Schottky Power Diodes Designed for Improved Breakdown Characteristics

A thesis submitted in fulfilment of the requirements for the degree of Doctor of Philosophy

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Declaration

I certify that except where due acknowledgement has been made, the work is that of the author alone; the work has not been submitted previously, in whole or in part, to qualify for any other academic award; the content of the thesis is the result of work which has been carried out since the official commencement date of the approved research program; any editorial work, paid or unpaid, carried out by a third party is acknowledged; and, ethics procedures and guidelines have been followed.

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Abstract

Silicon carbide (SiC) is a semiconductor material sold as substrates (like silicon is) for making semiconductor devices. It has advantages (compared to other semiconductors like silicon) regarding making devices that operate at high temperature, high electric fields and high current density.

Overall, the semiconductor industry continues to expand and SiC products are a growing part of this. In 2016, global semiconductor sales reached nearly US$340 billion (the highest ever) according to The Semiconductor Industry Association (SIA). Market growth is driven by the ever-increasing amount of semiconductor technology in devices the world depends on for working (as reported by SIA). Power electronic components such as semiconductor SiC power diodes used in cars for example are among the numerous areas where improvements in performance are continually sought. ‘Increasing electrification in vehicles generally – and in hybrid and electric vehicles specifically is energizing the market for power semiconductors in vehicles’ (IHS Markit report). The HIS report shows that the total market for power semiconductors (including discrete SiC power diodes) will increase from US$5.5 billion in 2016 to more than US$8.5 billion in 2022. An increasing trend towards electric cars in the coming years is expected to drive the demand for electronic components made from suitable semiconductor materials, including SiC. The advantage of SiC semiconductor chips is that they have high-reliability in harsh environments like the environment of the drive train of vehicles which includes the engine and connected components to deliver power to the wheels of vehicles. Moreover, the car industry is just one area where improvements in power semiconductor devices are sought. Anywhere where there is control, or high transmission voltage and current and voltage conversion, will benefit from improvement in diode performance. Two important aspects of Schottky diode performance are how much current it can deliver when in the forward bias mode and how much voltage it can withstand when in current blocking mode. Too much current (forward bias) or too much voltage (typically a reverse bias consideration) across the diode will cause it to break down.
Considering the value of the power semiconductor device market, the industry push for performance, and the possibilities that improvements in SiC materials bring to semiconductor research, SiC Schottky diodes (also called Schottky Barrier Diodes, SBD) were investigated to determine the influence of several factors that affect device performance. Minimising the loss of energy and maximising the possible delivered electric current and also blocking voltage capability by improving SiC Schottky diode electrical performance is an important area of semiconductor research and of value to industry. Breakdown in the forward and reverse bias modes will be the focus of this research but the other aspects will also be reported on too. For example, high forward current is desired but if it comes at the expense of high forward voltage then there will be high power loss in the diode which should ideally act as a switch with no power loss. Similarly, a high reverse bias is desired but if leakage current (reverse bias current) is high then again there is power loss.

This study uses finite element modelling and experimental investigation of different metals for forming improved Schottky contacts. Contact geometry and electrode edge isolation techniques are investigated to optimise designs. Schottky contact geometry is optimised in order to minimise the incidents of maximum current density within the diode structure, where breakdown occurs. Surface preparation and surface treatment prior to Schottky formation and in particular the surface treatments used to give a carbon-rich SiC surface, which in this research has been found to reduce the turn-on voltage of SiC Schottky diodes, is also investigated. Optimised geometry and electrode edge isolation improvements are demonstrated using silicon substrates and this improvement can be applied to any metal-to-semiconductor combination. A diode requires an Ohmic contact and this is also studied here with the approach of using selective etching to prepare the SiC surface. SiC diodes were fabricated and used for electrical testing to determine the electrical characteristics. Moreover, the effects of the quality of the SiC itself on the breakdown voltage was investigated (the major qualifier for crystal quality is the value of the density of the defect known as a micropipe and this value is called MPD (for micropipe density) and given in SiC wafer specifications from suppliers.
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Chapter 1 – Introduction

The properties of silicon carbide (SiC) make it particularly attractive for switched power electronic energy conversion, including, in particular, a wide bandgap, which allows operation at up to 10kV \(^1\) and junction temperatures in excess of 400°C. For these reasons, SiC devices are seen as the enabling technology for future energy conversion systems for a wide range of applications which cover diverse fields. These range from military to civilian industries \(\text{[2]}\) such as the development of high voltage, high frequency (HV-HF) power devices which extend the use of switch-mode power conversion to high voltage applications (e.g. power grid) and development in More Electric Aircraft (MEA) which involves removal of the need for on-engine hydraulic power generation, bleed air off-take and the deployment of power electronics in the starter/generation system of the main engine \(\text{[2, 3]}\). Furthermore, the development of Schottky power diodes based on SiC promises also to revolutionise the automobile industry such as the new type of automotive vehicles (e.g. hybrid and electric), grid-connected systems at distribution levels (up to 22kV) and high power density applications such as photovoltaic (PV) applications in aerospace systems \(\text{[2]}\) for harnessing solar energy \(\text{[4]}\).

The fabrication of Schottky power diodes in SiC is relatively straightforward. Bosch fabricates tens of thousands of silicon Schottky diodes for use in alternators. The use of Schottky diodes in cars is a good example of use in a high temperature environment where the SiC Schottky diode has been established as more reliable compared with the silicon-based Schottky diode \(\text{[5]}\). It is feasible to have an Australian SiC Schottky diode fabrication facility as the fabrication steps are few and capital costs for equipment are low.

At the moment, except for Griffith University where significant SiC development has been undertaken for more than 20 years, Australian researchers are limited when it comes to accessing prototype SiC devices. International companies that have developed power SiC devices include Global Power, ABB, Rohm, Siced (a joint venture between Infineon and Siemens) and Cree, Inc. These companies have laboratories in Europe and North America.
1.2 Schottky Diode

The Schottky diode has been available since the early twentieth century. It operates on the principle of utilising a metal semiconductor barrier to produce devices with a rectification of current [6]. A Schottky diode has a simple structure and is often used in power electronic applications. The structure of a Schottky diode has three components which are the Ohmic contact, the semiconductor substrate (in this case it is SiC) and the Schottky electrode. The arrangement of these three components is illustrated by Figs 1.1a, 1.1b and 1.1c.

As Fig. 1.1c shows, the structure of the diode is simple. When in operation the current will travel from the Ohmic contact through the substrate and reach the Schottky contact as illustrated by Fig.1.2.
Since the current flow will concentrate at the Schottky contact, the current density will be at the electrode’s surface and also at the edge (where the Schottky electrode meets the surface of the substrate), as in Fig.1.2. Hence, if the current density reaches a critical level which the materials of the Schottky electrode cannot withstand, the electrode will be destroyed and as a result, the diode will be destroyed with it. In summary, the Schottky electrode is an important component which will control the performance of the diode. The ideal Schottky electrode needs to be able to withstand as many cycles of current and last as long as possible in order for the diode to operate to the maximum capability.

The simple structure of Schottky diode also raises issues such as the magnitude of leakage current and breakdown effect as produced by the high electric field at the edges of the electrode. Normally, to reduce this effect, a diffused guard ring is formed around the perimeter of the Schottky contact.

Fig. 1.2. The direction of flow of current when the diode is in operation
Fig. 1.3. Diffusion guard ring to reduce effect of high electric field at edge of Schottky electrode

In fabricating the Schottky diode, it is important that the surface is clean in order to give intimate contact with the metal. The advantage of the Schottky diode is that due to its structure, it only needs low temperature processing for fabrication. In this way, high temperature processes such as impurity diffusion and impurity activation after ion-implantation can be avoided in the fabrication process [7].

1.3 Silicon Carbide (SiC)

Overall, the semiconductor industry continues to grow and SiC products are a part of this. In 2016, the global sales of semiconductors reached nearly USD$340 billion (the highest ever) according to the Semiconductor Industry Association (SIA). Market growth is driven by the ever-increasing application of semiconductor technology in devices the world depends on (as reported by SIA). Power electronic components such as semiconductor SiC power diodes used in cars, for example, are among the numerous areas where improvements in performance are continually sought. “Increasing electrification in vehicles generally – and in hybrid and electric vehicles specifically is energizing the market for power semiconductors in vehicles” (IHS market report). The IHS report shows that the total market for power semiconductors (including discrete SiC power diodes) will increase from USD$5.5 billion in 2016 to more than USD$8.5 billion in 2022. An increasing trend towards electric cars in the coming years is expected to drive the demand for electronic components made from suitable semiconductors.
SiC belongs to the IV-IV stable group of compound semiconductors. There are many polytypes of SiC. These include 3C-SiC, 6H-SiC, 4H-SiC and 2H-SiC, which are the ones most commonly used for devices. SiC has identical two-dimensional hexagonal layers which can form different types of SiC via different stacking sequences of the layers [6]. Fig. 1.4 illustrates the different stacking arrangements for 3C-SiC, 2H-SiC, 4H-SiC and 6H-SiC.

![Fig. 1.4. The stacking sequence of ABC with different types of SiC (adapted from [6])](image)

Fig. 1.4 shows a pattern by which we can identify whether the SiC material is of 3C (ABC), 2H (AB), 4H (ABCB) or 6H (ABCACB). Since two-dimensional SiC layers can form many different crystal structures just by different stacking of layers, it is also considered as being one-dimensional. Also, the crystal structure of SiC polytypes, such as the stacking of SiC bi-layers, has a strong influence on the physical and electrical properties of different SiC polytypes [8].
Table 1.1. Comparison of mechanical properties of three polytypes of SiC

<table>
<thead>
<tr>
<th></th>
<th>3C-SiC</th>
<th>4H-SiC</th>
<th>6H-SiC</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Bandgap [eV]</strong></td>
<td>2.390</td>
<td>3.265</td>
<td>3.023</td>
</tr>
<tr>
<td><strong>Lattice Constant [Å]</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>a</td>
<td>1.36</td>
<td>3.08</td>
<td>3.08</td>
</tr>
<tr>
<td>c</td>
<td></td>
<td>10.05</td>
<td>15.12</td>
</tr>
</tbody>
</table>
| **Effective Mass [m]

<table>
<thead>
<tr>
<th></th>
<th>3C-SiC</th>
<th>4H-SiC</th>
<th>6H-SiC</th>
</tr>
</thead>
<tbody>
<tr>
<td>m_e</td>
<td>0.68 – 0.25</td>
<td>0.37</td>
<td>0.69</td>
</tr>
<tr>
<td>m_h</td>
<td></td>
<td>0.94</td>
<td>0.92</td>
</tr>
<tr>
<td><strong>Mobility(@300K) [cm²/Vs]</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>μ_e</td>
<td>900</td>
<td>500</td>
<td>300</td>
</tr>
<tr>
<td>μ_h</td>
<td>20</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td><strong>Thermal conductivity (RT) [W/cm-K]</strong></td>
<td>3.0 – 3.8</td>
<td>3.0 – 3.8</td>
<td>3.0 – 3.8</td>
</tr>
</tbody>
</table>

Even though SiC is an important material for fabricating power devices due to its intrinsic properties as compared to silicon [9], not every polytype of SiC is well suited for the fabrication of power devices. According to Baliga, et al., 4H-SiC is superior compared to other polytypes of SiC. Hence, 4H-SiC is now the main material for fabrication of power devices and it is expected that it will remain so for a long time [10]. Due to its physical properties, 4H-SiC has superior electrical characteristics compared with traditional silicon material. Fig. 1.5 compares important properties of silicon with 4H-SiC. Silicon carbide has recently become available through the Cree Company as 150 nm wafers with a high quality layer of 4H n-type. It has advantages (compared to other semiconductors like silicon) when making devices that operate at high temperatures, high electric fields and high current density.
Table 1.2. Comparison of properties of silicon and 4H-SiC [6]

<table>
<thead>
<tr>
<th>Properties</th>
<th>Silicon</th>
<th>4H-SiC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy Band Gap (eV)</td>
<td>1.11</td>
<td>3.26</td>
</tr>
<tr>
<td>Relative Dielectric Constant</td>
<td>11.7</td>
<td>9.7</td>
</tr>
<tr>
<td>Thermal Conductivity (W/cm-K)</td>
<td>1.5</td>
<td>3.7</td>
</tr>
<tr>
<td>Electron Affinity (eV)</td>
<td>4.05</td>
<td>3.7</td>
</tr>
<tr>
<td>Density of States Conduction Band (cm⁻³)</td>
<td>$2.80 \times 10^{19}$</td>
<td>$1.23 \times 10^{19}$</td>
</tr>
<tr>
<td>Density of States Valence Band (cm⁻³)</td>
<td>$1.04 \times 10^{19}$</td>
<td>$4.58 \times 10^{19}$</td>
</tr>
</tbody>
</table>
In Table 1.2 above, the energy bandgap for 4H-SiC is approximately three times larger than silicon, which means that there is lower intrinsic carrier concentration at any temperature with 4H-SiC and a much smaller impact ionisation coefficient \( C \) at any given electric field in comparison to silicon. Also, the thermal conductivity for 4H-SiC is two times higher than for silicon, hence the device which uses 4H-SiC will have better performance in harsh environments such as extremely high temperatures, high pressure, higher dose of radiation and high toxic chemical exposure than devices fabricated with silicon.

