1, 11, 21, 31, 41, 51, 61, 71, 81, 91, 101.
The oxide material was SiO\textsubscript{2} and the CPW lines were of aluminum. Figure 5.14 shows the cause-effect diagram of the various factors affecting the characteristic impedance of the CPW during HFSS\textsuperscript{TM} simulation.

![Cause-effect diagram of various factors affecting CPW design](image)

**Fig. 5.14.** Cause-effect diagram of various factors affecting CPW design.

The HFSS\textsuperscript{TM} simulation structure is shown in Fig. 5.15. Because of symmetry of the CPW structure only *half the structure* was simulated from time, computer resource and mesh point-of-view. The ground line was of actual width and the signal line was half the size. With this half structure the simulated $Z_0$ was 100 Ω which is equivalent to 50 Ω for a full structure. It was observed that average $Z_0$ increases as the gap between the lines increases and it decreases as the width of the signal or the ground line increases. Also, any changes to the width of the signal line have greater influence on the value of average $Z_0$ than changes to the
width of the ground line. Multiple sets of line widths (ground and signal lines) and the gap between them result in average $Z_0 = 50 \, \Omega$. The final dimensions of the CPW was decided to be, gap = 40 $\mu$m, width of signal line = 78 $\mu$m and width of ground line = 160 $\mu$m to get an Average $Z_0 = 50 \, \Omega$ in 1 to 100 GHz frequency range with minimum standard deviation.

![CPW Design Schematic](image)

Fig. 5.15. HFSS™ design schematic of the CPW using half-structure.

5.5.2. Design of the “Line” standards of TRL Calibration

The other design goal was to design transmission lines of appropriate lengths for various frequency ranges required for the “Line” standards of TRL calibration technique. We are trying to measure crosstalk over a large frequency range from 1 GHz to 100 GHz; a single line will not correctly calibrate all parasitics at all
frequencies as the capacitance and inductances are frequency dependent. Hence lines with different lengths had to be designed to correctly calibrate the VNA at different frequencies. The effective permittivity of the structure $\varepsilon_{\text{eff}}$ was calculated from HFSS™ simulations corresponding to the CPW dimensions that resulted in 50 $\Omega$ characteristics impedance, and this $\varepsilon_{\text{eff}}$ value was used to calculate the line lengths for calibration. Figure 5.16 shows the relation between a particular frequency range and the corresponding line lengths, where $f_0$ is the center frequency at $\lambda/4$ for electrical length $\theta = 90^\circ$; $\lambda$ is the wavelength of a particular frequency for which the line length is designed. A line designed for a particular $f_0$ can calibrate up to $\pm0.9f_0$ (i.e. 90% of the center frequency). Equation 5.11 shows the relationship between two frequencies on both sides of $f_0$. If we start at 1 GHz frequency, then the first $f_0 = 1.4$ GHz and it can calibrate between 1 and 1.8 GHz. Similarly other $f_0$ can be calculated using Eq. 5.11. The line length for that particular $f_0$ is calculated using eqn. 5.12; where, $l$ = length of the calibration line for a particular frequency range corresponding to a particular $f_0$. The range of frequencies that are calibrated using each $f_0$ and the corresponding line lengths calculated using eqns. 5.11 and 5.12 [155] are shown in Table 5.2.

$$\frac{f_1}{f_2} = \frac{\theta_1}{\theta_2} = \frac{116}{64} = 1.8 \quad (5.11)$$

$$l = \frac{3 \times 10^8}{4f\sqrt{\varepsilon_{\text{eff}}}} \text{ in meter} \quad (5.12)$$
Fig. 5.16. Relationship between frequency and electrical length of a transmission line used to design the “Line” standards of the On-wafer TRL calibration kit.

Table 5.2 Line lengths for various frequency ranges used in the “Line” standards of On-wafer TRL calibration.

<table>
<thead>
<tr>
<th>$f_0$ GHz (HFSS)</th>
<th>$\varepsilon_{\text{eff}}$ (HFSS)</th>
<th>LINE LENGTH ($\mu$m)</th>
<th>FREQUENCY RANGE (GHz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.4</td>
<td>6.7</td>
<td>20696</td>
<td>1 - 1.8</td>
</tr>
<tr>
<td>2.52</td>
<td>6.7</td>
<td>11498</td>
<td>1.8 – 3.24</td>
</tr>
<tr>
<td>4.535</td>
<td>6.6</td>
<td>6437</td>
<td>3.24 – 5.83</td>
</tr>
<tr>
<td>8.165</td>
<td>6.4</td>
<td>3631</td>
<td>5.83 – 10.5</td>
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<td>26.45</td>
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<td>47.6</td>
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<td>85.7</td>
<td>6.44</td>
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<td>61.2 – 110.2</td>
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5.5.3. Mask Design for Fabrication

The last step of the design phase was to design the mask to fabricate the devices and calibration standards on the wafer. Autodesk™ software was used for mask design. The CPW has three lines in ground-signal-ground configuration, the
designed dimensions to have 50 Ω characteristic impedance in 1 GHz to 100 GHz frequency range are: width of ground lines = 160 µm, width of the signal line = 78 µm, and the gap between the ground and the signal lines = 40 µm. The mask dimensions of the CPW were drawn with a bias of 1 µm to achieve the designed dimensions taking into account the processing anomalies. Figure 5.17 (a) shows the mask layout with the actual device measurement section inside the dotted square and the TRL calibration section (rest of the mask), one DUT unit in Fig. 5.17(b), and the mask dimensions in a tabular form in Fig. 5.17(c).

There are six different device arrangements with spacing between the devices varying from 50 µm to 600 µm as shown in Fig. 5.17(a). The calibration section of the mask has the THRU, REFLECT, and LINE connections. In “Line” calibration the ports are connected by a 50 Ω transmission line with varying lengths to calibrate at different frequencies as shown in table 5.2. The mask was printed on a 5”x5”x0.090” Sodalime glass substrate with chrome drawn polygons.
The lines and the devices were 1 μm thick aluminum contacts fabricated by

5.6. Device Fabrication

The Schottky diodes (50 μm X 50 μm) and the on-wafer TRL VNA calibration kit as shown in the mask layout in Fig. 5.17 were fabricated on SOI wafers with different substrate resistivities, buried oxide thicknesses, and film thicknesses. The lines and the devices were 1 μm thick aluminum contacts fabricated by
evaporating aluminum directly on the silicon film and annealing at 400 ºC for 30 mins in forming gas ambient to form better contacts. The detailed processing steps are described in Fig. 5.18.

**Processing Steps to fabricate CPW – 1µm thick AL lines**

(Lift Off Process – Dark field Mask)

2. Chemicals *BOE (20:1), AZ400T, MIF300* (developer), *AZ4620* (Photo-resist)
3. Break the wafer into the required size and then clean both sides by putting in AZ400T for 10 mins heated at 160ºC. Rinse thoroughly in DI water and dry completely.
4. Dehydration bake at 120ºC for 15 min (to remove moisture).
5. *Spin* coat *HMDS* (transparent liquid) at 4000 rpm for 50 sec.
6. Put *AZ4620* and *spin* at 3000 rpm for 40 sec (7µm thick PR coating).
7. *Soft bake* (only when ready for Metal) at 85ºC/30 min slowly to have 90 deg step coverage else edges will be slanted.
8. Using *EVG620* expose for a dose ~ 500mJ/cm².
9. *Develop* using *MIF 300* for ~ 5 - 6 min.
10. *Rinse* with DI water, Dry and inspect under the microscope to check the sharpness of the edges. If not sharp then repeat steps 3 to 6.
11. *Bake* at 85ºC for 30 min, makes smooth profile, removes solvent and makes the resist stick to the surface thoroughly so that acid won’t etch it.
12. *Etch native oxide* by first putting the wafer in *BOE* for 15 sec, then put it in DI water for 1 min and then rinse thoroughly in DI water and dry.
13. *Deposit metal* AL- 10,000 A° using *Lesker 3 evaporator*.
14. *Liftoff* the unexposed layer (to bring out the contacts) using *AZ400T* (at 200ºC, set heater temp to 200C). Heat the hot plate to 200C – Put the Beaker with 400T – Put the wafer in 400T – Keep it on the hot plate for 10 min – put in the ultrasonic vibrator for 5 min – check for metal coming out. Make sure no water mixes with AZ400T. Removal takes around 10 to 15 mins.
15. *Rinse* thoroughly in DI water and dry.
16. Check under microscope for sharpness of edges.
17. *Anneal* the devices in a furnace at 400ºC/30 min to make better contacts.

Fig. 5.18. Processing steps for On-wafer TRL calibration kit and crosstalk measurement units.
5.7. Measurement

Microwave measurements were taken using an HP8500 VNA (Vector Network Analyzer) and the pico-probe station shown in Fig. 5.19. The probe station has two pico-probes, one for the input port and the other for the output port with three pins on each in ground-signal-ground configuration with 150 µm pitch between the probes. First the VNA calibration step was performed and then the measurement using the WinCal software. In “THRU” calibration connection, port1 and port2 are connected directly and it measures the transmission coefficients. The “REFLECT” calibration has the OPEN and SHORT connections of the probe pads; it measures the reflection coefficients with large load. *Open configuration was used for reflect calibration.* The measurements were carried out within 1 to 18.9 GHz frequency.

![Microwave measurement unit](image)  
(a) (b)

Fig. 5.19. Microwave measurement unit (a) HP8500 VNA (right) with Pico probe station (left), and (b) the probes with the sample.
5.8. Simulation Setup

Crosstalk was simulated using Silvaco ATLAS device simulator. Crosstalk was modeled using S-parameter simulation using the syntax

```
LOG OUTF=soi_S21_HeavySub_tox0p95.log MASTER GAINS S.PARAMS INPORT=source OUTPORT=drain WIDTH=100
SOLVE ac freq=1 fstep=10 mult.f nfsteps=4 name=source
SOLVE ac freq=1e6 fstep=2 mult.f nfsteps=25 name=source
```

5.9. Analysis of Experimental and Simulation Results

Fig. 5.20. Lumped element equivalent circuit model describing crosstalk in SOI substrate [23].

Substrate coupling in SOI can be modeled using a combination of resistors and capacitors as shown in Fig. 5.20 [23]. “1” is the input noise injecting node and “2” is the disturbed node. $C_{BOX}$ is the capacitance of the buried oxide, $C_{cp}$ and $R_{cp}$ are the coupling capacitors and resistors through the substrate between device 1 and 2. $R_I$ and $C_I$ are the coupling capacitor and resistor between the bottom of the BOX and the back substrate contact. The coupling though the Si film is neglected.
as the film is very thin with high sheet resistance. The resistors and capacitors in Fig. 5.20 are the main elements that affect the coupling. At frequencies above a few hundred MHz the BOX capacitor $C_{\text{BOX}}$ offers negligible impedance and the crosstalk is limited almost exclusively by the parallel combination of effective substrate resistance $R_{\text{cp}}$ and capacitance $C_{\text{cp}}$ [23]. The resistivity of the silicon handle wafer therefore becomes significant. If a high-resistivity silicon substrate (HRS) is employed, cross-talk will be controlled by $C_{\text{cp}}$ and should exhibit a 20 dB/decade frequency dependence. To understand the crosstalk effect on HRSOI, various factors influencing these components and thereby the coupling were studied. The substrate resistivities mentioned in all experimental results were supplied by the wafer manufacturer.