![Graph showing breakdown voltage vs. doping concentration for Si and 4H-SiC](image1)

*Fig. 1.5. The breakdown voltage for Si and 4H-SiC (Adapted from Baliga [9])*

![Graph showing critical electric field for breakdown vs. doping concentration for Si and 4H-SiC](image2)

*Fig. 1.6. The critical electrical field for breakdown of Si and 4H-SiC (Adapted from Baliga [9])*
Figs 1.5 and 1.6 show that there is plenty of room for development of a power Schottky diode when lowering the doping of the 4H-SiC substrate. For example, if we lower the doping to the value of $10^{15}$ cm$^{-3}$, the theoretical breakdown voltage is around 10,000 volts: in comparison with the current product that the industry is producing which obtains around 1,700 volts (Cree / Wolfspeed) [11]. Also, the breakdown voltage can be increased by reducing the level of doping. The important factor is that 4H-SiC has very high potential for improving the performance of the power Schottky diode but is unable to reach even one fifth of its breakdown capability.

The quality of the 4H-SiC material is of critical importance to breakdown voltage. Structural defects within the substrate include micropipes, dislocations, low-angle boundaries, voids, thermal decomposition cavities, misoriented grains and stacking faults. [12]. The critical parameter that leads to diode destruction during operation and needs serious consideration is the micropipe density (MPD) within the SiC substrate. The unit of micropipe density is micropipes / cm$^2$.

![Fig. 1.7. (a) 2D illustration of micropipes inside a SiC substrate (adapted from information in [12]), (b) X-TEM showing a micropipe [12]](image)
Fig. 1.8. Micropipes are distributed inside a SiC substrate as illustrated in this 3D schematic (adapted from information in [12]). However, the units of MPD are per unit area because of techniques that are used to determine MPD at a substrate’s surface.

Two types of bulk N-type SiC substrates are currently manufactured for commercial use. These are the substrates used (i) in the production of devices and (ii) for research purposes; both having a diameter ranging from 76.2 mm to 150 mm. The thickness options for both types range from 350µm (+/-25µm) to 500µm (+/-25µm) with the exception of the research substrate which can have a thickness of 5350µm (+/-25µm) in combination with a diameter of 150µm [13].

If the active area of the power diode is located exactly where the micropipes exist, the diode will be destroyed, hence with it will never reach it supposed potential as designed. According to Holland et al., it is important to know which factor is more dominant: that of the level of defects in the material or the doping of the substrate but defects are certainly detrimental to the Schottky diode reverse bias operation [14].

1.4 Forward and Reverse Bias with Implication for the Performance of the Schottky Diode

Two parameters are associated with the performance of the Schottky power diode. They are the forward and the reverse biases. An ideal diode would operate at maximum current for an indefinite period without breakdown. Fig. 1.9 illustrates the ideal I-V curve.
However, due to many factors, the I-V characteristic in real life is very different from the ideal I-V. Realistically, the diode’s performance will be affected by both forward and reverse breakdown and it cannot keep going indefinitely as in an ideal scenario. Fig. 1.10 illustrates a realistic I-V curve.

As Fig. 1.11 illustrates, there are many factors that need to be improved in order to improve the overall performance of the power Schottky diode.
1.5 Thesis Outline

This thesis initially discusses the background information and the current state of the art of the power Schottky diode as well as of the SiC materials. Further, finite element modelling (FEM) for determining diode geometry for optimum performance (for maximum current input versus breakdown capability); an alternative to guard-ring doping design for improving Schottky diode capability which includes FEM which simulate the laser ablation technique to enhance breakdown; materials analysis of surface treatment; and the carbon-rich surface for 4H-SiC including XPS, and Raman, are all discussed in detail. Experimental electrical characterisation which includes the I-V results, the relationship between SiC defects versus electrode design (including Ni contacts, MDP effect, and different Schottky metals) are also reported.

Chapter 2 provides a literature review which includes background information and the current state of the art of the power Schottky diode and SiC materials.
Chapter 3 discusses in detail, the use of finite element modelling (FEM) in determining the diode geometry for optimum performance, i.e. for maximum current input versus breakdown capability.

Chapter 4 discusses in detail, an alternative to guard-ring doping design for improving Schottky diode capability. FEM has been used to simulate a technique of laser ablation to enhance breakdown of the diode.

Chapter 5 presents experimental data on electrical characterisation of diodes which includes current–voltage measurements versus electrode design. Chapter 5 also contains an analysis by techniques including XPS and Raman spectroscopy of the surface treatment of 4H-SiC to form a carbon-rich surface. Chapter 5 also, looks at the relationship between micropipe defects in SiC versus electrode design (including Ni contacts, MPD effect, and different Schottky metals).

Chapter 6 summarises the results of this thesis and provides a recommendation for extending the research in the future.

Appendices

1.6 Original Scientific Contribution

1.6.1 Finding the optimum Schottky electrode geometry which enables the Schottky diode to deliver a higher current and have a lower turn-on voltage as well as larger breakdown voltage.

1.6.2 Establishing a fabrication process that produces Schottky diodes that can deliver high current with much longer time to breakdown. This was due to low MPD and surface preparation prior to Schottky metal deposition.

1.6.3 Finding the alternative to doping for forming a guard ring for the Schottky electrode. The trench guard ring is easier and quicker to fabricate, and bigger variation is possible.

1.6.4 Creating a carbon-rich surface for 4H-SiC to have better surface to contact quality which leads to better current–voltage performance and better reliability.
Chapter 2 – Literature Review

2.1 The Advantage of Silicon Carbide Versus Silicon and its Use in Schottky Power Diodes

2.1.1 Silicon carbide versus silicon
For many decades, silicon has been the main material used in power electronic semiconductor devices [1, 15]. However, due to its intrinsic properties, silicon (Si) cannot operate at high temperatures while maintaining high blocking voltage and rectification ratios. These shortcomings have been addressed through the use of silicon carbide (SiC) instead of Si. SiC has intrinsic properties which give it substantial advantages over Si for use in situations of high temperature, high power, high radiation and fast switching electronics [3, 15-19]. Moreover, SiC has advantages when being used to make system components for harsh environmental Microsystems. Hard-wearing micro-electro-mechanical-systems (MEMS) structures can be fabricated with all types of SiC such as single-crystalline, poly-crystalline and amorphous [20]. Recently, there has been significant study into incorporating SiC into the high power Schottky diode, because SiC Schottky diodes can be used at high voltage and high temperature without altering their electrical properties and, moreover, they can be operated at higher switching speeds compared to Si diodes [15, 16, 21-23].

2.1.2 Aspects for improving Schottky power diode performance
There have been many studies into how to improve a SiC Schottky diode’s performance. Those finding are summarised in the following paragraphs.

Schottky barrier height (SBH) is a fundamental quantity used to characterise metal-semiconductor contacts [16], and researchers have used it as a focal point for summarising Schottky contact studies [3, 16, 17, 24]. Apart from studying metal semiconductor Schottky contacts, researchers also study Ohmic contacts to SiC. (An Ohmic contact is essential to allow current in and out of the diode. It is the second contact in a Schottky diode). It is very difficult to form Ohmic contacts to p-type SiC materials through reducing the Schottky barrier height between the metal and SiC [3]. As a result, Cheung [3], proposed that instead of trying to reduce the barrier height,
we should try to reduce the barrier width via “high doping at the surface” to obtain an Ohmic contact to p-type SiC through the quantum mechanical effect of tunnelling. Also, according to Crofton et al. [25], p-type SiC with large bandgap forms a high Schottky barrier height (SBH) at its interface with a metal. Fig. 2.1 shows the typical energy band relationship between p-type SiC and metal. SiC has a high bandgap of 3.0 eV in combination with the value of electron affinity of 3.3 eV. Hence the correspondence with the position of the valence band is greater than 6 eV (away from the vacuum level) [26]. However, the work function of most metals is between 4 and 5.5 eV [26]. As a result, a high energy difference exists between the conducting carriers in the two materials (SiC and metal). The result is that a large SBH is formed at the interface of SiC. Pelletier et al. [26], found that p-type Ohmic contacts are not as well-developed or understood as n-type contacts. On the one hand, the large SBH that exists at the interface of metal-p-type SiC has resulted in the need for extremely heavy surface doping “since sufficient barrier lowering to enable Ohmic contact formation has not been achieved”. On the other hand, n-type SiC Ohmic contact has been developed with more success where specific contact resistances via doping can get to the value of $10^{-6} \, \Omega \, \text{cm}^2$ range [26]. The achievement is the result of the availability of high quality doped materials and is also due to the processes involving silicide formation which used metal such as Ni that appear to lower Schottky barrier heights at the metal-SiC interface [25].

Fig. 2.1. Energy band diagrams, as predicted from the Schottky-metal relationship, before and after contact, for a typical metal and p-type SiC. $E_F$ = Fermi level, $\phi_M$ = metal work function, $E_C$ = conduction band minimum, $E_V$ = valence band maximum, $E_g$ = bandgap, $\chi_S$ = electron affinity and $\phi_B$ = Schottky barrier height [3]
In a study by Ito, Tsukimoto and Murakami [27] on the realisation of “high performance Silicon Carbide (SiC) power devices”, an essential requirement was to develop “low-resistance Ohmic contacts to the p-type SiC”. Because reducing the barrier height to form an Ohmic contact is “extremely difficult” [27], they resorted to increasing the doping concentration of Al (p-type dopant) in 4H-SiC, by ion-implantation. After the experimentation, the researchers concluded that a low-resistance Ohmic contact “would be formed when there is a technique developed to eliminate the crystal defects formed in the 4H-SiC substrates after ion implantation” [27].

For n-type 4H-SiC, Baliga [9] was successful in fabricating an Ohmic contact by using a metal-semiconductor contact with low barrier height and a high doping concentration in the semiconductor to promote tunnelling current across the contact. For the metal-semiconductor contacts with high doping concentration level, the contact resistance ($R_c$) is determined by the barrier height and the doping level [9] using the equation

$$R_c = \exp \left( \frac{2 \varepsilon_\text{e} m}{h} \left( \frac{\phi_{\text{bn}}}{\sqrt{N_D}} \right) \right)$$

(2.1)

$h$: Planck constant

$\varepsilon_\text{e}$: Permittivity

$m$: Effective mass of electron (kg)

$N_D$: Doping level (cm$^{-3}$)

$\phi_{\text{bn}}$: Barrier height (eV)

Furthermore, Baliga [9], recommended that to take full advantage of the low on-resistance of the drift region in SiC devices, it is necessary to obtain a “specific contact resistance that is several orders of magnitude smaller than that of the drift region” [9]. According to the study, specific contact resistances of less than $1 \times 10^{-5}$ ohm-cm$^{-2}$ are desirable for n-type regions. Fig. 2.2 shows the relationship between specific contact resistance versus doping at metal-semiconductor contacts.
Baliga [9], has concluded that the specific contact resistance of $1 \times 10^{-5}$ W.cm$^2$ can be obtained with a doping concentration of $5 \times 10^{19}$ cm$^{-3}$, providing the barrier height is 0.6 eV. Also, high concentration doping can be achieved for the surface for n-type 4H-SiC by using “hot-implantation of nitrogen, phosphorous or arsenic followed by appropriate high temperature annealing”. This has confirmed that an Ohmic contact with low specific resistances can be obtained. Baliga, et al. has proposed that nickel and titanium can be used for the formation of Schottky barriers to 4H-SiC [9]. Deposited carbon or carbon-rich SiC surfaces formed by selective etching of SiC, or heat treatment to remove Si; and heat treatment of spun-on polymer or carbon ion implantation have all been used to include carbon in the Schottky electrode structure. In this project, I will focus on selective etching of the 4H-SiC surface to leave it carbon rich. The degree of etching will be controlled and this effect on electrical properties will be investigated. Experimental results will be included in TCAD modelling which will allow more sophisticated design when combined with characterisation of the materials of actual Schottky diode structures.

Fig. 2.3 illustrates the relationship between intrinsic carrier concentration (cm$^{-3}$) and temperature (1/K).
The intrinsic carrier concentration will have a value of $\sim 10^{-9}$ cm$^{-3}$ when at room temperature. Intrinsic carrier concentration will increase with temperature up to approximately $10^7$ cm$^{-3}$ at 666 K. Based on the information in Fig. 2.4, Ohmic contacts to n-type 4H-SiC (where $E_F$ is closer to $E_C$ than $E_V$) are possible by having a doping level such that $E_F$ is equivalent to one of the metals on the right hand side. No metals are shown which have a work function suitable for p-type 4H-SiC (i.e. where $E_F$ is close to $E_V$).
The equation for \((E_F - E_i)\) for an n-type semiconductor is:

\[
E_F - E_i = kT \ln \left( \frac{n_{no}}{n_i} \right)
\]  

(2.2)

\(E_F\): The Fermi level of semiconductor

\(E_i\): The intrinsic energy level of semiconductor

\(k\): Boltzmann’s constant

\(T\): Temperature in K

\(n_{no}\): The equilibrium carrier (electron) concentration in the semiconductor

\(n_i\): The intrinsic (no doping) carrier concentration in the semiconductor

This is the well-known equation for the energy difference between a semiconductor’s Fermi level and its intrinsic (mid-gap level). For a highly doped n-type semiconductor, \(E_F\) will be close to the bottom of the conduction band level \(E_c\). In SiC, it is possible to choose a doping level so that the Fermi levels of the SiC and the metal (coloured position in Fig. 2.4) line up. This will give a small difference in work functions of both and hence a small turn-on voltage at very high doping leads to an Ohmic contact.

Baliga [28] has shown that breakdown voltage decreases with rise in doping concentration (Fig. 2.5). However, the critical electric field for breakdown versus
doping concentration has the opposite effect. The critical electric field for breakdown increases with increasing doping concentration is shown in Fig. 2.6.

![Fig. 2.5. Breakdown voltage versus doping concentration. Adapted from [28]](image)

![Fig. 2.6. Critical electric field for breakdown versus doping concentration. Adapted from [28]](image)

Fig. 2.6 shows that theoretically, there is plenty of ground for a development of a power Schottky diode when lowering the doping of 4H-SiC substrate. For example, for $10^{15}$ cm$^{-3}$, the theoretical breakdown voltage is into the range of $10^4$ V, while currently, industry only produces power diodes up to 1,700V [30] and more recently Global Power have produced a commercial 3,300V Schottky diode. With low doping, high breakdown can be obtained and with high doping, low turn-on voltage can be obtained but this will also lower the breakdown voltage.
A study by Holland et al. [14], on GaAs Schottky diodes suggests that breakdown voltage is significantly affected by semiconductor material defects. GaAs defects are quantified by the parameter known as etch pit density (EPD) and GaAs with the lowest EPD could withstand significantly higher electric fields in reverse bias Schottky diode testing compared to GaAs of similar resistivity but higher EPD. This example of the effects of defects (EPD) in GaAs on GaAs Schottky diodes is comparable to the effects micropipe defects in SiC on SiC Schottky diodes because both defects show a direct effect on the respective current-voltage characteristics of diodes made from these materials.

SiC has many polytypes (with different arrangements of the Si and C atoms for the same stoichiometry) [3]. Cheung [3], stated that there are three polytypes that are most common for SiC. They are listed below:

- 3C-SiC
- 4H-SiC
- 6H-SiC

Amongst these polytypes, 4H-SiC has been found as the most appropriate for SiC Schottky power diode fabrication [9], because, with its higher vertical axis mobility, it is particularly suitable for vertical power devices [31]. Moreover, 4H-SiC’s larger bandgap, results in a much higher operating temperature and higher radiation hardness compared to other conventional materials [31]. 4H-SiC power diodes are available commercially [32] (e.g. from Wolfspeed – a Cree Company).

The significance of this study is that SiC has properties which are particularly attractive for switched power electronic energy conversion. With a wide bandgap, it allows operation at up to 10kV for junction temperatures in excess of 400°C [3, 32]. Also, SiC high power devices help enable future energy conversion systems: some examples for use being the automobile industry (hybrid and electric vehicles), grid-connected systems at the distribution level for the energy industry, in aerospace systems (power density application) and military applications [3].
The benefit of the silicon carbide Schottky diode lies in more efficient power handling than equivalent Si diodes as it provides more compact and efficient energy conversion technology with increase in power density.

2.2. Current State of the Art Design for Improving the Performance of Schottky Power Diodes

Over a period of time, many researchers have investigated methods to improve the performance of the Schottky power diode in terms of reducing leakage current, increasing breakdown voltage or reducing the damage to the Schottky electrode by reducing the electric field around the Schottky contact edge, etc. [23, 24-40]. Those designs started with simple improvements such as creating a metal field plate by overlapping Schottky metal over the oxide layer of the diode or using doping to make a guard ring or deploying a very complicated structure such as a merged pn / Schottky structure. These designs will be discussed in detail in the following sections.

2.2.1. Metal field plate over field oxide

Study [33] has shown that for Schottky diodes with high breakdown voltage, there is a requirement to have a termination around the edge of the Schottky electrode to reduce electric field crowding. Fig. 2.7 illustrates the design structure of the metal field plate. As reported by Saxena et al. [33], a Schottky diode was fabricated at Cincinnati with a simple metal field plate structure where the Schottky contact overlaps a thermally grown SiO\(_2\) layer (field oxide) to give the maximum electric field at any applied bias where \(E_{\text{max}}\) is at the SiO\(_2\)-metal interface. For this design, the lateral metal overlap on the oxide layer is equal to the thickness of the epitaxial layer of SiC [33]. Saxena et al. [33], reported that with this device structure, the breakdown voltage should “ideally not be affected by electric field crowding”.
Saxena et al. [33], showed that thermally grown oxide on SiC assists with surface passivation and helps with the removal of surface defects which are etched off after oxidation from the areas that are used to form a Schottky electrode.

The metal which is used to form the Schottky contact barrier plays an important role in determining the leakage current as well as the on-state voltage drop of a Schottky diode [9]. Since the power losses of a diode are dependent on temperature, the selection of the Schottky metal is based on the temperature of operation of the diodes. The on-resistance is low in forward bias; hence the majority of the voltage drop occurs across the metal-SiC Schottky barrier region [33]. This means the diodes that use metals which cause a larger Schottky barrier to SiC result, create a larger on-state voltage drop. For Schottky diodes that operate in a high temperature environment, those metals with larger Schottky barriers are still preferable since they provide lower leakage currents. In order for a Schottky diode to achieve a higher ON/OFF ratio, we should use metals that form larger Schottky barriers.

A static power-loss analysis for determining the optimum barrier height of the Schottky electrode, can be performed for rectifiers operating at a 50% duty cycle [34]. Hence, the maximum sum of the static power loss ($P_L$) dissipated during the on-state and off-state (per unit area) is provided by the following formula if the reverse current density adheres to the theoretical consideration provided by Itoh et al. [34]. The equation for
the maximum sum of static power loss ($P_L$) dissipated during the on-state and off-state per unit area was given as [41].

$$P_L = \frac{1}{2}(J_F V_F + J_R V_R)$$

(2.3)

$P_L$: Static power loss
$J_F$: Current density in forward bias
$J_R$: Current density in reverse bias
$V_F$: Voltage in forward bias
$V_R$: Voltage in reverse bias

2.2.2. Guard ring

Study [35] proposed the guard-ring structure as the edge termination for the high-voltage SiC Schottky diode. Ueno et al. [35], chose Al/Ti as the Schottky metal for investigating fabricated diodes with a guard ring. An illustration of the design is provided in Fig. 2.8.

![Schottky diode with guard-ring design structure](image)

**Fig. 2.8. Schottky diode with guard-ring design structure. Adapted from [35]**

The metal forms the Schottky contact with the n-type region and overlaps part of the guard-ring island. In plain view, the guard ring is seen as a circle surrounding the Schottky electrode (Fig. 2.9).
The reason for using a guard-ring design is to keep the electrical potential of the guard ring the same as the Schottky electrode. In this configuration, the maximum electric field ($E_{\text{max}}$) is applied at the edge of the guard ring [35] and not at the edge of the Schottky electrode (Fig. 2.8), hence, the breakdown voltage is determined by the mesa of the p-n junction.

Ueno et al. [35], reported that field plate length (Fig. 2.8) in SiC becomes shorter than in Si because of the smaller space charge region by about one order due to higher $E_{\text{max}}$ (by about one order). This means photo-alignment between the Schottky electrode metal pattern and the contact-hole pattern is more precise than in Si. Another advantage of the guard-ring structure is due to not using SiO$_2$, the guard-ring structure will not be affected by the process of annealing at high temperature in which metals will chemically react with silicon dioxide (SiO$_2$) (commonly used as the field plate insulator), as in other designs [35].

2.2.3. Floating metal field ring in combination with resistive Schottky barrier field plate

Bhatnagar et al. [36] investigated another way to improve the electrical characteristics of Schottky power diodes which specifically apply for SiC with the structures below.
- Floating metal field ring (FMR)
- Resistive Schottky barrier field plate (RESP)

Fig. 2.10. Floating metal field ring (FMR) structure for Schottky power diode. Adapted from [36]

In the case of the FMR design, the floating metal ring was used instead of the planar floating guard ring. The designated floating metal ring can be used to control the depletion layer contours as illustrated in Fig. 2.10. Another advantage of FMR termination is that this design helps reduce the processing cost because the fabrication for these rings can be done in the same process steps as those for the Schottky electrode [37]. SCR stands for Silicon Controlled Rectifier. This term was used in Fig. 2.10 to indicate that the device in the figure is a rectifier.

For the purpose of maximising the breakdown voltage, multiple rings should be used. These rings result in a higher breakdown voltage due to further contouring of the depletion layer. For this design, the spacing between rings is important because this determines the peak of the electric field, as illustrated in Fig. 2.11.
As illustrated in Fig. 2.12, in FMR termination, the peaks in the electric field occur at the edge of the main electrode \((E_{\text{main}})\) and at ring edges \((E_{\text{R1}}\) and \(E_{\text{R2}}\)). Thus, Bhatnagar [36], identified that the optimal design for the FMR termination should be arranged in a way that those electric field peaks match the edges of the main electrode as well as \(E_{\text{R1}}\) and \(E_{\text{R2}}\). Optimal design of the termination is obtained by comparing the value of the peak electric field at the main Schottky contact and the ring edges as a function of the ring spacing.
RESP termination had been demonstrated with the fabrication of high voltage GaAs Schottky diodes with breakdown voltage exceeding 1000 V [36].

Bhatnagar et al. [36] reported that by using the RESP principle for controlling of voltage gradient along the SiC surface, it should be possible to fabricate a diode which is able to reach a blocking voltage exceeding 95% of the theoretical value. Study [36] also reported that the breakdown voltage of SiC has a strong dependence on the surface condition. Thus, the RESP termination can be used to make a device with a breakdown voltage comparable to the theoretical breakdown voltage on the epitaxial layers of the same doping but “with markedly different surface conditions” and “make the reverse I-V characteristics independent of the processing condition” [36].

2.2.4. Optimisation of the oxide field plate
As well as using a floating guard ring structure, this design was aimed at improving diode reliability and performance by introducing an optimum thickness of field plate for the Schottky diode which is a composite layer of thermally grown oxide and plasma-enhanced chemical vapour deposition oxide [38]. A schematic of the diode is presented in Figs. 2.13 and 2.14.
Fig. 2.13. Schematic illustration of a diode with floating guard ring and enhanced field plate termination. Adapted from [38]

Fig. 2.14. Schematic showing the top-down view of diode structure with guard ring and enhanced field plate termination
There have been many designs for special field plate termination to minimise the field crowding at the edge of the Schottky electrode metal contact [33, 39-44]. Field plate edge termination is widely used even though it is not capable of improving high blocking voltage [38] in comparison to other edge termination techniques such as mesa, floating guard rings, and junction termination extension [44-46]. Another advantage of using field plate edge termination is that it is not required to have ion-implantation and high-temperature annealing processes. Thus, we can use field plate termination along with other termination techniques to provide further improvement for performance in terms of the breakdown voltage and reverse leakage current of the Schottky diodes. Sochacki et al. [47] observed that thermally grown silicon dioxide (SiO$_2$) is a commonly used insulating material in forming field plate edge termination. Gupta [38], suggested that there is a need to use other thicker dielectric materials to avoid the quantum mechanical tunnelling effect through field plate edge because of the limitation in thickness of SiO$_2$ due to the slow growth rate of the Si face of the SiC surface [38]. In the fabrication process, Gupta [38], used a capping of thick plasma enhanced chemical vapour which deposited (PECVD) SiO$_2$ over the thin thermally grown oxide. Moreover, the trapped carbon oxides from grown SiO$_2$ were removed by a process of vacuum annealing [38].

Due to the advantages of using a suitable metal guard ring or field ring (MGR) [38] around the active area of the main diode, the authors included the MGR structure into their design. Gupta [38] stated that the basic structure is designed in such a way that it is easy to transfer it into commercial production. The Schottky electrode is designed with a circular shape, with the field plate extended over the thermal oxide layer in which the width of the field plate of 50 µm is sufficient to neutralise the crowding effect at the Schottky electrode edge [38]. The guard ring is fabricated with the main diode as illustrated in Fig. 2.14.