To understand the factors affecting substrate crosstalk $S_{21}$ parameter between two Schottky diodes on various SOI substrates with varying substrate resistivities were measured using the measurement procedure described earlier. The effects of various factors were studied, such as: the spacing between the devices, substrate resistivity, oxide thickness, interface charges/traps i.e., effect of radiation, temperature, and light.

5.9.1. Effects of Device Spacing

Previous studies have shown that coupling through the substrate is related to the spacing between the devices [23]. In HRS substrates the crosstalk reduces as distance between the devices increases [19]. In order to understand the impact of spacing on HRSOI we had devices with varying spacing between them as shown in the mask layout in Fig. 5.17(a). The device separations were $d = 50 \ \mu\text{m}, 100$
µm, 150 µm, 200 µm, 250 µm, 300 µm, 400 µm, 500 µm, and 600 µm. The experimental results for effect of device separation for two different substrates with varying resistivity, BOX/film thickness are shown in Figs. 5.21(a, b) and the corresponding simulation results are shown in Fig. 5.21(c). The wafer parameters are given in Fig. 5.21(a, b). Both experimental and simulation results clearly show that the substrate coupling reduces as the separation between the devices increases. The total resistance between the devices increases as the separation increases which reduces the signal that can couple from one point to the other.
Fig. 5.21. Effect of device separation on crosstalk. Crosstalk ($S_{21}$) reduces as the separation between the devices increases in both experiments (from 50 µm to 600 µm) and simulations (10 µm to 200 µm). Experimental results for (a) $\rho_{\text{substrate}} = 1200 \ \Omega \text{cm}$, $t_{\text{BOX}} = 1 \ \mu\text{m}$, $t_{\text{Film}} = 145 \ \text{nm}$, and (b) $\rho_{\text{substrate}} = 33 \ \text{k}\Omega \ \text{cm}$, $t_{\text{BOX}} = 145 \ \text{nm}$, $t_{\text{Film}} = 1.25 \ \mu\text{m}$. (c) Simulation results for $\rho_{\text{substrate}} = 5000 \ \Omega \ \text{cm}$.
5.9.2. Effects of Substrate Resistivity

Figure 5.21 shows the effect of substrate resistivity on crosstalk. As the substrate resistivity increases the coupling resistance $R_{CP}$ between the devices also increases which lowers the coupling through the substrate. The experimental results also point to a fact that after a certain resistivity the crosstalk does not reduce significantly with further increase in substrate resistivity. Crosstalk reduces significantly from $\rho_{\text{substrate}} = 10 \, \Omega \cdot \text{cm}$ to 1.2 k$\Omega$ cm, but the reduction is not significant from 1.2 k$\Omega$ cm to 33 k$\Omega$ cm. The simulation results in Fig. 5.3 also show similar reduction in crosstalk from LRS ($20 \, \Omega \cdot \text{cm}$) to HRS (5000 $\Omega \cdot \text{cm}$) SOI. But for high frequencies above 10 GHz the substrate resistivity has little effect in preventing crosstalk.

![Figure 5.21](image1)

**Fig. 5.22.** Effect of substrate resistivity on crosstalk, (a) $\rho_{\text{substrate}} = 10 \, \Omega \cdot \text{cm}$, 1.2 k$\Omega$ cm, 24 k$\Omega$ cm, and 33 k$\Omega$ cm, (b) close-up view of the circled portion of Fig. 5.22(a). Significant reduction in crosstalk from 10 $\Omega \cdot \text{cm}$ to 1.2 k$\Omega$ cm but no significant reduction in crosstalk with further increases in resistivity.
5.9.3. Effects of Buried Oxide Thickness

Figure 5.23 shows the effect of BOX thickness on crosstalk. The oxide thickness controls the capacitance of the buried oxide (BOX) which is linked to the substrate crosstalk as shown in Fig. 5.20. Crosstalk was measured for two different samples with buried oxide thicknesses ($t_{BOX}$) of 145 nm and 1 µm and respective film thicknesses of 1.25 µm and 145 nm, as shown in Fig. 5.23(a). The substrate resistivity was 18 kΩ.cm and 24 kΩ.cm respectively i.e., both are HRSOI samples. Changing the BOX thickness did not have a significant impact on the crosstalk for HRSOI as observed by Raskin et al. [23]. Crosstalk was simulated for three different buried oxide thicknesses 0.145 µm, 0.4 µm and 0.95 µm for a fixed film thickness, as shown in Fig. 5.23(b). In LRSOI (20 Ω.cm) increasing the oxide thickness reduces the crosstalk at lower frequencies below 1 GHz. But the effect is not significant for high-resistivity substrates (5000 Ω.cm), similar to experimental results. So for HRSOI change in BOX thickness has little impact on substrate crosstalk.
Fig. 5.23. Effect of BOX thickness on substrate crosstalk, (a) experiment (b) simulation. In HRSOI change in oxide thickness does not significantly affect the crosstalk as observed in both simulations and experiments.

5.9.4. Effects of Radiation (Interface Traps/Charges)

Radiation has comparatively reduced effect on SOI devices due to the inherent structure with a buried oxide between the substrate and the film. Radiation creates interface traps and fixed oxide charges, as shown in Fig. 5.24(d). The radiation effects in HRSOI and LRSOI were simulated by varying the density of interface traps and charges. Interface traps are evenly distributed in the band gap at 26 energy levels within 0.05 eV to 0.5 eV from midband on both acceptor and donor side, for a total of 52 interface trap levels. Bulk traps represent the traps present in the substrate at various energy levels in the band gap. Bulk traps were also evenly distributed like the interface traps simulation. Interface and bulk traps had no effects on crosstalk in HR/LR-SOI simulations at different concentrations, as shown in Fig 5.24(c). On the other hand crosstalk increased at higher
concentration of fixed oxide charges ($10^{12}$ cm$^{-2}$ or more). Lower oxide charge concentration had little effect on crosstalk in HRSOI in the GHz range, as shown in Fig 5.24(b). These observations propose that moderate radiation doses (interface charges/traps) have little effect in HRSOI operating in the GHz frequency range. In actual measurements the samples were radiated with Co$^{60}$ radiation to create interface traps and oxide charges. Experimental results of a sample with $\rho_{\text{substrate}} = 18$ kΩ.cm and 1μm thick BOX showed almost negligible change in crosstalk at various device separations (50 μm, 100 μm, and 400 μm) and for different doses of Co$^{60}$ radiation: 5 krads, 25 krads, and 100 krads, as shown in Fig 5.24(a). The measurements were carried out immediately after the exposure to avoid room temperature annealing effects.
Fig. 5.24. Effect of radiation (interface traps/charges) on crosstalk. (a) Experimental results of sample radiated by Co$^{60}$ radiation at 5 krad, 25 krad and 100 krad, (b) simulation results for fixed oxide charges at the silicon and oxide interface, (c) simulation results for effect of interface traps and bulk traps, and (d) device cross section with oxide charges and band diagram of a p-type silicon with interface traps. Experimental results show radiation has little effect on crosstalk. Simulation results indicate interface traps have no effect on crosstalk even at very high densities but crosstalk increases for higher oxide charges ($10^{12}$ cm$^{-2}$).
5.9.5. Effects of Temperature

Increasing the substrate temperature creates more free carriers which increase the intrinsic carrier concentration \( n_i \) and the hole concentration and hence lowers the resistivity, as shown in Fig 5.25. A lowered substrate resistivity should increase the crosstalk. To understand the effect of temperature we heated two samples to 180°C (453K) and measured the \( S_{21} \) parameter at this elevated substrate temperature. The samples had \( \rho_{\text{substrate}} = 33 \text{k}\Omega\text{.cm} \) (see Fig 5.26(a)) and 24 kΩ·cm (see Fig 5.26(b)) and the same BOX/film thickness 1.25 µm/145 nm. Crosstalk between devices increased with temperature for device separations = 200 µm and greater, as shown in Fig. 5.26.

![Graph showing the effect of temperature on carrier concentration and resistivity](image)

**Fig. 5.25.** Effect of temperature on (a) carrier concentration and (b) resistivity.
Fig. 5.26. Effect of temperature on crosstalk. $S_{21}$ was measured on two samples with $\rho_{\text{substrate}} = 33 \text{k}\Omega\text{.cm}$ (a), and $24 \text{k}\Omega\text{.cm}$ (b) and same BOX/film thickness $1.25 \mu\text{m}/145 \text{nm}$ at $180^\circ\text{C}$ ($453\text{K}$). Crosstalk between devices increased with temperature for device separation $\geq 200 \mu\text{m}$.

5.9.6. Effect of Light

Light creates electron hole pairs and increases free carrier concentration, increased free carrier concentration reduces the resistivity and it should increase crosstalk. In order to test this hypothesis we measured $S_{21}$ in complete darkness, and then by shining light and laser, as shown in Fig. 5.27. There were no observable differences in crosstalk between light and dark measurements for samples with different resistivities and at different device separations. So light has minimal impact on HRSOI substrate crosstalk.
Fig. 5.27. Effect of light on crosstalk. $S_{21}$ was measured in complete darkness and also by shining light and laser on the devices. Crosstalk was almost the same with or without light. (a) $\rho_{\text{substrate}} = 33 \, \text{k}\Omega \cdot \text{cm}$, and (b) $\rho_{\text{substrate}} = 24 \, \text{k}\Omega \cdot \text{cm}$

5.9.7. Effect of Annealing

Figure 5.28 shows the effect of annealing on crosstalk. The devices and calibration structures were prepared by evaporating aluminum on SOI wafers in an e-beam evaporator. As a general practice the contacts were annealed after evaporation to remove any interface traps and anneal oxide charges created due to x-rays during e-beam evaporation. So to understand how annealing affects crosstalk we took two measurements, one before annealing the samples after metal evaporation and one after annealing the samples at 400°C for 30 mins in forming gas ambient. Crosstalk increased after annealing as shown in Fig. 5.28(a, b) for two different device separations $d = 300 \, \mu\text{m}$ and $d = 600 \, \mu\text{m}$; it is believed
to be due to the lowering of the contact resistance after annealing which can increase coupling.

Fig. 5.28. Effect of annealing on crosstalk. $S_{21}$ was measured before and after annealing the sample at 400°C/30 min in forming gas ambient. Crosstalk increased after annealing, (a) for separation $d = 300 \mu m$, and (b) $d = 600 \mu m$.

5.9.8. Effect of Device Types

There are different devices such as $pn$ junction diodes or Schottky diodes or MOSFETs on a single chip, so the question arises, does the type of device at the noise injecting node (input node) and at the disturbed node (output node) affect the crosstalk? To study this, several simulations were performed on a thick film (1 $\mu m$ film thickness) and thin BOX (145 nm BOX thickness) HRSOI wafer using different device types at the input and the output nodes as shown in Fig 5.29. There are five different combinations considered, they are: both input and output nodes are $n^+p$ diodes (see Fig. 5.29(a)), both input and output nodes are $n^+p$ diodes and isolated by an oxide (see Fig. 5.29(b)), both input and output nodes are
Schottky diodes (see Fig. 5.29(c)), Input node is $n^+p$ diode and output node is Schottky diode (see Fig. 5.29(d)), Input node is Schottky diode and output node is $n^+p$ diode (see Fig. 5.29(e)). The substrate is p-type with $N_A = 7 \times 10^{11}$ cm$^{-3}$, the film is p-type with $N_A = 1 \times 10^{14}$ cm$^{-3}$, the $n^+$ doping is $N_D = 10^{18}$ cm$^{-3}$.

The simulation results shown in Fig. 5.30 indicates that in the GHz frequency range the cross talk is same for all device types including the configuration with the oxide trench.

![Diagram](image)

Fig. 5.29. Cross sectional view of simulation structures used in the study of effect of device type on crosstalk. (a) In/Out both $n^+p$ diode (b) In/Out both $n^+p$ diode with oxide trench around the devices, (c) In/Out both Schottky diode, (d) Input node $n^+p$ diode and output node Schottky diode, and (e) Input node is Schottky diode and output node is $n^+p$ diode.
Fig. 5.30. Effect of device type on crosstalk. $S_{21}$ was simulated for different types of devices (Schottky and $pn$ diodes) with (a) same type of devices at input and output nodes, and (b) different types of devices at input and output nodes, with no substrate bias and no oxide/interface charges. In the GHz range the crosstalk is not affected by the input/output device types.

5.10. Crosstalk Reduction Techniques – Literature Review

Substrate crosstalk reduction techniques can be broadly classified into two main categories: (1) techniques that address the noise source i.e. the source of crosstalk, and (2) techniques that address the coupling of noise from source to other devices on the same chip. The first category of addressing the noise source involves innovative analog/digital circuit design techniques to suppress the noise generation or to suppress the effect of coupled noise at the receiver end, myriads of such circuits have been designed, and few examples are given in [162-164].

Substrate engineering falls into the second category. As discussed earlier in the introduction section of this chapter, substrate crosstalk is governed by the RC
circuit of the substrate and hence substrate resistivity and its structure play a role in defining the coupling of signal through the substrate. Su et al. proposed that the propagation of switching noise should be visualized as a three-dimensional phenomenon, with the type of substrate playing a crucial role in crosstalk effects [19]. Hence substrate engineering can be used to address substrate crosstalk. Various methods have since been proposed in this regard [19, 20, 23, 165-195]. The substrate engineering-based techniques can be broadly classified into two groups: (1) signal grounding paths to isolate the noise close to the noise source, and (2) interrupting the signal flow path through the conducting silicon by use of insulating or semi insulating regions.

5.10.1. Substrate Crosstalk Reduction using Signal Grounding Techniques

Various signal grounding techniques such as: p+ guard ring, deep trench, triple well, ground plane SOI etc. have been proposed to isolate the noise at the source [19, 165-168]. On epitaxial substrates with heavily doped substrates, the noise mostly propagates through the substrates. Su et al. proposed p+ guard ring on epitaxial substrates with n-well [19]. The effectiveness of the guard ring depends on its proximity to the sensitive circuits, when it is quiet and close and biased with dedicated package pins the crosstalk suppression is maximum compared to when it is far. Also the guard rings are more effective on lightly-doped substrates than heavily doped. They found reducing the inductance in the substrate bias to be the most effective way of minimizing substrate noise. p+ guard ring is a horizontal shielding using signal grounding method [150, 196]. Figure 5.31(a) shows an example of p+ guard ring isolation method.
The other popular grounding technique is the triple well or deep n-well in which the p-region is inside the well or the deep n-well itself is grounded as proposed by Joardar et al. [165], as shown in Fig. 5.31(b, d). Triple well is an example of vertical shielding method [150, 196].

Fig. 5.31. Various crosstalk reduction techniques using signal grounding methods, (a) $p^+$ guard ring, and (b) grounded deep n-well or triple well technique. (c) Cross talk reduction using SOI substrates. (d) Simulation results comparing crosstalk ($S_{21}$) using different isolation techniques [165].

5.10.2. Substrate Crosstalk Reduction by Interrupting the Signal Path

The other idea is to interrupt the coupling path between the noise source and the sensitive circuits by changing the resistivity of the path using insulating or
semi-insulating materials. The basic technique to reduce substrate crosstalk in this category is to increase the physical separation between the noisy digital circuits and the sensitive analog circuits [19]. But increasing the separation is effective in shielding the sensitive circuits when the substrates are lightly doped i.e., HRS substrates, see Figs. 5.21. The separation is not very effective on LRS substrates in the GHz freq range [19].

SOI wafers provide better crosstalk prevention ability than bulk substrates due to the oxide layer which acts as a highly resistive isolation structure interrupting the noise path [20, 169], see Fig 5.31(c). But the degree of isolation provided by the SOI technique worsens considerably if the handle wafer is not grounded [165]. Joardar et al. showed that junction isolation can provide equal or better crosstalk isolation than SOI structure in LRS wafers [165], see Fig. 5.31(d). The degree of isolation decreases with frequency in all cases because the impedance \((1/2\pi fC)\) due to the MOSFET gate, \(pn\) junctions, and buried oxide capacitances decreases.

Later, Raskin et al. showed that SOI wafers with HRS substrates provide the best crosstalk isolation among all types of substrates because the signal path can be effectively interrupted by the higher substrate resistivity [23]. Figure 5.3 compares the crosstalk in various types of substrates and shows the effectiveness of HRSOI. They have also shown the use of guard ring in HRSOI to reduce crosstalk (see Fig. 5.32(a)).

Hiraoka et al. proposed a crosstalk reduction structure (Supporting Substrate Guard Ring: SSGR) using the HRSOI substrate [172] (see Fig. 5.32(b)). The
performance gains were 11 dB from the basic SOI structure and 7.5 dB from the conventional guard ring (GR) structure at 10 GHz.

![Crosstalk reduction using SOI substrates](image)

Fig. 5.32. Crosstalk reduction using SOI substrates (a) guard ring (GR) [23], and (b) supporting substrate guard ring (SSGR) [172].

### 5.10.3. Substrate Crosstalk Reduction using Surface Passivation Techniques

Even though HRSOI has been proposed as one of the best substrate for crosstalk reduction, it has drawbacks. The HRSOI wafers in their basic form are not highly effective in preventing crosstalk as they are sensitive to the oxide charges in the BOX which at various bias conditions (as happens in power devices during normal operations) form a conducting channel at the BOX/substrate interface by accumulating or inverting that region and thereby degrading the crosstalk prevention capabilities of HRSOI, also in HRSOI the crosstalk is limited by the silicon relaxation capacitance that causes a frequency dependent contribution [197]. Reyes *et al.* proposed the surface conduction phenomenon [198, 199] and Wu *et al.* experimentally verified the same [200], and Lederer *et al.* highlighted the effect of DC bias on RF losses in substrates [201]. Hence the BOX/Substrate interface is considered to play a major role in crosstalk...
and much research has been conducted in this regard to contain the surface conduction channel at the BOX interface to lower the crosstalk. These are called surface passivation techniques and various such techniques have been proposed [181-194].

![Diagram](image_url)

Fig. 5.33. Crosstalk reduction in SOI substrates using surface passivation techniques, achieved by adding a layer of polysilicon / amorphous Si / nanocrystalline particles / trap rich layer etc. below the BOX.

One of the ways to achieve surface passivation is by adding a poly-Si layer below the BOX at the substrate interface. This polysilicon layer hinders the formation of the accumulation or inversion layer near the interface and also increases the resistivity of the substrate close to the interface and hence reduces crosstalk [184-186].

Another way to achieve surface passivation to prevent the formation of the channel at the BOX/Substrate interface is by having a very high trap density in the band gap and possibly an increased band gap. This is achieved by depositing a thin amorphous layer at the BOX/substrate interface [189] or damaging the silicon
surface by bombarding the interface with heavy dose of high energy argon [187, 188].

Lederer et al. proposed surface passivation in HRSOI and oxide covered HR substrates by using a rapid thermal anneal (RTA)-crystallized layer of silicon [190]. The proposed method consists in the LPCVD-deposition of amorphous silicon followed by Si-crystallization at 900°C with RTA. This method achieves low surface roughness and a high stability over long thermal anneals and also up to 10 kΩ.cm local resistivity.

Surface passivation in HRS silicon was also achieved by covering the Si surface at the BOX interface with a thin ferroelectric film. This is achieved by covering the surface by Ba$_{0.25}$Sr$_{0.75}$TiO$_3$ (BSTO) thin films deposited using pulsed laser deposition [191].

Hamel et al. proposed a buried ground plane SOI (GPSOI) structure to counteract the surface conduction to reduce substrate crosstalk. In their method a 2 Ω/square metal-silicide buried ground plane was placed between below the BOX in a regular SOI wafer. This SOI substrate can be manufactured by bonded silicon technology in a similar manner to that for silicon on metal-silicide on insulator (SMI or SSOI) substrates [166].

Recently Chen et al. [194] have proposed addition of a nanocrystalline film below the BOX as a surface passivation layer in HRSOI.

Some researchers have addressed the issue of conducting channel at the interface by creating metallic Faraday cages which completely surround the noise source and shunt the signal to ground. In one approach, the Faraday cage structure
consists of a ring of grounded vias encircling sensitive or noisy portions of a chip. The via technology features high aspect ratio through-wafer holes filled with electroplated Cu and lined with a silicon nitride barrier layer. This Faraday cage structure showed crosstalk suppression of 40 dB at 1 GHz and 36 dB at 5 GHz at a distance of 100 µm. [181]. This solution is attractive as a post-process module, particularly in a silicon carrier structure, or system on a package (SOP). Isolation is limited at high frequency by the inductance of the vias [182]. In another approach the Faraday cage is comprised of a buried metal tungsten silicide ground plane beneath the buried oxide layer to form the bottom of the cage, and vertical metal-lined $n^+$ polysilicon-filled trenches in the active silicon layer to form the cage walls [183]. Examples of Faraday cage structures are shown in Fig. 5.34.

![Diagram](image)

(a)              (b)

Fig. 5.34. Crosstalk reduction using Faraday cage structures. (a) Faraday cage using through-wafer grounded vias [181], and (b) metal-lined polysilicon filled trench used in the GPSOI with the Faraday cage structure [183].
5.10.4. Substrate Crosstalk Reduction - Other Techniques

Although much importance is given to higher substrate resistivity to minimize substrate crosstalk, Ankarcrona et al. have shown that very low resistivity substrates have significant lower crosstalk for all frequencies, compared to both high-resistivity and medium-resistivity substrates mainly due to effective shunting of the signal to ground through the low-resistive substrate. Additional advantage of the low-resistivity substrate is that the crosstalk is insensitive to relaxation effects, due to the high doping concentration [173, 202].

Joardar in 1995 [170] and Yeh et al. in 2004 [171] have shown that simple pn junction can be used for noise isolation using triple well or deep n-well on a p-type substrates. The pn junction capacitance acts as an effective isolation structure.

Coupling can be reduced by locally increasing the resistance by a very large factor. One of these methods, that of high-energy proton bombardment, converts local resistivity to greater than 20 kΩ.cm and has been used to demonstrate improved Q of planar spiral inductors [174]. The local conversion of silicon to porous silicon [175] results in regions which are essentially completely insulating. Porous silicon trenches which go completely through the wafer reduce crosstalk in p+ substrates to the measurement limit. As these regions are thick, the capacitive crosstalk is much less than that in the thin buried oxide of SOI wafers. The improvement for p substrates is not as effective [176]. Another approach is the ‘silicon on glass’ method of [180] where the active layers are transferred to a glass substrate and the silicon is completely removed. Drayton et al. proposed
micromachined packages for higher isolation where the substrate is thinned from
the backend after circuit fabrication [195].