2.2.5. High-K dielectric-based field plate edge termination
This design basically uses a field plate termination which extends from the Schottky electrode overlap on the high-K dielectric layer which replaces the thermally grown SiO$_2$ layer. The reason is that the high-K materials relax the equipotential contours under the filed plate edge and in turn make the electric field reduce by up to 88% and
result in a major drop in field enhancement factor (defined as a ratio of electric field at the midpoint of the active region under the Schottky contact to the electric field underneath the Schottky contact edge at the same depth) [48]. The drop is determined case by case as reported by Shankar [48]; the field enhancement factor decreases with an increase in the dielectric constant of the field plate dielectric. For example, field enhancement factor values range from 6.6 for SiO$_2$, 4.4 for Si$_3$N$_4$, 3.4 for Al$_2$O$_3$ and 2.2 for HfO$_2$ [48].

The structure of the high-K dielectric-based field plate edge termination design is illustrated in Fig. 2.15.

Fig. 2.15. Schematic of a Schottky diode structure with high-K dielectric replacement of silicon dioxide field plate base edge termination. Adapted from [48]

It has been reported that although the use of a SiO$_2$ based field plate is popular with silicon devices, it does not fare well when used with SiC devices [49]. The reason is that it suffers dielectric breakdown due to the low dielectric constant of SiO$_2$ which has the value of K = 3.9. Other high-K dielectrics such as Si$_3$N$_4$, Al$_2$O$_3$ and HfO$_2$ have been reported as alternative materials to address this issue [49-51].

2.2.6. Bevel oxide field plate

The design adopts common design features such as field plate edge termination and the extension of the Schottky metal overlap of the oxide field plate. However, in Fig. 2.16, there is an improvement in design which utilises a bevelled oxide field plate as illustrated for a GaN Schottky diode.
In this design, the bevel field plate was used as a junction termination technique to improve the breakdown voltage of the Schottky diode. The authors [52] suggest that to further improve the effect that the oxide field plate has been providing, the bevel structure for the oxide field plate is adopted by gradually increasing the thickness of the field oxide, as suggested by Brezeanu et al. [53]. The gradual increase in oxide thickness is illustrated in Fig. 2.17.

To maximise the breakdown voltage, there are two variables for the bevel oxide field plate that needed to be considered. They are the bevel width and the oxide thickness.
Sundaramoorthy [52], reported that there is a dependence of the breakdown voltage on the bevel width such as with the increase of the bevel width (Fig. 2.17), electric crowding does not occur at the edge of the Schottky contact. However, the depletion width is increased which causes the smoothing of the distribution of the electrical peak [52]. It is also reported [52] that the value of the electric field at the edge of the contact is lower than the breakdown field strength of the material. The maximum breakdown voltage was evident at different thicknesses of the oxide layer for different bevel widths [24]. Thus, there is a clear indication of the influence of the bevel angle between the material and bevel surface. The sharpness of the edge termination is defined by the bevel angle which results in that the width of the electric field contours is at the junction as reported by Sundaramoorthy [52]. As in the report, the lower the angle: the wider are the electric field contours and the electric field peak that occurs inside the oxide layer [52].

2.2.7. Boron-implanted edge termination

This early design (1996) used the highly resistive edge termination layer to fabricate a high performance Schottky diode. The designed diode structure is illustrated schematically in Fig. 2.18.

![Fig. 2.18. Schematics showing a cross-section of a Schottky diode with a boron implanted edge termination layer. Adapted from [54]](image)

The highly resistive layers were fabricated by implantation of boron (B⁺). Then, as shown by Itoh, a heat treatment was used to improve the crystallinity of the implanted
layers [54]. As shown by Alok et al. [55], Ar+ can also be used for implantation to form highly resistive amorphous layers at the edge termination with a Schottky diode. However, this device also has a large leakage current density even in low reversed bias voltage which possibly occurs because of the damage from the implantation process within the implanted edge layers. The leakage current will result in high power loss during turn-off stages [55]. Hence, boron is better used for forming the edge termination layer for this structure. Itoh [54], reported that the B⁺ implanted to form edge termination layers for the Schottky diode has resulted in an increase in voltage that approaches the theoretical values in breakdown voltage without increasing leakage current densities.

2.2.8. Merged pn / Schottky structure
This design aims to address factors missing in other designs such as surge current overload, thermal runaway, and the lack of avalanche clamping. For these purposes, the design uses a merged p-n /Schottky diode structure. As per Bjoerk et al. [56], a PN structure with low Ohmic contact resistance is used in parallel with the Schottky structure for extending the handling of peak current and also giving avalanche energy capability while not compromising the dynamic performance of the Schottky diode [56]. The proposed structure is illustrated by Fig. 2.19.

Fig. 2.19. Schottky diode with merged pn/Schottky structure. Adapted from [56]
In this design, the Schottky interface is used for low current operation while the pn interface is used for high current operation. Originally, a floating p island was designed for the silicon Schottky diode to lower the leakage current for the diode by shielding of the Schottky interface. In using this structure in the SiC Schottky diode [56], however, the merged p-areas can be used as a Bi-polar Junction Transistor (BJT) emitter structure by means of a low Ohmic connection to the p regions. Bjoerk et al. [56], also reported that there are two advantages from using embedded p-doped islands. The first advantage is the ability of building a bi-polar current path during the surge current condition when the threshold voltage of the SiC pn junction is reached. The second advantage is during the reverse operation; the avalanche breakdowns are positioned at the edge of the p areas. Thus, this results in a homogenous avalanche breakdown throughout the active area of the diode.

The operation of the diode under normal operation will be like a Schottky diode with a positive temperature coefficient [56]. Under surge conditions, the conventional Schottky diode will reach conduction limits, due to thermally increasing differential resistances, which will result in the destruction of the device due to thermal runaway; the pn/Schottky merged structure’s peak forward current continues to increase with a forward voltage characteristic dominated by the bi-polar conduction. Moreover, it is reported in [56] that the merged pn Schottky design can withstand a substantial avalanche current at the breakdown situation, while this is not viable in designs without the pn/Schottky structure. The reason is due to the low resistivity and the design of the p island in the merged Schottky structure. This, in turn guarantees an onset of the avalanche before the electric field at the Schottky interface gets to the destruction point.

2.3. Summary

Most of the designs for improvement of the performance of the Schottky diode were discussed in regard to their operation. However, those designs, even the simplest improved structures, still need increased steps in fabrication. The more performance enhancement a design provides, the more difficult it is to fabricate it. Not all the designs with minimal cost for commercialisation of the design are practical for mass production. Many of the designs involve multiple processing steps from metal deposition,
annealing, implantation and annealing again, etching, etc. Those steps add to the complexity of the process. Adding them to a basic diode process is not practical for mass production which is a key to commercialisation of the design.

The improved designs focus on the metal guard ring, floating metal ring, and field plate edge termination and extend into the use of a complicated structure such as pn / Schottky, etc. However, there is no research on designs that consider other aspects such as a geometrical design for the Schottky electrode or an alternative to guard-ring structures in a more direct and simple approach in terms of fabrication and cheaper cost while still helping to enhance the performance of a Schottky diode.
Chapter 3 – Optimisation of Schottky Electrode Geometry

The geometry of the Schottky contact electrode is important in the design of Schottky power diodes in regard to the maximum allowed current and electric field. This work focuses on the optimum shape of the Schottky contact geometry and uses finite element modelling to determine the effects of the shape on the electrical characteristics of a diode. The investigation considers the typical situation where the contact is smaller than the substrate area (usually a square). Simulations were run with different contact shapes ranging from a perfect square to a perfect circle, with the size of the diode substrate (die) and the distance between the edge of the die and edge of the Schottky contact as a constant. The different models were examined and compared with the magnitude of the occurrence of the maximum current density (for a particular output current, constant for all geometries). Hence, the breakdown regions at current density approaching the critical value for breakdown (most likely destruction of a diode) due to high current density were determined. The hypothesis here is that there is an optimum geometry that can be determined for the highest current that a given diode substrate could deliver. The hypothesis taken further, is that there is an optimum geometry for the Schottky contact and it should be neither a perfect square nor a perfect circle, but an intermediate geometry. This geometry gives the optimum distribution of current density around the edge of the Schottky contact. Investigations were performed using Synopsys TCAD. The forward and reverse bias situations were investigated to optimise the effect of electrode geometry on both characteristics.

3.1. Introduction

There were many studies in the past which examined ways of improving the performance of Schottky power diodes. Those studies ranged from design of a guard ring [35], to utilising metal field place termination [33] in order to improve the breakdown voltage. However, those improved designs are relatively complicated (regarding fabrication) and hence costly, compared to a basic operational diode structure. In the structure of a Schottky diode, the Schottky electrode plays an important role in diode capability: which relates to the breakdown voltage (critical electric field in reverse bias and maximum current density in forward bias). Baliga [28],
stated that the theoretical breakdown is much higher than real life devices: which indicates that there is much potential for improvement of structure and optimisation of materials. This chapter will focus on one structural aspect, Schottky electrode geometry. In considering only the substrate material [57], according to Kim et al. [4], breakdown occurs at a sharp electrode corner which means that a diode will break down and will be destroyed, possibly before it can reach its theoretical breakdown electric field. In this study, the Schottky electrode design will be examined with Synopsys TCAD to find the optimum geometry for the improvement of the breakdown voltage and the maximum operating current in forward bias for a Schottky power diode of basic operational design.

3.2. Modelling

3.2.1. Modelling design

In order to avoid prohibitively long simulations, the modelling work for this investigation was undertaken with scaled down diode geometry. This significantly reduces the simulation times required for the many models investigated and still demonstrates the proposed process for optimum Schottky electrode design. The diodes investigated by modelling were designed as shown in Fig.3.1 with the dimension of the square shaped substrate represented by edge length, W, and thickness, t, in unit of µm. The Schottky contact is placed centrally on the substrate and has the dimension of D (see Fig. 3.1 a) as the width and length in unit of µm for a square contact, and then adjusted for corner rounding with the radius R (µm). The Ohmic contact at the bottom of the diode structure has the dimensions of W x W (the die area).

3.2.2. Modelling parameters

The metal chosen for the Schottky electrode in these simulations is titanium (Ti) with its characteristic metal work function of 4.33 eV and resistivity of 4.2x10^{-5} Ωcm. The substrate in the simulations is n-type 4H-SiC with doping concentration (n) of 1 x 10^{16} cm^{-3}. The Ohmic contact is the Synopsys TCAD ideal Ohmic contact which contributes zero resistance to the electrical characteristics of the diode. Hence, it is not necessary to specify the physical parameters for it. The modelling design parameters are illustrated with Figs 3.1a and 3.1b.
The simulations were carried out with a range of Schottky electrode geometry starting with a near square shaped electrode and then with different rounding corner values until the geometry gets near to being a circle, as shown in Fig. 3.2. The dimensions for the diode used for the main investigation of this chapter were $W = 10 \, \mu\text{m}$, $d = 2.5 \, \mu\text{m}$ and $t$ (thickness) = $3 \, \mu\text{m}$. (Note that $d$ represents the minimum distance from the edge of the electrode to the edge of the substrate). The values of $R$ used were, $0.25 \, \mu\text{m}$, $0.5 \, \mu\text{m}$, $0.75 \, \mu\text{m}$, $1 \, \mu\text{m}$, $1.25 \, \mu\text{m}$, $1.5 \, \mu\text{m}$, $1.75 \, \mu\text{m}$ and $2 \, \mu\text{m}$. Fig. 3.3 shows a quarter section of a 3-D model used for one of the diode structures modelled. The example used shows the meshing used and shows current density distribution. The highest current density can clearly be seen to occur near the contact edges. Later figures in this chapter, showing similar results for current density distribution are in plan view only, as this is sufficient to show the location of the highest current density regions of the diodes (because they occur at the surface).

![Diode modelling design parameters](image)

**Fig. 3.1.** Diode modelling design parameters. (a) Shows the full plan view, (b) shows expansion of the corner geometry
Fig. 3.2. Plan view of Schottky diode showing the five Schottky electrodes used in the simulations. The value $R$ is the radius used to form a fillet at the corners of an otherwise square electrode. In this study, $R$ changes from 0.25µm for a small rounded corner to 2µm which transforms the geometry from a near-square to a near-circle in shape. The distance between the edges of the Schottky electrode to the edge of the substrate is kept at constant $d$.