5.11. Proposed Crosstalk Reduction Technique

In the previous section various methods to reduce crosstalk in SOI and HRSOI
wafers have been discussed. The main criteria from the above discussion are to
increase the overall substrate resistivity and to prevent the formation of the
conducting layer near the BOX/Substrate interface and to disrupt the signal flow
path from the noisy source to other sensitive circuits.

Air has the lowest dielectric constant and if it is used as a dielectric then the
corresponding capacitance will be much less than any other dielectric and also it
acts as an insulator. So if there are air gaps introduced in the substrate below the
BOX at the BOX/Substrate interface then the coupling capacitance $C_{cp}$ shown in
Fig. 5.20 will be the lowest compared to other dielectrics and being an insulator, it
will also increase the overall coupling resistance $R_{cp}$; consequently the overall
coupling will be less. In order to show the feasibility of this approach, various
structures were simulated as shown in Fig 5.35. In one structure the air gap was
placed separately only below the input and output nodes and in another structure
the air gap was all along the distance between the input and output nodes. The
input port is the noise injecting port and output port is the affected node and the
goal is to measure the coupling from input to output for structures with and
without air gaps. The simulated HRSOI structure has an HRS substrate with
doping concentration of $N_A = 7 \times 10^{11}$ cm$^3$, film doping concentration of $N_A = 10^{14}$
cm$^{-3}$, BOX thickness $t_{BOX} = 145$ nm and film thickness $t_{film} = 1$ µm. The ports are 100 µm apart as shown in Fig 5.35.

The simulated results are shown in Fig 5.36 and it clearly shows a reduction in crosstalk at all frequencies with the air gap below the BOX, even in the GHz range. The longer the air gap is, the better is the crosstalk prevention. The approach was also simulated on an LRSOI wafer of similar configuration but with substrate resistivity $N_A = 10^{14}$ cm$^{-3}$ and the effect of air gap in reducing crosstalk is more prominent in LRSOI.

Fig. 5.35 SOI cross sections to study the effect of air gap on substrate crosstalk.
Fig. 5.36 Effect of air gap on substrate crosstalk for different substrate doping, (a) HRSOI, \( N_A = 7 \times 10^{11} \text{ cm}^{-3} \), (b) LRSOI, \( N_A = 10^{14} \text{ cm}^{-3} \); crosstalk reduces with air gap.

5.12. Conclusion

Substrate coupling in high-resistivity SOI substrates was studied and the effects of various factors such as: substrate resistivity, separation between devices, buried oxide (BOX) thickness, radiation, temperature, annealing, and light on crosstalk was studied using both experiments and simulations. Both experiments and simulations showed that crosstalk reduces as substrate resistivity increases. HRSOI has better substrate coupling prevention capability than LRSOI substrates but in HRSOI wafers crosstalk did not reduce significantly beyond a certain resistivity. Substrate crosstalk is directly related to the separation between the devices on all types of substrates. The farther apart the devices are, the lower the crosstalk between them. The thickness of buried oxide does not affect the crosstalk significantly as evident from experiments and simulations. Experimental results for substrate bias showed reduction in crosstalk with both positive and negative substrate bias but simulation results did not show any significant change.
with bias. Radiation (interface traps and oxide charges) seems to have little effect on crosstalk. Simulation results also indicate interface traps have no effect on crosstalk even at very high concentrations but simulations for oxide charges showed an increase in crosstalk at higher concentrations ($10^{12}$ cm$^{-2}$). In experiments, crosstalk increased with temperature when device separations were 200 µm or greater. Annealing the sample increased the crosstalk. There was no observable difference in crosstalk between light and dark.

From the experiments it can also be deduced that after a certain resistivity, in this case 1 kΩ.cm further increase in resistivity of HRS wafers does not show any significant reduction in substrate crosstalk in the GHz frequency range. Also various factors such as light, radiation, temperature, and BOX thickness do not significantly alter the crosstalk in HRS wafer.

A new approach to reduce crosstalk has been proposed, which uses air gaps at the BOX/substrate interface to reduce crosstalk. Larger air gaps are more effective in reducing crosstalk than smaller ones present only below the noisy and the sensitive devices. Impact of air gap in reducing crosstalk is more prominent in LRSOI than HRSOI.
CHAPTER 6. A NOVEL RESISTIVITY MEASUREMENT TECHNIQUE FOR HIGH-RESISTIVITY SILICON

6.1. Introduction

High-resistivity silicon (HRS) substrates are important for low-loss, high-performance microwave and millimeter wave devices in high-frequency telecommunication systems. The highest resistivity of up to ~10,000 ohm.cm is Float Zone (FZ) grown Si which is produced in small quantities and moderate wafer diameter. The more common Czochralski (CZ) Si can achieve resistivities of around 1000 ohm.cm, but the oxygen content in Czochralski crystals can lead to thermal donor formation with thermal donor concentrations \( \sim 10^{15} \text{ cm}^{-3} \). This is significantly higher than the background dopant concentration \( (\sim 10^{12} - 10^{13} \text{ cm}^{-3}) \) of such high-resistivity Si and can lead to resistivity changes and possible type conversion of high-resistivity p-type silicon to n-type [8-10]. Owing to their very low doping concentrations and presence of oxygen in CZ wafers, HRS wafers pose a challenge in resistivity measurement using the conventional techniques such as: four-point probe and Hall measurement. The goal of this research is to highlight the challenges in resistivity measurement of HRS substrates using the traditional resistivity measurement methods such as: four-point probe, Hall measurement, and Capacitance-Voltage method and propose a novel simple measurement technique for accurate resistivity measurement of HRS substrate.
6.2. Literature Review: Challenges and Proposed Resistivity Measurement Techniques for High-Resistivity Silicon

In the past, researchers have proposed various approaches to address the challenges in resistivity measurements of high resistivity materials, they are: floating portions of the circuitry [24], ac [25] and dc "bootstrapping" [26, 27], use of differential electrometers [28], double modulation [29], ac guarding [30], and dc guarding [31]. The guarded approach involves the use of a high input impedance unity gain amplifier between each probe on the sample and the external circuitry, thus permitting measurement with standard laboratory differential voltmeters [203]. Resistivity can be indirectly determined from Capacitance-Voltage (C-V) measurements. It is used extensively for doping profile calculation of silicon wafers. It can be used in two configurations; series or parallel mode [11]. We found series C-V is preferable for HRS substrates due to high substrate resistance; as mentioned in [11]. Parallel C-V does not show correct C-V plots at high frequencies as substrate resistance begins to dominate, as discussed in chapter 4, section 4.2.1.

6.3. Challenges in Resistivity Measurement of HRS Wafers

Resistivity is one of the fundamental parameters of HRS wafers that should be measured accurately. The low doping concentration and presence of oxygen in CZ HRS wafers create challenges in resistivity measurement. During this research it was observed that it is very difficult to accurately and consistently measure the resistivity of HRS wafers using the standard four-point probe or Hall measurement method.
6.3.1. Four-Point Probe Measurement

Four-point probes (4PP) are routinely used for semiconductor material characterization to measure semiconductor resistivity and sheet resistance of thin conducting layers and wafers [11]. The four-point probe method was originally proposed by Wenner [204] and then Valdes adopted it for semiconductors [205]. It is commonly used in the collinear configuration where the four probes are arranged in a straight line with equal spacing; the two outer probes carry the current and the two inner probes measure the voltage. Previous studies have shown that very high resistive materials are difficult to measure using this method [11]. Similar difficulties were observed during our experiments using a Keithley 2400 system attached to a Signatone four-point probe and the measured resistivities were not within the expected range. Two different samples from the same wafer were used for measurement: one annealed at 400°C/30 min in forming gas ambient and the other without annealing. These wafers had a polished front surface and an unpolished back surface and measurements were taken on both sides. Resistivity was calculated from the slope of the $I-V$ plot. $I-V$ data were not linear and the inbuilt software of the tool employs curve-fitting technique to approximate the data into a linear plot through the origin and then measures the slope of the straight line to calculate the resistivity. The measured resistivities for different samples are shown in Table 6.1 and a sample screenshot of tool’s output is shown in Fig. 6.1. The expected resistivity as supplied by the manufacturer was $\approx 1 \ \text{k}\Omega\cdot\text{cm}$, but that value was never obtained during our measurements.
Table 6.1 Measured resistivity data from the Keithley 2400 system connected to a Signatone four-point probe system.

<table>
<thead>
<tr>
<th>Observation #</th>
<th>Without Anneal – Polished Surface</th>
<th>Without Anneal – Unpolished Surface</th>
<th>Annealed – Unpolished Surface</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6.56</td>
<td>5.71</td>
<td>50.09</td>
</tr>
<tr>
<td>2</td>
<td>10.67</td>
<td>NA</td>
<td>49.22</td>
</tr>
</tbody>
</table>

Fig. 6.1. Sample $I$-$V$ and resistivity measurement output of Keithley 2400 system connected to Signatone four-point probe (a) annealed sample – unpolished surface (b) bare silicon sample – polished surface. $I$-$V$ plots are not linear indicating non-Ohmic contacts.

$I$-$V$ measurements from the instrument indicated that contacts are no longer Ohmic, they show mostly Schottky type behavior and we believe that plays a role in the inaccurate measurement. Similar Schottky type behavior was also observed.
by researchers during four-point probe measurements of silicon carbide (SiC) samples, another high-resistive material [206]. The measurements were also repeated using multiple instruments and similar results were observed. Also the measurements took a long time to settle down to a steady value and were affected by illumination as also observed for SiC [207].

6.3.2. Hall Effect Measurement Method

Hall Effect measurement is a widely used semiconductor characterization technique due to its simplicity and ability to accurately measure resistivity, carrier densities and mobility in semiconductors [208]. It is based on the Hall Effect discovered by Hall in 1879 [209]. Hall, using the principle of Lorentz force, discovered that a small transverse voltage appeared across a current-carrying thin metal strip in an applied magnetic field. This helps to find the carrier concentration and its polarity directly. Hall technique uses the van der Pauw [210, 211] method for sheet resistance measurement. HRS samples are known to be difficult to measure using four-point probe or van der Pauw methods [11].
Fig. 6.2. A sample Hall measurement output of an HRS substrate (expected resistivity of ~1 kΩ·cm) using silver paste contacts. (a) Hall parameters (b) I-V plots for 100 nA current. I-V plots are non linear, non overlapping indicating non-Ohmic contact. The measured data were inaccurate and non-repeatable.
Hall measurements were made using ECOPIA Hall effect measurement system HMS 3000 and using silver paste along with thin copper wires to form contacts between the sample holder and the HRS substrate, see Fig. 6.3(a). The screen shots from the instrument are shown in Fig 6.2. But the Hall measurements did not provide the expected resistivity and carrier concentration. The current-voltage plots were not Ohmic, the Hall coefficients did not match and the results were not repeatable. Hence the measured resistivity using silver paste was inaccurate. Next, Hall measurements were made using gold contacts. The results were more promising than those using silver paste, the $\rho_{\text{substrate}} = 755$ ohm.cm. The results are summarized in Table 6.4.

6.3.3. Hall Measurement using Indium Contacts

In previous Hall techniques silver paste was used directly on the HRS surface to connect the sample to the Hall probe pads using copper wires. Silver is a good conductor but silver paste has organic compounds in it and it may not be forming a good Ohmic contact. Indium is found to form good Ohmic contact with silicon [212]. It was decided to use Indium as contact material. Also careful sample preparation avoiding surface contamination and native oxide is a key to proper measurement. A 1cm x 1cm square Si sample was cleaved. The sample was cleaned using Acetone, Methanol and Isopropyl alcohol followed by DI water rinse and proper drying. Before placing the Indium the sample was etched in a 50:1 dilute HF for 30 seconds to remove the native oxide. Then circular indium discs were placed on the four corners of the square sample and heated to 160°C for 2 mins. Indium melted and fused to the silicon surface forming a strong
contact. Then the sample was connected to the sample holder using thin gold wires and silver paste, as shown in Fig. 6.3(b). The measurements were taken using a Hall set-up with 1 Tesla magnet and a high impedance voltmeter. Current in the range of 50 nA to 200 nA was suitable for this sample, other current values showed erroneous result. The average resistivity was $2.693 \text{k}\Omega \text{cm}$ and the doping was p-type with $N_A=7.22\times10^{12} \text{ cm}^{-3}$. The Hall measurements using Indium contact are summarized in Table 6.2. The measured data are consistent within a small range and the Hall coefficients matched. The measured resistivity was not very close to the expected value but was not too far off like the previous Hall measurements. This indicates that the Indium contacts work better for HRS substrates for Hall measurements. But the variation of resistivity with applied current points to a non-linear current-voltage relationship.

![Fig. 6.3. Hall measurement – sample (1x1 cm) and sample holders (a) gold and silver paste contacts – Ecopia HMS-3000 instrument, (b) Indium contact.](image-url)
Table 6.2 Summary of Hall measurement data using Indium contact.

<table>
<thead>
<tr>
<th>Current (nA)</th>
<th>Resistivity (kΩ.cm)</th>
<th>Doping Type</th>
<th>Doping Concentration (cm⁻³)</th>
<th>Mobility (cm²/V.s)</th>
<th>Magnetic Field (Gauss)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>2.784</td>
<td>p-type</td>
<td>6.37x10¹²</td>
<td>352.45</td>
<td>2860</td>
</tr>
<tr>
<td>100</td>
<td>2.782</td>
<td>p-type</td>
<td>7.38x10¹²</td>
<td>-</td>
<td>2860</td>
</tr>
<tr>
<td>100</td>
<td>2.743</td>
<td>p-type</td>
<td>7.2x10¹²</td>
<td>316.17</td>
<td>3800</td>
</tr>
<tr>
<td>200</td>
<td>2.461</td>
<td>p-type</td>
<td>7.94x10¹²</td>
<td>319.67</td>
<td>2860</td>
</tr>
<tr>
<td>Average =</td>
<td>2.693</td>
<td>p-type</td>
<td>7.22x10¹²</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

6.3.4. Resistivity from Doping Profile: C-V Measurement Method

Resistivity can also be determined from the doping profile or the average doping concentration of a silicon substrate [11]. Capacitance–Voltage technique is a well established method for doping profiling. The space charge region width dependence on applied bias is the core of C-V technique. It can be used with Schottky barrier diodes with deposited metals, mercury, and liquid electrolyte contacts, pn junctions, MOS capacitors, MOSFETs, and metal-air-semiconductor structures [11]. In this research, C-V technique was used to determine doping profiles of HRS substrates using Schottky barrier diodes and MOS capacitors with aluminum contacts annealed at 400ºC/30 min in forming gas. The doping
profile was different for both test structures and the doping polarity was n-type for p-type Si due to oxygen donor formation as discussed in chapter 4. Also the fast electron-hole pair generation rate in HRS substrates due to the low doping concentration created a challenge to drive the device into deep depletion in the MOS capacitor based C-V. These challenges highlight the difficulties of using the C-V technique for HRS wafers.

Measurements were made using MOS capacitors on an HRS bulk silicon wafer with 100 nm thick gate oxide and 900 µm diameter circular aluminum gate contact (gate area \(A_{\text{Gate}} = 6.36 \times 10^{-3} \text{ cm}^2\)). MDC probe station attached to an HP4284 high precision capacitance measurement instrument was used for C-V measurement. Series \(C_S\)-V method was used as it is more accurate for HRS samples, refer to chapter 4, section 4.2.1 for details.

Steps to calculate doping profile from C-V [11]:

- Measure series \(C_S\)-V at 100 kHz and at very high DC bias sweep rate so that the device goes into deep depletion. Plots were least noisy at 100 kHz frequency, hence chosen.
- Calculate \(1/C^2\) vs. \(V\) from the above \(C_S\)-V plot as shown in Fig. 6.4 (a).
- Calculate the depletion width \(W\) for each gate bias using
  \[
  W = \frac{K_S \varepsilon_0 A_{\text{Gate}}}{C_S}, \quad \text{where } A_{\text{Gate}} = \text{gate area}, \ K_S = \text{relative permittivity of silicon} = 11.9, \ \varepsilon_0 = \text{relative permittivity of vacuum} = 8.854 \times 10^{-14} \text{ F/cm}. \ C_S \text{ is measured by the instrument and depends on the gate bias as depletion width varies with applied bias.}
• Calculate doping concentration for each depletion width \( W \) i.e. using

\[
N_A = \frac{2}{K_z e_0 A^2 \left( d\left( \frac{1}{C^2} \right) / dV \right)},
\]

where \( N_A \) = doping concentration, \( V = \) applied DC gate bias, \( d(1/C^2)/dV = \) slope of \( I/C^2 \) vs. \( V \) plot.

The substrate doping is n-type and the average doping concentration from the doping profile plot in Fig. 6.4(b) is \( N_D \approx 10^{14} \) cm\(^{-3} \) which is equivalent to 133 \( \Omega \).cm for equivalent boron doped and 44 \( \Omega \).cm for equivalent phosphorous doped sample [11]. Annealing the sample to make good contacts changes the doping polarity due to thermal donor creation which dominates in very lightly doped samples and makes it difficult to measure the actual profile and hence the intended resistivity.

![Graphs](image)

Fig. 6.4. (a) \( C_S - V \) and \( 1/C_S^2 - V \) plots (series method), (b) doping profile from \( C_S - V \) for HRS with \( \rho_{\text{manufactured}} \approx 1 \) k\( \Omega \).cm. Doping is n-type and average \( N_D=10^{14} \) cm\(^{-3} \).
6.3.5. Resistivity Extraction from C-V Measurement Method

The aim is to explore a method to calculate the substrate resistivity from parallel \((C_P-V)\) and series \((C_S-V)\) measurements at very high frequencies and compare the results with other measurement methods. Figure 6.5(a) shows the circuit representation of the actual device (Schottky Diode) and the corresponding series and parallel equivalent circuits are shown in Fig 6.5 (b) and (c) respectively [11]. “C” in Fig. 6.5(a) can be the oxide capacitance in case of an MOS structure or the junction capacitance in case of a Schottky diode. Series \(C_S-V\) method assumes the DUT as a series circuit and measures the equivalent series capacitance \(C_S\) and the equivalent series resistance \(R_S\). Parallel \(C_P-V\) method assumes the DUT as a parallel circuit and measures the equivalent parallel capacitance \(C_P\) and conductance \(G_P\). Table 6.3 summarizes the formulas for equivalent series and parallel circuits, which will be used in resistivity extraction from C-V measurements. As \(f \to \infty \Rightarrow R_S \to r_S\), where \(r_S\) consists of both substrate resistance and contact resistance. The instrument provides \(C_S, R_S, C_P,\) and \(G_P\) as the measured values. The gate oxide thickness is 100 nm and the wafer thickness \(t_{\text{wafer}} = 725 \, \mu\text{m}\), gate area \(A_{\text{Gate}} = 6.36 \times 10^{-3} \, \text{cm}^2\) (gate contacts are 900 \(\mu\text{m}\) diameter circular aluminum dots). All calculations were made with the device in accumulation at \(V_{\text{Gate}} = +20\) V. The wafer was grown as p-type but after annealing at 400ºC/30 min to improve the contact quality, it got converted to n-type due to thermal donor creation, as discussed in Chapter 4.
Fig. 6.5. (a) Actual device, (b) parallel equivalent circuit, and (c) series equivalent circuit of a Schottky diode.

Table 6.3 Summary of formulas for series and parallel equivalent circuits [11].

<table>
<thead>
<tr>
<th>Circuit Type</th>
<th>General Formula</th>
<th>When $\omega \to \infty$ ($\omega = 2\pi f$, i.e., $f \to \infty$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parallel Measurement</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
| $C_p$ | $C_p = \frac{C}{(1 + r_s G)^2 + (\omega r_s C)^2}$ | $C_p = \frac{C}{(\omega r_s C)^2} = \frac{l}{\omega^2 r_s^2 C}$
$=> C = \frac{l}{\omega^2 r_s^2 C_p}$
$=> r_s = \frac{l}{\omega \sqrt{C C_p}}$ |
| $G_p$ | $G_p = \frac{G(1 + r_s G) + r_s (\omega C)^2}{(1 + r_s G)^2 + (\omega r_s C)^2}$ | |
| Series Measurement | | |
| $C_s$ | $C_s = C \left[ 1 + \left( \frac{G}{\omega C} \right)^2 \right]$ | $C_s = C$ |
| $R_s$ | $R_s = r_s + \frac{l}{G \left[ 1 + \left( \frac{\omega C}{G} \right)^2 \right]}$ | $R_s = r_s$
$\rho_{\text{measured}} = R_s \frac{A_{\text{Gate}}}{t_{\text{wafer}}}$ |
Proposed steps to calculate resistivity from measured $C_S$ and $C_P$ values.

- Measure $C_P$ and $C_S$ at a very high frequency i.e., at $f = 1$ MHz, the maximum frequency allowed by the instrument.

- Calculate resistance using $r_s = \frac{1}{\omega \sqrt{C C_P}}$ where $C = C_S$ as mentioned in Table 6.3.

- Calculate resistivity, $\rho_{\text{calculated}} = r_s \frac{A_{\text{Gate}}}{t_{\text{wafer}}}$.

Steps to calculate resistivity from measured resistance.

- Measure $R_S$ at a very high frequency i.e. at $f = 1$ MHz, the maximum frequency allowed by the instrument.

- Calculate resistivity, $\rho_{\text{measured}} = R_s \frac{A_{\text{Gate}}}{t_{\text{wafer}}}$.

Figure 6.6(a) shows the above calculation in a graphical form, where $C_S$, $C_P$, $\rho_{\text{calculated}}$ and $\rho_{\text{measured}}$ were plotted against different frequencies. The figure shows that at high frequencies the calculated and measured resistivities tend to coincide.

At 1MHz, $\rho_{\text{calculated}} = 202.25 \ \Omega \text{cm}$ and $\rho_{\text{measured}} = 220.22 \ \Omega \text{cm}$. 
Fig. 6.6. (a) Resistivity extraction from series and parallel C-V measurements for a bulk HRS wafer with $\rho_{\text{manufactured}} \approx 1 \ \Omega\cdot\text{cm}$. (b) Parallel C-V, and (c) Series C-V at different frequencies. $C_S$ and $C_P$ values from these plots at +20V (accumulation) are used to calculate the resistivity in (a).
Table 6.4 Summary of resistivity measured by different methods for a bulk silicon sample with 1000 $\Omega$.cm manufacturer specified resistivity.