Fig. 3.3. A quarter cut of the TCAD-modelled diode which shows the meshing and the relative current density on the surface as well as within the substrate. This example is for $R = 0.25µm$, $W = 10µm$, $d = 2.5µm$, $t = 3µm$, $n = 10^{16} \text{ cm}^{-3}$

3.2.3. Results and discussion

The simulations were performed and data extracted (as illustrated in Fig. 3.4), from all models at forward current ($I_f$) of 0.002 amps showing the value of the instance of maximum current density and the electric field for each diode. A relative comparison
of the maximum current density is required in the linear region of the current–voltage characteristics and on inspecting the characteristics, the value at 0.002 amps, is suitable for comparing all diodes. The results are illustrated by Figs 3.5 and 3.6 below. The maximum current density ($J_{\text{max}}$) changes with the changing value of $R$ (the corner radius parameter which transforms the corners of the Schottky geometry from a square to a circle). Figs 3.5 and 3.6 show the maximum current density concentrating at the corners of the Schottky electrode for $R$ equals 0.25µm and then spreading out and around the edges of the Schottky electrode as the value of $R$ increases. Fig. 3.7 shows the location of an example of the cross-section of a Schottky diode that is shown in more detail in Figs 3.8(a) and 3.8(b). These figures further demonstrate that the location of the highest current density is near the edges of the Schottky electrode.

Fig. 3.4. Schematic illustration of the application of forward and reverse bias in determining the current–voltage characteristics of bulk Schottky power diodes using TCAD. The substrate has thickness $t$. $V_f$ is the forward bias. $V_r$ is the reverse bias.
Fig. 3.5. Current density at the surface of Schottky diodes (a) $R = 0.25\mu m$, (b) $R = 0.5\mu m$, (c) $R = 0.75\mu m$ and (d) $R = 1\mu m$ for forward current $I_f = 0.002A$. $W = 10\mu m$, $d = 2.5\mu m$, $t = 3\mu m$, $n = 10^{16} \text{cm}^{-3}$.

(The scale bars indicate the maximum current density in each instance). (NOTE: In (c) a black marker has been superimposed on the figure to demonstrate the location of the edge of the Schottky electrode)
Fig. 3.6. Current density at the surface of Schottky diodes (a) $R = 1.25\,\mu\text{m}$, (b) $R = 1.5\,\mu\text{m}$, (c) $R = 1.75\,\mu\text{m}$ and (d) $R = 2\,\mu\text{m}$ for forward current $I_f = 0.002\,\text{A}$. $W = 10\,\mu\text{m}$, $d = 2.5\,\mu\text{m}$, $t = 3\,\mu\text{m}$, $n = 10^{16}\,\text{cm}^{-3}$. (The scale bars indicate the maximum current density in each instance). (NOTE: In (b) a black marker has been superimposed on the figure to demonstrate the location of the edge of the Schottky electrode).
Fig. 3.7. Isometric view of 3-D modelling which shows current density around the Schottky electrode with the cross-cut (x-axis) section of Fig. 3.8 indicated between A and B. $R = 1.25 \mu m$, $W = 10 \mu m$, $d = 2.5 \mu m$, $t = 3 \mu m$, $n = 10^{16}$ cm$^{-3}$

Fig. 3.8. Current density distribution. The cross-cut (X-axis) of the modelled diode (a) shows the full cross-cut and (b) shows a zoomed-in section where the corner of the Schottky geometry is as indicated in Fig. 3.7

With data from Fig. 3.9 below, Table 1 has been constructed to show the relationship between maximum current density and forward bias versus the transformation of the Schottky electrode via the changing of value $R$ at forward current = 0.002 amps. As mentioned previously, and shown in Fig. 3.9, this value of current was chosen for...
comparing different electrode geometries because it is conveniently positioned in the linear region of all the current–voltage plots.

Fig. 3.9. I-V Characteristic for diodes with R values ranging from 0.25 µm to 2 µm. W = 10µm, d = 2.5µm, t = 3µm, n = 10^{16} cm^{-3}

Table 3.1. The relationship between maximum current density versus the transformation of the Schottky electrode via the changing of value R (µm). The model parameters are: W = 10µm, d = 2.5µm, t = 3µm, n = 10^{16} cm^{-3}

<table>
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<tr>
<th>Geometry Type – R</th>
<th>Vf at Ir = 0.002 amps</th>
<th>Jmax at Ir = 0.002 A (x10^4 A/cm^2)</th>
</tr>
</thead>
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<td>1.78</td>
<td>2.797</td>
</tr>
<tr>
<td>0.50</td>
<td>1.79</td>
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</tr>
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<td>0.75</td>
<td>1.80</td>
<td>2.324</td>
</tr>
<tr>
<td>1.00</td>
<td>1.82</td>
<td>2.098</td>
</tr>
<tr>
<td>1.25</td>
<td>1.84</td>
<td>1.946</td>
</tr>
<tr>
<td>1.50</td>
<td>1.86</td>
<td>2.015</td>
</tr>
<tr>
<td>1.75</td>
<td>1.89</td>
<td>2.648</td>
</tr>
<tr>
<td>2.00</td>
<td>1.92</td>
<td>2.936</td>
</tr>
</tbody>
</table>
Data from Table 3.1 shows that with the changing of the value for corner rounding (R), the value for maximum current density at forward current $I_F = 0.002$ amps is reduced with the broader rounding corner ($0.25\mu m \rightarrow 1.25\mu m$) and then with further increases in R, the maximum current density increases abruptly to a much higher value when the geometry of the Schottky comes close to being the shape of a circle. The optimum value for R (where the maximum current density for a fixed value of current, is the lowest) for the Schottky electrode can be identified by using Fig. 3.10 below.

![Graph showing maximum current density vs. R](image)

**Fig. 3.10.** Schottky diode TCAD modeling results for maximum current density at forward current $I_F$ of 0.002 amps versus R (radius of curvature of the Schottky electrode corner). $W = 10\mu m$, $D=5\mu m$, $d = 2.5\mu m$, $t = 3\mu m$, $n = 10^{16} \text{ cm}^{-3}$. (Note: $R=2.5$ corresponds to $2R=d$ and therefore a circle contact)

Fig. 3.10 shows that the point with lowest incidence of maximum current density is when the value of R equals 1.25µm (for D=5 µm). Moreover, the ON-resistance for these geometries are presented in Table 3.2 below, which shows that when changing from a sharper corner to rounder shaped corner, the ON-resistance is increasing: which means that it will use more power for the ON stage, but this change is relatively small as shown in Table 3.3.
Table 3.2. Relationship between changes in Schottky electrode (R values) versus ON resistance. 
$W = 10\mu\text{m}, d = 2.5\mu\text{m}, t = 3\mu\text{m}, n = 10^{18} \text{ cm}^{-3}$ ($V_{\text{TO}}$ is Turn-on voltage)

<table>
<thead>
<tr>
<th>R ($\mu\text{m}$)</th>
<th>$V_{\text{TO}}$ (V)</th>
<th>ON-resistance (Ω)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.25</td>
<td>1.78</td>
<td>475</td>
</tr>
<tr>
<td>0.50</td>
<td>1.79</td>
<td>482</td>
</tr>
<tr>
<td>0.75</td>
<td>1.80</td>
<td>485</td>
</tr>
<tr>
<td>1.00</td>
<td>1.82</td>
<td>498</td>
</tr>
<tr>
<td>1.25</td>
<td>1.84</td>
<td>510</td>
</tr>
<tr>
<td>1.50</td>
<td>1.86</td>
<td>518</td>
</tr>
<tr>
<td>1.75</td>
<td>1.88</td>
<td>530</td>
</tr>
<tr>
<td>2.00</td>
<td>1.92</td>
<td>540</td>
</tr>
</tbody>
</table>

3.2.3.1. Forward reverse bias current–voltage characteristics

The comparison between all diodes ($W=10\mu\text{m}, D=5\mu\text{m}$) with Schottky geometry ranging from R equals 0.25µm to R equals 2µm is provided by Fig. 3.9. In this figure, in the ON stage (considering the forward current $I_F$ to be well in the linear I-V region), each geometry will have an equivalent forward voltage which determines the ON-resistance. The higher ON-resistance means that the geometry will waste more energy in the ON stage operation. There is usually a compromise when trying to design for optimising both the turn-on and the breakdown voltage. The best geometry which gives the best ON-resistance may not provide the best reverse bias breakdown voltage.
Table 3.3. Shows the relationship between the geometry values (R) versus the power consumed by the diode in the ON stage at \( I_f \) equals 0.002A. \( W = 10\mu m, d = 2.5\mu m, t = 3\mu m, n = 10^{16} \text{ cm}^{-3} \)

<table>
<thead>
<tr>
<th>R (\mu m)</th>
<th>Power (mW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.25</td>
<td>3.56</td>
</tr>
<tr>
<td>0.50</td>
<td>3.58</td>
</tr>
<tr>
<td>0.75</td>
<td>3.60</td>
</tr>
<tr>
<td>1.00</td>
<td>3.64</td>
</tr>
<tr>
<td>1.25</td>
<td>3.68</td>
</tr>
<tr>
<td>1.50</td>
<td>3.72</td>
</tr>
<tr>
<td>1.75</td>
<td>3.76</td>
</tr>
<tr>
<td>2.00</td>
<td>3.84</td>
</tr>
</tbody>
</table>

Fig. 3.11. Results of TCAD modelling showing the relationship between power (W) and R (\mu m), for different shaped diodes at the ON stage of \( I_f \) equals 0.002 amps. \( W = 10\mu m, d = 2.5\mu m, t = 3\mu m, n = 10^{16} \text{ cm}^{-3} \) 

TCAD modelling was also used to determine reverse bias characteristics for varying ‘R’. These are shown in Fig. 3.12.
A review of Figs 3.9, 3.11 and 3.12 shows that for a balance between a good turn-on voltage, where the diode will use less power while obtaining a good breakdown, is the geometry with $R = 1.25 \mu m$: for the example investigated here ($W = 10 \mu m$, $d = 2.5 \mu m$, $t = 3 \mu m$, $n = 10^{16} \text{ cm}^{-3}$). This is scalable for geometry. There is approximately a 3% change in power consumption for $R = 0.25 \mu m$ to $R = 1.25 \mu m$ but the breakdown voltage is double. With the geometry at $R = 1.25 \mu m$, the diode obtained a turn-on voltage at 0.8 volts while having the largest breakdown at around -68 volts.
Table 3.4. Results obtained using TCAD modelling for breakdown voltage and $J_{\text{max}}$ at $I_f = 0.002$ amps versus change in geometry ($R$). $W = 10\mu m$, $d = 2.5\mu m$, $t = 3\mu m$, $n = 10^{16} \text{ cm}^{-3}$

<table>
<thead>
<tr>
<th>Geometry Type – $R(\mu m)$</th>
<th>Voltage-breakdown (Volts)</th>
<th>$J_{\text{max}}$ at $I_f = 0.002A$ ($x10^4 \text{ A/cm}^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.25</td>
<td>-33.0</td>
<td>2.797</td>
</tr>
<tr>
<td>0.50</td>
<td>-44.9</td>
<td>2.791</td>
</tr>
<tr>
<td>0.75</td>
<td>-45.0</td>
<td>2.424</td>
</tr>
<tr>
<td>1.00</td>
<td>-53.2</td>
<td>2.010</td>
</tr>
<tr>
<td>1.25</td>
<td>-68.2</td>
<td>1.946</td>
</tr>
<tr>
<td>1.50</td>
<td>-63.0</td>
<td>1.929</td>
</tr>
<tr>
<td>1.75</td>
<td>-60.2</td>
<td>2.648</td>
</tr>
<tr>
<td>2.00</td>
<td>-57.0</td>
<td>2.936</td>
</tr>
</tbody>
</table>

3.2.3.2. The scalability of the experimental model

In order to test that the device in this simulation can scale up, (for example scaling as reported in Loh, et al. [58]) for example, such as scaling up to the realistic size which may be $1000 \mu m \times 1000 \mu m \times 300 \mu m$ (Width x Length x Height) for the substrate, the model has been scaled up two times in terms of every dimension for both the substrate and the Schottky contact and run with several different geometries to obtain the data. The results show that the ratio of ON-resistances is 2 when comparing the ON-resistance of the original size diode, versus the 2 times scaled diode.

3.3. Conclusion

Using simulation by TCAD, the optimum electrode has been identified as a shape of neither a square nor a perfect circle. The geometry has to be compromised in order to obtain a best balance between forward turn-on and reverse breakdown voltage: the best geometry is obtained when value $R$ equals 1.25 $\mu m$ and 2.5 $\mu m$ for the 2 x scaled model. For the ratio of $R/(D/2)$ which is the value that reflects on the transformation of
the Schottky electrode ranging from a circle to a square (with \( R/(D/2) = 1 \), giving a circle, and \( R/(D/2) = 0 \), giving a square, see also Figs 3.1 (a), 3.1 (b) and 3.2). Results show that the optimum shape is for \( R/(D/2) = 0.5 \). The distance from the edge of the Schottky electrode was kept constant as this is likely the parameter that has manufacturing limitations that affect Schottky electrode positioning on the substrate die. Results were compared for a fixed ON-current. Results show that power consumption by the diodes does not change significantly for the different shapes of Schottky electrode. The most affected parameter is reverse breakdown voltage which can vary significantly (~100\% difference) for the different electrode shapes tested. The maximum current density in forward bias can also be significantly different, but closer to 50\% variation for the electrode shapes investigated. This investigation has demonstrated a process for determining the optimum shaped electrode that should be manufactured for a diode that is used only in reverse bias (e.g. a radiation detector) or the exact geometry in diodes where forward bias operation is critical or can be used to determine a design where both forward and reverse bias are important.
Chapter 4 – Improvement of Schottky Power Diode Performance by Surround Trenching of Schottky Contact

This work aims to further improve the performance of power diode through the alternative approach of using trenching around the optimised Schottky electrode. This approach was investigated in this study by using NASTRAN, a finite element modelling (FEM) method software package. The modelling was done with the building of samples with different geometries into two types (the first without trenching around the Schottky electrode and the second with trenching around the Schottky electrode) with the same current throughput for every model from both groups. The results show that there is significant improvement in the trenching samples, as the Schottky electrode that is trenched can take as much as two times the current in comparison to the non-trenched samples.

4.1. Introduction

Improvement of the overall performance for the SiC Schottky power diode has been investigated by many researchers. One of the main research aspects is finding a way to improve the breakdown voltage in the reverse bias, which has the potential to be as large as $10^4$ volts [28]. In terms of its physical structure, Schottky contact geometry and materials [59-61] also play a role in determining whether the diode will have a better breakdown voltage or not. The theoretical breakdown can be approached (by improved SiC material in particular, as well as geometry, which is the focus of this work) as long as the Schottky contact can survive the maximum current density at the specified maximum operating current or voltage. A current or voltage that is too high will cause deteriorating effects on the contact and destroy it before the diode itself reaches the potential breakdown within the substrate. In this study, it will be shown that by using a certain geometry, the Schottky diode can obtain better breakdown where the maximum current density is distributed more evenly around the edge of the Schottky contact. For many years, device engineers have used a way to reduce maximum current density by using a guard ring and field plate termination [33, 35, 57]. The method reported here is similar to these in effect and lends itself to being easily incorporated into a manufacturing process. This research aims at improving the
Schottky contact's ability to deliver more current by the simple method of trenching around the contact.

4.2. Modelling

4.2.1. Modelling design
Optimum electrode geometry can help to reduce the maximum current density (for a given ON-current) which concentrates on the edge of the Schottky contact. This research will enable a rigorous approach to the design of models for the simulations of different electrode geometries. These are in line with the results shown in Fig. 4.1 which shows the finding of maximum current density versus “changing of the geometry” (changing radius of curvature of the electrode corners): using NASTRAN according to the design reported in the previous chapter. These models were constructed with the geometry of the Schottky electrode ranging from square to circle where SiC was used as the material for the simulation. For convenience, with regard to the meshing for finite element modelling, the dimensions of the models were kept small but with the same aspect ratio as large diodes formed using standard substrate thickness. The small-sized models serve to demonstrate the process for determining the optimum geometry for the electrode given other diode parameters. Provided a uniform scaling factor is applied in all directions, the results can also be linearly scaled.
Fig. 4.1. Example of “maximum current density” versus “changing of the geometry” of the Schottky contact. Obtained using FEM models of Schottky diodes with Schottky electrode shape changing from square to circle using NASTRAN

The simulation models were designed with Schottky geometry ranging from square to circle with and without trenching around the edge of the Schottky contact. For every Schottky contact geometry, two models were built: one trenched and one non-trenched. The data acquired with the simulation shall be compared in terms of maximum current density between non-trenched models versus trenched models. Fig.4.2 shows a 3D illustration of the Schottky diode model with a square contact with trenching. Fig.4.3 shows a schematic cross-cut view of a diode model that includes trenching around the Schottky electrode.

Fig. 4.2. Schematic of a 3D Schottky diode with trenching around the square Schottky contact (shown in black)
NASTRAN, a finite element modelling (FEM) software, was used for the investigation’s forward bias (purely resistive effects past the turn-on voltage point) breakdown simulation. All models had the same input current, which is illustrated in Fig. 4.4.

The geometry of the Schottky electrode is designed as in Fig. 4.5. Details of the data are in Table 4.1 below.
Fig. 4.5. Design for Schottky electrode geometry. This is relevant to the Schottky electrode only. R1, R2, R3 and R4 are the radius of the degree of corner rounding.

Table 4.1. Detailed information of the radius of the degree of corner rounding for the Schottky electrode design used in the simulation

<table>
<thead>
<tr>
<th>Radius of the degree of corner rounding</th>
<th>Description of Schottky electrode geometry</th>
<th>Measurement (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>Circle</td>
<td>2.5</td>
</tr>
<tr>
<td>R2</td>
<td>Rounded Corner</td>
<td>1.25</td>
</tr>
<tr>
<td>R3</td>
<td>Rounded Corner</td>
<td>0.625</td>
</tr>
<tr>
<td>R4</td>
<td>Square</td>
<td>0</td>
</tr>
</tbody>
</table>

The dimensions of the Schottky barrier diode model used for simulation in this chapter are illustrated in Fig. 4.6.
The model of the simulated Schottky diode (Fig. 4.6) has the following parameters: the substrate has contact (A) with a dimension of 5x5 µm$^2$ with a thickness (C) of 0.5 µm. The substrate (F), has a dimension of 13 x 13 µm$^2$ with a thickness (D) of 3.5 µm. The trench has a width (B) of 1 µm and a depth (E) of 0.5 µm. The resistivity of the substrate is 150 Ω.µm and the metal is assumed as being at an equipotential.

4.2.2. Results and discussion

4.2.2.1. Comparison of current density in models without trenching compared to models with trenching. The current in the simulation was constant. Fig. 4.7 to Fig. 4.14 show the simulation results of current density for different simulated models with different geometry for the trenched and non-trenched models.
Fig. 4.8. Current density for square geometry with radius of R4 with trenching (see also Fig. 4.5 and Table 4.1). The maximum current density value at the corner is 14.7 µA/µ².

Fig. 4.9. Current density for rounded corner geometry with radius of R3 without trenching (see also Fig. 4.5 and Table 4.1). The maximum current density value at the corner is 23.5 µA/µ².

Fig. 4.10. Current density for rounded corner geometry with radius of R3 with trenching (see also Fig. 4.5 and Table 4.1). The maximum current density value at the corner is 12.3 µA/µ².
Fig. 4.11. Current density for rounded corner geometry with radius of R2 without trenching (see also Fig. 4.5 and Table 4.1). The maximum current density value at the corner is 28.4 µA/µm²

Fig. 4.12. Current density for rounded corner geometry with radius of R2 with trenching (see also Fig. 4.5 and Table 4.1). The maximum current density value at the corner is 13.7 µA/µm²

Fig. 4.13. Current density for circle geometry with radius of R1 without trenching (see also Fig. 4.5 and Table 4.1). The maximum current density value is 43.1 µA/µm²
Fig. 4.14. Current density for circle geometry with radius of R1 with trenching (see also Fig. 4.5 and Table 4.1). The maximum current density value is 21.8 µA/µm²

4.2.2.2. FEM results of non-trenched and trenched models.

The results from the simulation with FEM for the non-trenched and trenched models are presented in Tables 4.2 and 4.3.

Table 4.2. Results from FEM simulation for non-trenched models with different R values

<table>
<thead>
<tr>
<th>FEM results for non-trenched models</th>
</tr>
</thead>
<tbody>
<tr>
<td>Models with R values of</td>
</tr>
<tr>
<td>------------------------</td>
</tr>
<tr>
<td>R1</td>
</tr>
<tr>
<td>R2</td>
</tr>
<tr>
<td>R3</td>
</tr>
<tr>
<td>R4</td>
</tr>
</tbody>
</table>
Table 4.3. Results from the FEM simulation for trenched models with different R values

<table>
<thead>
<tr>
<th>FEM results for trenched models</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Models with R values of</td>
<td>Maximum Current Density Value (µA/µm²)</td>
</tr>
<tr>
<td></td>
<td>R1</td>
</tr>
<tr>
<td>R1</td>
<td>21.8</td>
</tr>
<tr>
<td>R2</td>
<td>13.7</td>
</tr>
<tr>
<td>R3</td>
<td>12.3</td>
</tr>
<tr>
<td>R4</td>
<td>14.7</td>
</tr>
</tbody>
</table>

From data acquired from the FEM simulations (Tables 4.2 and 4.3); the comparison of the maximum current density values between non-trenched and trenched models is presented in Fig. 4.15.

Fig. 4.15. Comparison of maximum current density values of the non-trenched models versus trenched models with geometry ranging from square to circle (R values from R4 to R1. See Tables 4.1, 4.2 and 4.3)
In comparing the maximum current density curves of the trenched and non-trenched models, there is a big difference between those two types of models. The trenched models give much lower maximum current density in comparison to the non-trenched models for a given diode current. In comparison to the non-trenched models, the FEM simulations show that the trenched models give as much as 50% lower maximum in current density values. This means that a diode with a trenched Schottky electrode can take as much as two times the current in comparison to a diode with a non-trenched Schottky electrode: before the contact gets destroyed by the current.

4.3. Conclusion

The FEM results have shown that by employing trenching around the edge of the Schottky contact, we will be able to improve the ability of the contact so that it can take as much as two times the amount of current. However, this will depend on which geometry is chosen. For example, in fabricating the Schottky electrode, only the optimum geometry will deliver the best result. Different geometries will give different percentage improvements in the ability of the Schottky electrode to withstand maximum current density. However, regardless of the geometry of the trenched Schottky electrode, the ability to withstand maximum current density is still better than that of the non-trenched Schottky electrode (given they are at the same size, same type of metal, same metal thickness as well as using the same substrate). This means that in a Schottky electrode of the same area, the electrode with trenching around its edge will be able to withstand two times more current before failure. The results given here demonstrate that the specifications of a power diode can be improved by using the Schottky electrode design method proposed.
Chapter 5 – Results of Experiments

In this study, Schottky contact geometry is optimised in order to minimise the incidents of maximum current density within the diode structure where breakdown occurs. Surface preparation and surface treatment prior to Schottky contact formation, and in particular the surface treatments used to give a carbon-rich SiC surface, which in this study has been found to reduce the turn-on voltage of SiC Schottky diodes, are also investigated. Optimised geometry and electrode edge isolation improvements are demonstrated using silicon substrates and this improvement can be applied to any metal-to-semiconductor combination. A diode requires a Schottky contact and an Ohmic contact which is also studied here to confirm that it has no effect on the diode’s I-V characteristic. Furthermore, the use of selective etching to prepare the SiC surface for improving the Ohmic contact surface is studied as well. SiC diodes were fabricated and used for electrical testing to determine the electrical characteristics. Moreover, the effects of the quality of the SiC itself on the breakdown voltage were investigated (the major qualifier for crystal quality is the value of the density of the defect known as a micropipe and this value is specified as MPD (for micropipe density) and provided in SiC wafer specifications from suppliers.

SiC is expensive and difficult to dice into pieces because it is extremely hard. By fabricating and testing silicon Schottky diodes, for some of the experimental work, to investigate diode geometry effects on I-V characteristics, silicon substrates were used to test the computer-modelled designs. Considering only geometry, the effect of geometry variations has the same trend, i.e. poorly designed diodes behaved worse than those that were designed well. Whether the semiconductor was Si or SiC, the same trends in regard to electrode geometry were observed. (A limited number of SiC devices and an extensive number of Si diodes were tested to show this). For experimental work on the effectiveness of trench guard rings, laser ablation processes were conducted by the candidate at The School of Mechatronic Engineering, Universiti Malaysia Perlis (UniMAP), Main Campus Ulu Pauh, Perlis, Malaysia.

SiC wafers (no epitaxial layer) of different resistivity and defect density were purchased from University Wafer Inc. The approach used for investigating a ‘slab’ of
4H-SiC semiconductor without any epitaxial layer was deliberate so that the effect of different properties could be determined. Note that 4H is a polytype of SiC where the Si and carbon atoms have a hexagonal arrangement. 4H–SiC has been shown to give the highest electrical breakdown values. Other polytypes that are common are 6H and 3C (where ‘C’ indicates a cubic arrangement) and the stoichiometry of all polytypes of SiC is such that there are 50% Si atoms and 50% C atoms in a unit volume. Commercial SiC Schottky diodes use one or more epitaxial layers and while this does reduce the series resistance, it adds too much complexity for this investigation, which is focused on optimising Schottky electrode design and fabrication steps and the effects of defects in the SiC on the electrical characteristics of diodes. Of particular interest is the relative influence of defects and electrode geometry.