<table>
<thead>
<tr>
<th>Method</th>
<th>Four-Point Probe</th>
<th>Hall (Silver Paste Contact)</th>
<th>Hall (Gold Contact)</th>
<th>Hall (Indium Contact)</th>
<th>C-V Doping Profile</th>
<th>C-V Extraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resistivity</td>
<td>6.5k$^a$, 5.7k$^b$, 50k$^c$</td>
<td>Undetermined</td>
<td>755</td>
<td>2.69k</td>
<td>133</td>
<td>220</td>
</tr>
<tr>
<td>Average Doping</td>
<td>NA</td>
<td>Undetermined</td>
<td>9.1x10$^{12}$</td>
<td>7.22x10$^{12}$</td>
<td>$10^{14}$</td>
<td>NA</td>
</tr>
</tbody>
</table>

$^a$ polished surface, $^b$ unpolished surface, and $^c$ unpolished surface after annealing

6.4. Proposed Solution Methodology

In previous sections, various challenges associated with different resistivity measurement techniques involving HRS substrates were highlighted. Due to very low substrate doping concentration the probe tips are most probably not forming an Ohmic contact during these measurements and causing erroneous results. It is believed that the contact resistance and the types of contact, Ohmic or Schottky, play a significant role in the observed measurement anomalies. The strategy is to understand the nature of contacts during standard four-point probe or Hall techniques and find a way to either avoid the contact problem or take into account the contact resistances and separate them from the final measurement to get the actual substrate resistance.
A new approach based on Impedance Spectroscopy (IS) [213] is proposed to extract resistivity. IS has been used to characterize silicon for varied characteristics: characterize resistivity, density of surface states and shallow states [214], defect profile characterization in high purity FZ crystals [215], characterize surface states [216], improved C-V characterization using electrochemical IS [217]. In IS a particular device structure is used to measure the material characteristics such as resistance and capacitance and then a mathematical model is fitted to the experimental data to extract the device parameters as described in detail in the following section. In this research both real and imaginary components of impedance vs. frequency are used for modeling and curve fitting to extract the device parameters compared to just the real or imaginary parts; this approach results in a more accurate parameter extraction. The other aspect of this approach is to extract resistivity of high resistivity CZ crystals using a process that does not involve high temperature steps such as thermal oxide growth or contact annealing; as they are found to create thermal donors affecting the substrate resistivity. Also the goal was to use conventional equipments and have simpler processing steps using regular devices such as MOS capacitors or Schottky diodes. In order to achieve a non-oxide gate it was decided to use a dielectric layer that can be formed without any thermal step, has uniform thickness without defects, and creates a strong bond with silicon. After much research two polymers were used to create a dielectric film by spin coating, they are, PMMA (Poly Methyl Methacrylate) and Polystyrene (PS) [218, 219]. Both of them have relative dielectric constant of 2.6 and create a strong uniform thin film
on silicon. The details of this approach and the use of polymer films are covered in the subsequent sections.

6.5. A Novel Approach to Extract Resistivity of HRS Based on Impedance Spectroscopy

Impedance Spectroscopy (IS) is a small-signal measurement of linear electrical response of material (including electrode effects) and subsequent analysis of response to yield information about physiochemical properties of the system [213]. It is mostly measurement and analysis of impedance vs. frequency. But it also involves analysis of admittance, modulus and dielectric constant vs. frequency. IS is mainly a frequency domain analysis, but sometimes measurements are performed in time domain and Fourier transformed to frequency domain [213]. There are mainly two types of IS: (a) Electrochemical Impedance Spectroscopy (EIS), and (b) Non Electrochemical Impedance Spectroscopy. In this research Non Electrochemical Impedance Spectroscopy approach is used.

Impedance of a circuit using a time varying signal is a complex quantity with both real and imaginary parts. Figure 6.7(a) shows a complex impedance \( Z(\omega) \) and its components. In Cartesian form the complex impedance \( Z = R + jX \), i.e., the sum of real part \( R \) (resistance of the circuit) and the imaginary part \( X \) (reactance of the circuit, which can be the capacitive reactance \( X_C = 2\pi fC \) or inductive reactance \( X_L = 2\pi fL \) as shown in Fig. 6.7(b)), \( f \) is the frequency of the input signal, \( C \) is the capacitance and \( L \) is the inductance. Complex impedance of a series RL and RC circuit is shown in Fig. 6.7(b). In polar form the complex
impedance can be represented by its magnitude \( |Z| = \sqrt{R^2 + X^2} \) and phase 
\[ \theta = \tan^{-1}\left(\frac{X}{R}\right). \]
The complex impedance \( Z(\omega) \) is a frequency dependant term and its magnitude and phase vary with frequency. The frequency variation of complex impedance \( Z(\omega) \) is represented by a Bode or Cole-Cole or Nyquist plot. In this research Bode plot is used to represent the frequency variation of magnitude and phase of \( Z(\omega) \). It was observed that phase vs. frequency plot is more sensitive to circuit parameters and helps in more accurate modeling.

(a) Fig. 6.7. Complex Impedance of a circuit. (a) Impedance vector \( Z \), magnitude \( |Z| \), and phase \( \theta \). (b) Impedance of a series RL and RC circuit.
6.5.1. Impedance Spectroscopy Methodology and Process Flow

Fig. 6.8. Impedance Spectroscopy process flow.

The general process flow for Impedance Spectroscopy is shown in Fig. 6.8. The process flow is described with reference to the current research for ease of explanation. In this approach the complex impedance Z(ω) of the sample is measured using a MOS capacitor or Schottky diode structure for f = 0.1Hz to 10MHz at ac voltages between 5-25mV using a Solartron 1260 Impedance Analyzer. Then an equivalent circuit is created based on the physical device model, see Fig. 6.8. The equivalent circuit represents the device as series and parallel combination of resistances (R) and capacitances (C). The device can have a dielectric layer either on the top surface only or on both surfaces along with metal contacts. A mathematical model, in the form of a transfer function in the Laplace domain representing the physical model and the equivalent circuit is
derived. The measured data are then plotted in two plots (a) impedance magnitude (in decibel) vs. frequency, and (b) phase (in degree) vs. frequency. Then the mathematical model was curve fitted to the measured plot using MEISP [220] and Matlab software using CNLS (Complex Non-Linear Least Square) algorithm to extract the device parameters (R’s and C’s). The phase diagram is found to be more sensitive to circuit parameters. The derivation of the mathematical model and the equivalent circuit is an iterative process until a proper match is found and it may differ between devices and experimental conditions. Once the substrate resistance is extracted, the resistivity is calculated using Eqn. 6.1. In this method the substrate resistivity can be extracted accurately as it takes into account the effect of contacts and other device components. The resistivity is

\[ \rho = R_{\text{fitted}} \left( \frac{\text{Area}}{\text{Thickness}} \right) \]  

(6.1)

In this research, various device structures were investigated for resistivity extraction following the Impedance Spectroscopy approach.

1. Bare HRS sample with mechanical contacts on top and bottom (S1).
2. HRS sample with only top gate oxide and silver paste bottom contact (S2).
3. Bare HRS sample with Teflon film on both sides and mechanical contacts (S3).
4. HRS sample with thin PMMA film on both sides and gold contacts (S4).
5. HRS sample with thin polystyrene film on both sides and gold contacts (S5).
6. HRS sample with thin polystyrene film on top side only and gold contacts on both sides (S6).
7. HRS sample with thick PMMA film on both sides and aluminum contacts (S7).
8. HRS sample with only aluminum contacts on both sides without any dielectric layers – Schottky contacts (S8).
9. HRS sample with thermal oxide on both sides and aluminum contacts (S9).

6.5.2. Experimental Setup

Fig. 6.9. Impedance Spectroscopy tool set-up.

Courtesy: Dr. R. Richert’s Lab in ASU

Details of the sample holder

Solartron 1260
The measurements were carried out using a Solartron 1260 Impedance Analyzer. Figure 6.9 shows the instrument set-up for impedance spectroscopy, (a) the equipment rack, (b) Solartron 1260 instrument, (c) the details of the sample holder with connections for input and output port for the Solartron 1260 through the 3 tubes, and two circular 2 cm diameter brass plates to hold the sample as shown in the close-up view in Fig. 6.9(c). Before each measurement, the Solartron 1260 was calibrated using a standard Teflon film as per the estimated total device capacitance. This calibration data were used to remove the error due to measurement system parasitic resistances and capacitances from the measured data to get the actual device characteristics. A very low ac voltage between 5 mV to 25 mV was used for impedance measurement, so that the measurement is done in the linear region of current-voltage characteristics.

The various devices types used are mentioned in the previous section 6.5.1. Different sample cleaning methods were used to check the effect on measurement, samples S4, S5, and S6 of section 6.5.1 were cleaned using Piranha etch (3:1 ratio of sulphuric acid (H$_2$SO$_4$) and hydrogen peroxide (H$_2$O$_2$)), samples S7, S8, and S9 of section 6.5.1 were cleaned with RCA1 (5:1:1 ratio of water, ammonium hydroxide (NH$_4$OH), and hydrogen peroxide (H$_2$O$_2$)) and RCA2 (6:1:1 ratio of water, hydrochloric acid (HCL), and hydrogen peroxide (H$_2$O$_2$)) cleaning method. The samples were 2.5cm x 2.5cm and 3cm x 3cm pieces cleaved from the original wafer with $\approx$ 1 k$\Omega$.cm resistivity.

The PMMA and polystyrene thin films were coated using a spinner, PMMA film was hard baked at 170°C for 15 mins and the polystyrene sample was soft
baked at 60°C for 2 minutes, then both were vacuum dried for 12 hrs to remove solvent before the metal contact deposition. The process details for each polymer film used in spin coating of various samples are mentioned in table 6.5. 300 nm thick metal contacts (aluminum or gold) were deposited using Lesker e-beam evaporator. The PMMA and polystyrene coated samples were not annealed after metal deposition, but the Schottky contact sample and the gate oxide samples were annealed at 400°C for 30 min in forming gas ambient. No mask was used for contact formation, a simple process using brown tapes at all sides of the sample was used to make the 2cm x 2cm square metal contacts, see Fig 6.10 for samples.

Table 6.5 Summary PMMA/polystyrene coated sample details.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Solution</th>
<th>Spin Speed / Time</th>
<th>Film Thickness (nm)</th>
<th>Metal Contact</th>
<th>Contact Area (cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S4</td>
<td>4% PMMA in anisole</td>
<td>4500 rpm / 30sec</td>
<td>200</td>
<td>Gold</td>
<td>2.66</td>
</tr>
<tr>
<td>S5</td>
<td>4% polystyrene in toluene</td>
<td>4500 rpm / 30sec</td>
<td>334</td>
<td>Gold</td>
<td>3.42</td>
</tr>
<tr>
<td>S6</td>
<td>4% polystyrene in toluene</td>
<td>4500 rpm / 30sec</td>
<td>380</td>
<td>Gold</td>
<td>2.89</td>
</tr>
<tr>
<td>S7</td>
<td>6% PMMA in anisole</td>
<td>3500 rpm / 40sec</td>
<td>600</td>
<td>Aluminum</td>
<td>4.0</td>
</tr>
</tbody>
</table>
6.5.3. Impedance Spectroscopy – Bare HRS without Any Contacts

The first experiment was to try the easiest option that is to put the 2cm x 2cm piece of HRS wafer between the two metal plates of the sample holder. This forms two Schottky contacts on both sides of the wafer and can be represent by a series arrangement of 3 parallel RC circuits $R_{\text{dep1}}C_{\text{dep1}} - R_{\text{sub}}C_{\text{sub}} - R_{\text{dep2}}C_{\text{dep2}}$ as shown in Fig. 6.11(a) and the fitting mathematical model is given by the impedance transfer function $Z(s)$ in Eqn. 6.2, where $R_{\text{dep1}}C_{\text{dep1}}$ = parallel combination of resistance and capacitance of the depletion layer due to the top Schottky contact, $R_{\text{sub}}C_{\text{sub}}$ = parallel combination of substrate resistance and capacitance, and $R_{\text{dep2}}C_{\text{dep2}}$ = parallel combination of resistance and capacitance of depletion layer due to the bottom Schottky contact. The mathematical model was curve fitted to the experimental data using MEISP and MATLAB software using CNLS algorithm, the fitted results are shown in Fig 6.11(b). After curve fitting, the modeled parameters are $R_{\text{dep1}} = 8.75 \times 10^5 \ \Omega$, $C_{\text{dep1}} = 3.42 \times 10^{-10} \ \text{F}$, $R_{\text{sub}} = 2.44 \times 10^3 \ \Omega$, $C_{\text{sub}} = 2.46 \times 10^{-10} \ \text{F}$, $R_{\text{dep2}} = 4.88 \times 10^6 \ \Omega$, $C_{\text{dep2}} = 6.75 \times 10^{-10} \ \text{F}$. 

Fig. 6.10. HRS substrates (a) gold contact, and (b) aluminum contact.
Using Eqn. 6.1, for $R_{\text{sub}} = 2.44 \, \text{k}\Omega$, thickness = 741 $\mu\text{m}$, and Area = $3.14\text{cm}^2 \Rightarrow$ substrate resistivity $\rho_{\text{sub}} = 103 \, \text{k}\Omega\cdot\text{cm}$. This is a very high value compared to the expected value of around $1 \, \text{k}\Omega\cdot\text{cm}$. The mechanical contacts do not form a uniform strong contact with the silicon and the contact resistance dominates, which is believed to affect the overall measurement. Hence, only mechanical contact on bare silicon is not suitable for resistivity extraction using Impedance Spectroscopy.

$$Z(s) = \frac{R_{\text{dep}1}}{1 + (R_{\text{dep}1}C_{\text{dep}1})s} + \frac{R_{\text{sub}}}{1 + (R_{\text{sub}}C_{\text{sub}})s} + \frac{R_{\text{dep}2}}{1 + (R_{\text{dep}2}C_{\text{dep}2})s} \quad (6.2)$$

Fig. 6.11. Impedance Spectroscopy: bare Si with mechanical probe contacts only. (a) Device structure and equivalent circuit, (b) curve fitting, measured and model.

6.5.4. Impedance Spectroscopy – HRS with Top Gate Oxide and Al Contact

The second experiment was based on a MOS capacitor structure with no bottom contacts. The devices had 900 $\mu\text{m}$ diameter aluminum gates on 112 nm
thick SiO$_2$ grown on the polished side of the wafer. Silver paste was used to contact the top gate and the back side to a sample holder having coaxial cable connections as shown in Fig 6.12(c). The approximate contact area is 0.196 cm$^2$ ($\approx$ 5 mm diameter silver paste). It can be represented by a series arrangement of $C_{ox}$-$R_{sub}C_{sub}$-$R_{dep}C_{dep}$ as shown in Fig. 6.12(a) and the fitting mathematical model is given by the impedance transfer function $Z(s)$ in Eqn. 6.3, where $C_{ox}$ = oxide capacitance of the top gate oxide, $R_{Sub}C_{Sub}$ = parallel combination of substrate resistance and capacitance, and $R_{dep}C_{dep}$ = parallel combination of resistance and capacitance of depletion layer due to the bottom Schottky contact (silver paste on silicon). The mathematical model was curve fitted to the experimental data using MEISP and MATLAB software using CNLS algorithm, the fitted results are shown in Fig 6.12(b). After curve fitting, the modeled parameters are $C_{ox}$ = 1.39x10$^{-9}$ F, $R_{sub}$ = 2.88x10$^3$ Ω, $C_{sub}$ = 3.25x10$^{-12}$ F, $R_{dep}$ = 6.57x10$^3$ Ω, $C_{dep}$ = 1.38x10$^{-10}$ F. Using Eqn. 6.1, for $R_{sub}$ = 2.88 kΩ, thickness = 760 µm, and Area = 0.196 cm$^2$ ⇒ substrate resistivity $\rho_{sub}$ = 7.52 kΩ.cm. Though this resistivity is high compared to the expected value of around 1 kΩ.cm, but it is not excessively high like the mechanical contacts.

This experiment showed that avoiding direct contacts to the substrate or making strong metal silicon contacts can yield better results. So it was decided to use a dielectric layer that can be formed without any thermal step, has uniform thickness without defects, and creates a strong bond with silicon. In subsequent experiments, proper contact formation was the main focus.
Fig. 6.12. Impedance Spectroscopy – Si sample with top gate oxide and Al contact and bottom silver paste contact. (a) Device structure and equivalent circuit, (b) curve fitting measured and model, (c) device in the sample holder.

6.5.5. Impedance Spectroscopy – Bare HRS with Teflon Sheets on Both Sides

The next experiment was to use a dielectric layer between the silicon and the sample holder metal contacts, on both sides, to make a capacitive structure and
avoid the issues due to contact imperfections. So the easiest option was to use a thin Teflon sheet (100 µm) as a dielectric on both sides of the silicon sample. Figure 6.13 shows the device structure and the equivalent circuit in (a) and the impedance vs. frequency in (b). But the results were inconclusive, it was mainly dominated by the Teflon film as an insulator and no equivalent circuit could be properly fitted to the measured data.

![Teflon Film and Si Equivalent Circuit](image)

Fig. 6.13. Impedance Spectroscopy – Si sample with Teflon film as top and bottom gate dielectric and mechanical contacts. (a) Device structure and equivalent circuit, (b) impedance vs. frequency plot - inconclusive.

### 6.5.6. Impedance Spectroscopy – HRS with Polystyrene and PMMA Thin Films and Gold Contacts

In order to address the contact issue and avoid thermal oxide which may cause resistivity changes due to thermal donor formation as we studied earlier; a new approach using polymer film as dielectric was examined. Two types of devices
were fabricated, one with a thin film of PMMA or polystyrene on both top (smooth) and bottom (rough) surfaces of HRS substrate and another with the polymer film only on the top surface of the HRS substrate, as shown in the device schematic in Fig. 6.14. There were 3 samples used in this experiment: (a) 334 nm spin coated polystyrene film on both sides using 4% polystyrene solution in toluene, (b) 380 nm spin coated polystyrene film on smooth surface only using 4% polystyrene solution in toluene, and (c) 200 nm spin coated PMMA film on both sides using 6% PMMA in anisole. All samples had evaporated gold contacts on both sides. All film thicknesses were measured by ellipsometry.

Fig. 6.14 Device schematics with top and bottom polymer dielectrics and the corresponding fitted equivalent circuit.

Then the equivalent circuit and the mathematical model were derived using IS approach as shown in Fig. 6.14 and Eqn. 6.4, respectively. It was found that all three devices used in this experiment can be modeled as a series combination of $R_{contact}C_{TopGate}R_{sub}C_{sub}R_{film/dep}C_{film/dep}$. $R_{contact}$ = contact resistance, $C_{TopGate}$ = top gate capacitance, $R_{sub}C_{sub}$ = parallel combination of substrate resistance and
capacitance, and $R_{\text{film}}C_{\text{film}} = \text{parallel combination of leakage resistance and capacitance of bottom dielectric, if present}$, and $R_{\text{dep}}C_{\text{dep}} = \text{parallel combination of resistance and capacitance of depletion layer due to the bottom Schottky contact (Gold).}$ The mathematical model was curve fitted to the experimental data using MEISP and MATLAB software using CNLS algorithm, the fitted plots are shown in Fig 6.15(a, b, c). When the thin film (dielectric) is present on both sides of the HRS substrate, the extracted resistivity is 1.13 kΩ.cm for PMMA and 1.24 kΩ.cm for polystyrene, which is very close to the desired resistivity $\approx$ 1 kΩ.cm. But when the film is on the top surface only, the extracted resistivity is 2.03 kΩ.cm. It is believed, without the bottom dielectric the depletion layer due to the Schottky contact is in series with the substrate affects the results. The results are summarized along with the device cross sections in Fig. 6.15(d).

\[
Z(s) = R_{\text{Contact}} + \frac{1}{C_{\text{TopGate}}s} + \frac{R_{\text{sub}}}{1 + (R_{\text{sub}}C_{\text{sub}})s} + \frac{R_{\text{film/dep}}}{1 + (R_{\text{film/dep}}C_{\text{film/dep}})s} \quad \text{(6.4)}
\]
Fig. 6.15. (a, b, c) Resistivity extraction from IS using curve fitting for various dielectrics. (d) Device cross section with extracted Si resistivity.

6.5.7. Impedance Spectroscopy – HRS with PMMA Thick Films and Al Contacts on Both Sides

The next approach was to use a thicker polymer film and aluminum contact for resistivity extraction to see the effect of film thickness and different contact material types. A thicker PMMA film (600nm) using 6% PMMA in anisole was
spin coated on both top (smooth) and bottom (rough) surfaces of HRS substrate as shown in the device schematic in Fig. 6.16(a). The equivalent circuit and the mathematical model were derived using IS approach as shown in Fig. 6.16(a) and Eqn. 6.5, respectively. The device can be modeled as a series combination of $R_{\text{top}}C_{\text{top}}-R_{\text{sub}}-R_{\text{bot}}C_{\text{bot}}$. $R_{\text{top}}C_{\text{top}}$ = parallel combination of leakage resistance and capacitance of top PMMA film, $R_{\text{sub}}$ = substrate resistance, and $R_{\text{bot}}C_{\text{bot}}$ = parallel combination of leakage resistance and capacitance of bottom PMMA film. The substrate could have been modeled by a parallel RC circuit like previous cases but a resistive ($R_{\text{sub}}$) circuit gives a better matching between the experiment and the model. The mathematical model was curve fitted to the experimental data using MEISP and MATLAB software using CNLS algorithm, the fitted plots are shown in Fig 6.16(b). With a thicker film (dielectric) on both sides of the HRS substrate, the extracted substrate resistivity is 1.45 kΩ.cm, close to the previous values and the expected resistivity $\approx$ 1 kΩ.cm.

$$Z(s) = \frac{R_{\text{top}}}{1 + (R_{\text{top}}C_{\text{top}})s} + R_{\text{sub}} + \frac{R_{\text{bot}}}{1 + (R_{\text{bot}}C_{\text{bot}})s} \quad (6.5)$$
Fig. 6.16. Impedance Spectroscopy – HRS sample with thick PMMA film (600nm) on both sides and aluminum contacts. (a) Device structure and equivalent circuit, (b) curve fitting - measured and model.