5.1 Most Suitable Schottky Metal for Enhancing Schottky Diode Performance

The silicon carbide (SiC) Schottky diode is well-known for operating in high temperature environments and at high voltage without changing its intrinsic properties. Also, with its ability for fast switching speed, it has huge applications within many industries such as power, aerospace, automotive and military. Improvements to the SiC Schottky diode provide better power handling and benefits in terms of more compact and efficient energy conversion technology with an increase in power density. Any studies on how to improve SiC Schottky diodes involve study of its I-V characteristic and its turn-on voltage, as well as its reverse breakdown voltage and the reverse leakage currents. Due to different metal work functions for different metals, the Schottky metal plays an important role in influencing the I-V characteristic of the Schottky diode [29]. As part of the experiment, both the Ohmic contact and the Schottky contact were investigated and trials of different metals for fabrication of the Schottky contact were conducted. The research data for analysis was acquired with an Agilent 2723A-USB and a Keithley 2410 source meter. A Schottky diode with titanium as the Schottky contact metal which obtained a low turn-on voltage of 0.25 volts while having a breakdown voltage of -600 volts was successfully fabricated. The findings of this research indicated that titanium is overall the most suitable metal to use in high power SiC Schottky diode fabrication and there is still room for
improvement on the reverse breakdown voltage with titanium, where tungsten was better in that it had Schottky diodes with a lower leakage current.

5.1.1 Solution methodology

There are two components to the silicon carbide Schottky diode.

- The first component is the metal Schottky contact which is placed on top of the polished side of the SiC substrate. This contact determines the I-V characteristic of the diode.
- The second component is the Ohmic contact which obeys Ohm’s law and should have very low resistance: its purpose being to give electrical contact to the device for applying an electric field and enabling the current to flow.

![Schottky diode structure](image)

**Fig. 5.1.** Schottky diode structure for testing the effect of different Schottky metals. (The Ni contact was formed by Ni deposition and heat treatment before the Schottky metal was deposited for each case)

In this study, 4H-SiC was used as the material for the fabrication of the Schottky diodes under review. 4H-SiC has been proven to be the most appropriate polytype of SiC for making high capacity diodes; it is easier and more economical to produce as well as being more widely available [9, 24, 32].

Choosing a metal for fabricating Schottky contacts was based on Fig. 2.4 [29] which shows the 4H-SiC energy band diagram compared with the workfunction of a number of Schottky metal candidates.
Based on Fig. 2.4, the Schottky contact was investigated by using different metals with a range of metal workfunctions to see how they will behave under forward and reversed bias. Schottky contacts were formed with different metals such as Ti (workfunction 4.33 eV), Ni (5.10 eV), W (4.55 eV), and Pt (5.65 eV). This suggests that Ti (compared to the other metals investigated) gave the lowest workfunction difference for the n-type SiC used in this experiment.

Because the quality of the surface of Schottky contact will affect the leakage current, the turn-on voltage and the maximum ON-current, the experiment was also concerned with investigating how to obtain the best SiC surface preparation method to improve those factors.

5.1.2 Solution implementation
The SiC (silicon carbide) wafers used in this investigation were 2-inch diameter, single side polished and n-type with a concentration of $1 \times 10^{16}$ cm$^{-3}$. The wafers were diced so that in experimental work size of the SiC substrates were 1 cm x 1 cm. The thickness of the substrate is 258 µm. The SiC substrates were coated with Ni on the back of the wafer to make an Ohmic contact.

The fabrication process was broken into three stages according to the following order: testing the Ohmic contact; fabrication of the Schottky contact; diode testing and data acquisition. The reason for proceeding in this order is that after deposition of the Ohmic contact metal, the sample needs be annealed in the furnace so that a good Ohmic contact is formed. However, the Schottky contact metal should not be annealed because this would most likely lead to deterioration of its Schottky characteristics.

5.1.2.1 Ohmic contact (Ni) testing
The investigation was conducted on batches of SiC substrates with Ni pre-deposited by DC sputtering, as an Ohmic contact on the entire back of the samples. For each batch, an Ohmic test was carried out on two random samples (after heat treatment of these alone) to make sure that the Ohmic contact from this batch was of good quality. If the tests confirmed that the Ohmic contacts were in good condition, the rest of the Ohmic contacts from the batch would not be etched but only annealed in a furnace.
To test the quality of the Ohmic contact, the Ni layer of the Ohmic contact was etched to remove strips of Ni (substrate edge to edge) leaving Ni islands (Fig. 5.3) which could then be tested by using probes to connect to any two isolated islands. Their I-V characteristics were observed using a Tektronix curve tracer.

Fig. 5.3. Isolated Ni-Ohmic contacts formed by etching

The actual fabrication steps are described in the steps below.

5.1.2.1.1 Cleaning the SiC surface in preparation for Ni coating
The entire contact surface was cleaned to allow the best possible current conduction. The surface of Ni was cleaned with acetone then re-rinsed with isopropanol and left under running deionised (DI) water for approximately 5 seconds before being dried by a pressurised nitrogen gas gun. All steps were carried out carefully. As soon as the cleaning process was complete, the sample was put into a pre-cleaned glass container for storage. The purpose was to minimise contamination to the samples.

5.1.2.1.2 Depositing photoresist on the Ni surface
After the cleaning process, the samples were located with photoresist AZ1512.

The setting for the deposition was as follows:
- Speed: 3,000 rpm
- Acceleration: 300 rpm/s
- Time: 30 seconds.
After the spinning finished, the samples were immediately removed from the spinner and put on a hot plate for the soft-bake process.

5.1.2.1.3 Soft-bake
The purpose of soft-baking is to prevent chemical change in the resist material as well as to improve resist adhesion. Moreover, the soft-bake process also helps in stabilising light absorbance characteristics, as in photolithography solvent removal reduces the variability of the resist process to exposure. Furthermore, when the soft-bake is higher or longer the variance in linewidth will be reduced. However, overdoing it will reduce the sensitivity of photoresist to exposure.

The setting for the soft-bake process is:

- Time: 2 minutes
- Temperature: 95\(^\circ\) C.

After the soft-bake process was done, the samples were ready for exposure.

5.1.2.1.4 Photolithography
The samples were exposed using a contact mask aligner (Fig. 5.4).
The mask used was aligned on top of the sample’s surface which was coated with a layer of photoresist and then the mask and sample were brought into contact. The samples were exposed for 60 seconds. The duration of the exposure was not a critical parameter because the patterns were relatively large.

5.1.2.1.5 Developing
The exposed samples were developed with AZ400K: DI water (1:4) developer for 20 seconds.

After development, the samples were immediately soaked in DI water for 45 seconds. While soaking, the samples were agitated to ensure that there was no developer residual on the samples. After that, the samples were rinsed under running DI water and dried with a pressurised nitrogen gas.

5.1.2.1.6 Ni etching
The etching was done in the fume cupboard. In order to obtain the isolated islands as planned, Ni etchant was used to etch the Ohmic Ni surface. The Ni etchant was a 4:1 solution of HCl:HNO₃. The samples were soaked in Ni etchant for 1 minute. Afterwards, these samples were soaked in DI water for 30 seconds and were then put under running DI water for approximately 15 seconds.

A surface examination was done with an optical microscope to make sure that the desired results had been achieved.
5.1.2.1.7 Annealing

After the samples were etched to give the required pattern, they were loaded into a furnace which was at 900°C. Fig. 5.5 to Fig. 5.8 show the preparation of the furnace, the inserting of samples into the furnace and the appearance of the samples after the annealing process.

Fig. 5.5. Furnace at 900°C for annealing etched samples. The furnace is approximately 1.5 m long and 3 inches in diameter. Samples were loaded using a glass rod and placed near the centre. Forming gas of 3% hydrogen in nitrogen and 2 l/min was used to prevent oxidation.

Before the samples could be put into the furnace, a forming gas of 3% hydrogen in nitrogen and a flow rate of 2 l/min was set up. To further prevent oxidation during the annealing process, each sample was sandwiched between two larger pieces of Ti-coated silicon substrates because Ti is a gatherer of oxygen. (The entire Ni layer was in intimate contact with a Ti coated silicon substrate).
After the preparation, the samples were put into a furnace for 5 minutes.
The samples shown after annealing (the square is the SiC) in Fig. 5.8 indicate the amount of oxidation (turning green) of the titanium pieces. It was a good vacuum simulation in that the samples indicated that there had been some adherence to both of the titanium pieces when they were separated. Small weights were stacked on the sample during annealing to help limit any gas flow into the Ni-to-Ti contact region.

5.1.2.1.8 Ohmic test and conclusion
The test was conducted by connecting one probe to one island and the other probe to a different island of the patterned Ohmic contact and examining the I-V characteristics with a Tektronix curve tracer. Fig. 5.9 and Fig 5.10 show the test schematic and the Tektronix curve tracer which was used for testing the patterned Ohmic contact.

The resistance measured between a set pair of dot contacts before any heat treatment was 900,000 Ω. After furnace annealing at 900°C at 5 minutes, the resistance between the same pair of contacts, reduced to 300 Ω and after furnace annealing at 900°C for 10 minutes, it reduced to 60 Ω. The magnitude of this reduction is a qualitative indication of the effect of the heat treatment.
The results obtained after testing showed a linear curve which fitted in with the behaviour of an Ohmic contact. Therefore, it is concluded that the Ni-Ohmic contact for the batch of SiC with deposited Ni was in good condition. The specific contact resistance of the Ni to SiC was investigated using an appropriate test structure.

5.1.2.2 Schottky contact fabrication

Four different metals were used for the fabrication of the Schottky diode samples. These were Ni, Ti, W and Pt. The Schottky diodes with Ni, Pt and Ti as the Schottky electrode, were exposed with the same mask; while the Schottky electrode samples with W were fabricated as a whole piece without going through photolithography because of difficulty with using photoresist in the sputtering system. (The other metals were evaporated). The details for W-sample fabrication will be provided in the W Schottky diode fabrication section.
5.1.2.2.1 Ni Schottky contact fabrication

5.1.2.2.1.1 Surface cleaning for SiC
As with any sample for microfabrication, the surface, on which photoresist will be deposited, must be clean to make sure that there are no particles stuck to it. The process was done in a fume cupboard with acetone, isopropanol and flowing DI water. After cleaning, the samples were dried off with a pressurised nitrogen gas gun and then stored in a clean glass petri dish.

5.1.2.2.1.2 Photoresist deposition
After the cleaning process, the samples were deposited with photoresist AZ1512.

The setting for the deposition is as follows:
• Speed: 3,000 rpm
• Acceleration: 300 rpm/s
• Time: 30 seconds.

After the spinning was finished, the samples were immediately removed from the spinner and put on a hot plate for the soft-bake process.

5.1.2.2.1.3 Soft-bake
The purpose of soft-baking was discussed in the Ni Ohmic testing section. The setting for the process in this session was 2 minutes duration with the temperature at 95° C. After the soft-bake process was done, the samples were ready for exposure.

5.1.2.2.1.4 Photolithography
The following pattern is used for patterning Ni, Pt and Ti samples.
Fig. 5.11. Mask pattern for Schottky electrode with Ni, Pt and Ti as Schottky contact metal. The dimension of the mask is 1 cm x 1 cm

The pattern was aligned with the sample in the contact mask aligner. The exposure time was 50 seconds. After exposure to UV light, the samples were moved to the fume cupboard for development.

The exposed samples were developed with AZ400K (1:4) developer. The duration for the development was 20 seconds.

After developing, the samples were immediately soaked in DI water to stop the development for 45 seconds. While soaking in DI water, the samples were shaken gently to make sure that there was no developer residue on the samples. Afterwards, the samples were rinsed under running DI water and dried with the nitrogen.

5.1.2.2.1.5 Ni Schottky metal deposition
After development, the samples were adhered to a glass slide with photoresist and sent for Ni metal deposition (by e-beam evaporation). Normally, this process takes around 3 hours to complete. The lift-off process was done with acetone and isopropanol. The samples were put into a container of acetone and to hasten the process the container was agitated in an ultrasonic bath. After the lift-off process was complete, isopropanol was used to rinse the samples and once again they were rinsed under running water for around 15 seconds. The finished sample was then ready for testing and data acquisition. Fig.5.12 shows the sample from this fabrication batch with Ni and a top Au layer.
5.1.2.2.2 Pt Schottky contact fabrication
All the processes used for fabrication of Ni Schottky diodes (substrate cleaning, photoresist deposition and photolithography) were repeated for Pt Schottky diode fabrication.

5.1.2.2.2.1 Pt Schottky metal deposition
After development, the samples were adhered to a glass slide with photoresist and sent for Pt deposition (also by e-beam evaporation). When the samples were returned, the lift-off process was done in the same way as with the Ni batch. However, there was one issue that went unnoticed until the lift-off process was completed. It had been found that evaporated Pt does not adhere well to SiC, hence, during the lift-off process, acetone had peeled off a considerable number of the Pt electrodes. Thus, there were only 3 workable diodes in this batch.
Figs. 5.13 and 5.14 show the actual samples that are still workable after the lift-off process. These samples were ready for further testing.

5.1.2.2.3 Ti Schottky contact fabrication
All the processes used for fabrication of Ni Schottky diodes (substrate cleaning, photoresist deposition and photolithography) were repeated for Ti Schottky diode fabrication.