6.5.8. Impedance Spectroscopy – HRS Sample with Only Al Contacts on Both Sides (Schottky Contacts)

It was discussed previously that the contact imperfection plays a major role in measurement difficulties, so to address that issue it was decided to make metal contacts by evaporating 300 nm aluminum on both surfaces of the HRS substrate as shown in the device schematic in Fig. 6.17(a). The contacts were annealed at 450°C in forming gas ambient for 30 minutes. The equivalent circuit and the mathematical model were derived using IS approach as shown in Fig. 6.17(a) and Eqn. 6.6, respectively. The device can be modeled as a series combination of $R_{top}C_{top}-R_{sub}-R_{bot}C_{bot}$. $R_{top}C_{top}$ and $R_{bot}C_{bot}$ = parallel combination of leakage resistance and capacitance of the top and bottom Schottky depletion layers respectively, $R_{sub}$ = substrate resistance. The mathematical model was curve fitted
to the experimental data using MEISP and MATLAB software using CNLS algorithm, the fitted plots are shown in Fig 6.17(b). The substrate could have been modeled by a parallel RC circuit like previous cases but only resistive ($R_{\text{sub}}$) circuit gives a better matching between the experiment and the model. With aluminum contacts on both sides of the HRS substrate, the extracted substrate resistivity $\rho_{\text{sub}} = 2.24 \ \text{k}\Omega\cdot\text{cm}$ higher than expected but similar to the results obtained by one side coated polystyrene structure in section 6.5.6. The high resistive depletion layers on both sides might be causing an increase in the measured substrate resistivity. So the suggestion is to avoid direct contact to the silicon surface and use a dielectric layer.

$$Z(s) = \frac{R_{\text{top}}}{1 + (R_{\text{top}} C_{\text{top}})s} + \frac{R_{\text{sub}}}{1 + (R_{\text{bot}} C_{\text{bot}})s}$$ (6.6)

Fig. 6.17. Impedance Spectroscopy – HRS sample with only aluminum contacts on both sides. (a) Device structure and equivalent circuit, (b) curve fitting - measured and model.
6.5.9. Impedance Spectroscopy – HRS with Thermal Oxide and Al Contacts on Both Sides

It was also decided to try a device with gate oxide on both sides of the HRS substrate for Impedance Spectroscopy as it is the best dielectric on silicon even though it involves high temperature steps which may affect HRS substrate due to thermal donors. Thermal oxide (47 nm) was grown on both sides of the HRS substrate and 300 nm aluminum contacts were evaporated on both sides as shown in the device schematic in Fig. 6.18 (a). The equivalent circuit and the mathematical model were derived using IS approach as shown in Fig. 6.18 (a) and Eqn. 6.7, respectively. The device can be modeled as a series combination of RC-$R_{\text{sub}}$. $RC = \text{parallel combination of leakage resistance and capacitance of top oxide layer}$, $R_{\text{sub}} = \text{substrate resistance}$. This particular model is different from previous models but it best fits the measurement for this structure in this experiment compared to an RC-R-RC or RC-RC-RC structures as used in previous models. The mathematical model was curve fitted to the experimental data using MEISP and MATLAB software using CNLS algorithm, the fitted plots are shown in Fig 6.18(b). With a gate oxide (dielectric) on both sides of the HRS substrate, the extracted substrate resistivity $\rho_{\text{sub}} = 1.46 \, \text{k}\Omega\cdot\text{cm}$, close to the expected value $\approx 1\, \text{k}\Omega\cdot\text{cm}$.

$$Z(s) = \frac{R}{1 + RCs} + R_{\text{sub}} \quad (6.7)$$
Fig. 6.18. Impedance Spectroscopy – HRS sample with thermal oxide (47nm) on both sides and aluminum contacts. (a) Device structure and equivalent circuit, (b) curve fitting - measured and model.

6.5.10. Impedance Spectroscopy - Summary of All Experiments

Impedance Spectroscopy analysis for all different device types are summarized in Fig 6.19 and Table 6.6. It shows, using a dielectric layer on both sides yields a more accurate result close to the expected value $\approx 1k\Omega.cm$.

Fig. 6.19. Summary of all Impedance Spectroscopy measurements.
Table 6.6 Summary of all Impedance Spectroscopy measurements.

<table>
<thead>
<tr>
<th>Device Type</th>
<th>Fitted Equivalent Circuit</th>
<th>Mathematical Model</th>
<th>Resistivity (kΩ.cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bare silicon and mechanical contacts both sides</td>
<td>RC-RC-RC</td>
<td></td>
<td>100</td>
</tr>
<tr>
<td>Oxide on top and silver paste contacts both sides</td>
<td>C-RC-RC</td>
<td></td>
<td>7</td>
</tr>
<tr>
<td>Teflon film and mechanical contacts both sides</td>
<td>Did not work</td>
<td>Not Available</td>
<td></td>
</tr>
<tr>
<td>PMMA film (200 nm) both sides and gold contacts</td>
<td>R-C-RC-RC</td>
<td></td>
<td>1.13</td>
</tr>
<tr>
<td>Polystyrene film (334 nm) both sides and gold contacts</td>
<td>R-C-RC-RC</td>
<td></td>
<td>1.24</td>
</tr>
<tr>
<td>Polystyrene film (380 nm) on top and gold contacts both sides</td>
<td>R-C</td>
<td></td>
<td>2.03</td>
</tr>
<tr>
<td>PMMA film (600 nm) both sides and aluminum contacts</td>
<td>RC-R-RC</td>
<td></td>
<td>1.45</td>
</tr>
<tr>
<td>Bare silicon and aluminum contacts both sides</td>
<td>RC-R-RC</td>
<td></td>
<td>2.24</td>
</tr>
<tr>
<td>Oxide both sides (47nm) and aluminum contacts</td>
<td>RC-R</td>
<td></td>
<td>1.46</td>
</tr>
</tbody>
</table>
6.6. Conclusion

In this chapter, various commonly used resistivity measurement techniques such as four-point probe, Hall measurement method, C-V characterization technique were used to measure the resistivity of high-resistive silicon and it was shown that it is very difficult to measure the resistivity of HRS wafers using these techniques. The measured resistivity differed for each technique. The Schottky nature of the contact was found to pose a major challenge in these measurements.

A novel resistivity measurement technique based on Impedance Spectroscopy was proposed, which provided a more accurate result close to the expected value. Various device structures were used during IS and it was found that measurement using a mechanical contact to the substrate is not suitable. Evaporated aluminum contacts on both sides work better but the measurement is not completely accurate due to the Schottky nature of the contacts. Using a dielectric such as a thermal oxide or a polymer on both sides of the HRS substrate provides a more accurate result close to the expected value. It was shown that HRS substrate with spin-coated polymer film such as polystyrene and PMMA along with aluminum or gold contacts on both sides can be used as an effective test structure to extract resistivity using IS. Using the dielectric layer only on one side of the substrate does not yield accurate result. The polymer films avoid any thermal steps thereby reducing the possibility of thermal donor creation in HRS wafers which are known to change the polarity and resistivity of low doped p-type substrates. This novel technique is simple, uses regular capacitive structure and entails very simple and minimal processing. The samples and the contacts can be larger,
covering most of the sample area, unlike the Hall measurement method. So this Impedance Spectroscopy based approach using polymer films can be used for resistivity measurement as it takes into account the contact effects and other device related anomalies and avoids thermal donor creations steps.
CHAPTER 7. CONCLUSION AND FUTURE WORK

7.1. Conclusion

High-resistivity silicon wafers are gaining importance in the modern era of mobile technology and high-performance system-on-chip circuits due to their ability to lower the coupling between devices and provide low-loss substrates for high speed and system integration. This research is focused on the characterization of high-resistivity bulk and SOI wafers to understand the C-V behavior of these wafers, understand the coupling reduction abilities, and to explore various ways to measure the resistivity of these wafers.

The C-V characteristics of HRSOI were studied in detail by experiments and simulation with a metal contact directly on the film. Various factors affecting the C-V characteristics were studied: frequency, size of the top film contact, effect of the contact size and the substrate size, film thickness, film and substrate doping concentrations, carrier lifetimes, contact work-function, and type of film contact i.e., Schottky or Ohmic, radiation, light, temperature and annealing. The doping type of HRSOI substrate can undergo a reversal from p- to n-type at low substrate doping concentration due to the formation of oxygen thermal donors after annealing. The C-V plots showed spreading of capacitance following an “S” shape at a particular bias mostly where the capacitance changes from a value proportional to the contact area to a value 5 to 10 times larger. The spreading is mainly due to the floating body and the contact being directly on the film, and the RC transmission line behavior of the film/BOX/substrate interface. The capacitance spreading is not observed when there is a gate oxide on the silicon
film. This shape of the C-V plot is mainly due to the Schottky contact and its work-function. The RC transmission line behavior of the film and the substrate plays a significant role in the bias spreading and the shape of the C-V characteristic. At higher frequencies the ac signal flows very close to the contact due to the low-pass filter nature of the RC circuit and spreads less into the other part of the film giving smaller capacitances than at a lower frequency.

Substrate coupling in high-resistivity SOI substrates was studied and the effects of various factors such as: substrate resistivity, separation between devices, buried oxide (BOX) thickness, radiation, temperature, annealing, and light on crosstalk was studied using both experiments and simulations. Both experiments and simulations showed that cross talk reduces as substrate resistivity increases. HRSOI has better substrate coupling prevention capability than LRSOI substrates but in HRSOI wafers crosstalk did not reduce significantly beyond a certain resistivity.

A new approach to reduce crosstalk has been proposed, which uses air gaps at the BOX/substrate interface to reduce crosstalk. Larger air gaps are more effective in reducing crosstalk than smaller ones located only below the noisy and the sensitive devices. Impact of air gap in reducing crosstalk is more prominent in LRSOI than HRSOI. Another approach is to use a porous layer at the BOX-substrate interface which can lower the coupling.

Owing to their very low doping concentrations and the presence of oxygen in CZ wafers, HRS wafers pose a challenge in resistivity measurement using the conventional techniques such as: four-point probe and Hall measurement. It was
shown with measurement that it is difficult to measure the resistivity of HRS wafers accurately and repeatedly using the commonly used resistivity measurement methods such as four-point probe, Hall measurement, capacitance-voltage methods. A novel resistivity measurement technique based on Impedance Spectroscopy was proposed and implemented, which provides a more accurate result close to the expected value. Various device structures were used during IS and it was found that measurement using a mechanical contact to the substrate is not suitable. Evaporated aluminum contacts on both sides work better but the measurement is not completely accurate due to the Schottky nature of the contacts. Using a dielectric such as a thermal oxide or a polymer on both sides of the HRS substrate provided a more accurate result close to the expected value. It was shown that HRS substrate with spin-coated polymer film such as polystyrene and PMMA along with aluminum or gold contacts on both sides can be used as effective test structure to extract resistivity using IS. Using the film on only one side of the substrate does not yield accurate results. These polymer films avoid any thermal steps thereby reducing the possibility of thermal donor creation in HRS wafer which are known to change the polarity and resistivity of low-doped p-type substrates. This novel technique is simple, uses regular capacitive structure and entails very simple minimal processing. So this Impedance Spectroscopy based approach using polymer films can be used for resistivity measurement as it takes into account the contact effects and other device related effects.
7.2. Future Work

The suggested crosstalk minimization technique using airgap below the BOX can be experimentally implemented. The proposed Impedance spectroscopy approach using polymer dielectrics can be further verified and refined to make it an industry applicable product using HRS samples with various substrate resistivities.
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