5.1.2.2.3.1 Ti Schottky Metal deposition
After development, the samples were adhered to a glass slide with photoresist and sent for Ti deposition. When the samples were returned, the lift-off process was done in the same way as with the Ni and Pt batches. When conducting the lift-off process, the photoresist on the samples did not peel off as easily as it was supposed to. With some gentle rubbing, it took approximately one hour to remove the photoresist. Fig. 5.15 shows SiC Schottky diodes with Ti as the Schottky contact metal before the lift-off process. Fig. 5.16 shows the Schottky diodes with Ti as Schottky metal after the lift-off process.
5.1.2.2.4 W Schottky contact fabrication
The final batch of samples for fabrication was for those where the Schottky electrode had W as the contact metal. W was deposited for the whole surface of the SiC substrate. W was different to the other metals because it was sputter deposited and the others were evaporated and sputtering would have damaged the resist if lift off was done because the energy of the arriving metal atoms is high and hence the temperature of the sample is high. After that, it was formed into different-sized square electrodes using a saw to form trenches. This was a different approach to using the mask pattern of Fig. 5.11 (used for the Ni, Ti and Pt electrodes).

5.1.2.2.4.1 W Schottky metal deposition
Before sending the samples for metal deposition, the edges of the samples had to be covered with photoresist to prevent W from the Schottky contact shorting with Ni from the Ohmic contact. After covering all the edges of these samples with photoresist, the samples were soft-baked on a hot plate at 110°C for 5 minutes to increase adhesion of the samples to the glass panel.

5.1.2.2.4.2 Preparing for dicing into multiple diodes
After the lift-off process, using a dicing saw, one sample was used to create the design seen in Fig. 5.17.
Before the sample was diced it had photoresist deposited on the W surface to protect the surface from getting damaged.

The photoresist deposition was carried out similarly to the other batches but there were changes as follows.

The soft-bake was conducted for a longer time (30 minutes) at $95^\circ$ C. The reason for this was that this photoresist would be acting as a protective coating for the W surface in the dicing process.

5.1.2.3 Diode testing
The test was carried out with a Tektronix 571 curve tracer which can be used to provide a voltage of up to 100 V. The purpose was to check all the diodes on all the samples to make sure that they were all good before proceeding to the data acquisition stage.

The Tektronix 571 curve tracer is easy to set up and run. The only shortcoming is that results only show up on the screen: there was no means to dump the test data for further analysis. The setup of Tektronix curve tracer in preparing for the diode testing was shown in Fig. 5.18.
The samples were tested by adhering the samples’ Ohmic contacts to the copper side of blank PCBs by using silver paint, which is highly conductive. Thus, the PCB acted as the cathode and the SiC Schottky contact acted as the anode. Fig. 5.19 illustrates the connection wiring for the characterisation test setting for the Schottky diodes.

Most of the diodes from the fabricated batches worked apart from the Pt batch which had only three working diodes.

5.1.2.4 Data acquisition
In order to obtain the forward bias and the reserved bias of all the diodes, the following two equipment items were used:
1. Agilent 2723A-USB current–voltage system
Agilent 2723A-USB provides a voltage ranging from -20 volts to 20 volts, with the maximum current output per channel being 120mA. Initially, there was too much noise during the acquisition: which was subdued after using co-axial cable to connect the probes and the Agilent channel.

All the diodes were tested and the data acquired was dumped out in the ‘csv’ format for later analysis as illustrated by Fig. 5.20.

![Fig. 5.20. Data acquisition with Agilent unit, 2723A-USB](image)

2. Keithley 2410 source meter
The advantage that the Keithley has over the Agilent is that the Keithley has a larger voltage range of sweeping and it has a maximum current output of 1A. Also, the Keithley can dump the acquired data in text format for storage and later stage analysis. Hence, the Keithley was used to measure the breakdown voltages for those diodes.
5.1.3 Results and assessment of results

To help with analysis, charts were constructed where the same metal but different-sized diodes were plotted together. Further charts plotted different metals but with similarly-sized diodes to obtain a clear picture of how they behave in forward bias as well as in reverse bias.

The following figures (Figs. 5.22, 5.23, 5.24) show the forward bias of each of the Schottky contact metals.

**Fig. 5.22.** A comparison of Ni’s different-sized diodes’ turn-on voltage for increasing Schottky contact area (N1 smallest, N8 largest) – see Appendix 2.
Fig. 5.23. A comparison of Ni’s different-sized diodes turn-on voltage (Batch 2) for increasing Schottky contact area (N1 smallest, N8 largest) – see Appendix 2

It is clear that the forward bias for Schottky diodes with Ni as the Schottky electrode metal is higher than 0.5 volt. It is estimated that the turn-on voltage for Ni is around 0.8 volt to 1 volt.
Fig. 5.24. A comparison of Pt’s different-sized diodes’ turn-on voltage for increasing Schottky contact area (N1 smallest, N8 largest) – see Appendix 2

In this example of Pt as the Schottky electrode metal, in comparison to the other metals, it is interesting to note that even though Pt is considered to have the highest metal work function, the turn-on voltage should be much higher than what is indicated in the graph (turn-on voltage ranges from 0.75 to 0.9 volt).
Fig. 5.25. A comparison of W's different-sized diodes' turn-on voltage for increasing Schottky contact area (A16 smallest, A1 largest) – see also Appendix 2

Fig. 5.25 shows Schottky diodes with W as Schottky electrode metal has turn-on voltage of 0.6 volt to 0.8 volt.

Fig. 5.26. A comparison of Ti's different-sized diodes' turn-on voltage for increasing Schottky contact area (N1 smallest, N8 largest) – see also Appendix A2.1 and A2.2
Based on the observation, Ti has very low turn-on voltage. The turn-on voltage ranges from 0.15 volt to 0.3 volt.

![I-V Curve (Ni,Pt,Ti,W)](image)

**Fig. 5.27. Comparison of the turn-on voltage between Ni, Pt, Ti and W**

In Fig. 5.27, through comparison between the turn-on voltage of Ni, Ti, W and Pt, Ti clearly is a choice for Schottky metal contacts due to its very low turn-on voltage. Of the four metals tested, Ti has the lowest workfunction difference compared to the SiC conduction band edge and therefore is expected to have the lowest turn-on voltage. That it is considerably lower than for the other three metals suggests that the Fermi level of the SiC must be such that the workfunction difference is minimal. However, as seen in Fig.2.4, which is an energy band diagram of those metals and 4H-SiC, the turn-on voltage for Ni and Pt is not as expected. However, W and Pt had very similar turn-on voltage.
According to the diagram in Fig. 2.4, the turn-on voltage of these metals is closer to Ti in the following order (W, Ni, Pt). Experimental results have shown that the order is Ti, W, Pt then Ni. This unexpected behaviour will be discussed later.

In examining the I-V curve (Fig. 5.29) for the breakdown voltage of Ni, Ti, W and Pt, the following results had been obtained. Ni and Pt diode samples had poor reverse bias behaviour. They both broke down at near 25 volts. W and Ti diode samples performed better with W holding out up to near-150 volts before it broke down. For Ti, because of the auto-current limit on the Keithley 2410, data results could not be obtained after -150 volts. Hence, a Keithley with a higher power curve tracer was used for the reversed breakdown measurement. The disadvantage was that as it was an old model, it could not dump the acquired data, hence the reversed breakdown voltage for Ti – B3S1N2 had to be captured from the screen manually (see Appendix 2).

Fig. 5.30 shows the captured reversed bias of the Schottky diode with Ti as the Schottky electrode metal (B3S1N2).
According to breakdown function theory, the behaviour of Schottky diodes with Ni and Pt as Schottky electrode metals in the reversed breakdown current, was as expected. Their unexpected behaviour in the forward bias can be explained as being affected by Fermi-level pinning. According to Han and Lee [62], who conducted research on the 4H-SiC n-type, surface band bending increases about 0.75 eV with Ni deposition. This results in the shifting of the Fermi-level towards the valence band edge. This can be used to explain the behaviour of the Ni. Moreover, another research group [63] has conducted research on localised Fermi-level pinning by defect states. The group conducted their investigation on arrays of Ni, Pt, and Ti Schottky diodes on n-type 4H-SiC. They found that defects located in the thin layer near the epitaxial 4H-SiC cause the inhomogeneity. Also, during their investigation, there was a surprising variation within various samples in terms of the Schottky barrier height and reversed leakage current. Based on this finding, there is a chance that the behaviour of Pt was affected by defects in the n-type 4H-SiC.

Lastly, there is also a micropipe issue with SiC. This is a well-known defect of SiC which means there is a chance that the samples of SiC which were used to fabricate a Schottky electrode with Pt had micropipe defects and this caused the anomaly that had been seen in the result.

Overall, Ti is the most potential candidate for Schottky electrode material because of its low turn-on voltage and high reversed breakdown voltage.
5.1.4 Summary for Section 5.1
A Schottky diode with Ti as the Schottky electrode metal which obtained a low turn-on voltage of 0.25 volt with a breakdown voltage of 600 volts was fabricated. Thus, Ti is the metal of choice for fabricating Schottky diodes but there is also space for improvement for the breakdown voltage. Ti is the most suitable metal when compared to the other metals (Ni, Pt, W) which gave high turn-on voltage or low breakdown voltage and high reverse current.

Ti gives the best I-V characteristic and it is also good at adhering to the SiC. Pt peels off and does not adhere well to the SiC surface. Moreover, Ti is a tough material that can withstand high heat and a hard operating environment but is more prone to oxidation.

5.2 Electrical Characterisation of Metal Contacts to 4H-SiC Enhanced by Pre-Metalisation Surface Treatment

Using electrical current through solutions of HF/ethyl glycol (HF/EG) and HF/H$_2$O, 4H-SiC substrate samples were etched to alter the surface stoichiometry to make a carbon-rich surface. The effect of these treatments on Schottky current–voltage characteristics was investigated. This work was conducted under the guidance of Professor Cao at The Vietnamese Academy of Science and Technology (VAST), Hanoi. After etching, the processed samples were inspected using AFM, XPS, Raman spectroscopy and electrical (current–voltage) tests between pairs of contacts (of a fixed pattern) on the surface. The results show that in comparison to the unetched samples, the current across the surface of the etched samples is approximately two times higher in the HF/EG etched sample and approximately twenty times higher in the HF/H$_2$O etched sample. This experimental work shows that selective etching has altered the surface electrical conductivity and surface roughness. Etching selectively removed silicon atoms leaving a carbon-rich surface. The presence of a carbon-rich interfacial layer between the Schottky metal and the semiconductor will likely lead to a lower barrier height and hence a lower turn-on voltage which in turn will use less power for a given ON-current.
5.2.1 Introduction to the experiment
Ohmic contacts to silicon carbide typically require high temperature processing [64] in order to obtain contact resistances that are suitable for device (e.g. Schottky power diode) operation. It is well established that semiconductor surfaces determine a metal-semiconductor contact’s behaviour [65, 66]. Surface properties that lead to defects, altered bandgap, and addition of an interfacial layer with resistive or insulating properties can all have a significant effect and even dominate a contact’s electrical characteristics. Substrate surfaces as prepared by a supplier will typically go through some cleaning processes but the behaviour of electrical contacts is largely determined by the supplier’s crystal growth and surface finishing. In spite of the theory that it is based on the physics of a semiconductor crystal in contact with a metal, real contacts do not behave well. Surfaces are the reason; the crystal comes to an end and in doing so, is not the same as the bulk. A chemical surface treatment to terminate dangling bonds [67] etc., passivating defect states is common. However, determining the appropriate chemistry for doing so is not well established for different semiconductors. Silicon carbide is used for power devices and the Schottky diode is the most basic and an essential part of power electronics. The two metal contacts to a Schottky diode have different objectives; the Schottky contact should dominate the current–voltage (I-V) characteristic. The only other feature should be the effect of the substrate resistance when the diode is on (well into the forward bias). Carbon as a deposited layer is much reported [68, 69] for enhancing electrical properties of semiconductor devices. This experiment investigates the effects of selective etching of 4H-SiC, using electrochemistry in different solutions: to change the surface stoichiometry, surface roughness, surface conductance and metal-to-4H-SiC electrical characteristics. It is possible, just as in the case for silicides to silicon substrates, to modify a semiconductor’s surface.

5.2.2 Methodology
The experiment was carried out by etching the substrate surface with combinations of HF, ethyl glycol (EG), H₂O and electrical current (3 mA/cm²) through the solutions. 4H-SiC was used for the experiment. These were prepared as previously, with a Ni Ohmic (after heat treatment) contact on the entire back of the sample. This was necessary for the electrochemistry to occur and was also used later for electrical testing. The timing for the etching was 30 minutes with comparison of different
solutions of HF/ethyl glycol and HF/H$_2$O. After etching, the processed samples were inspected by AFM, XPS, Raman spectroscopy and electrically tested and then compared with the un-etched samples.

5.2.3 Results and discussion

Inspection with AFM, XPS and Raman spectroscopy of un-etched and etched samples is provided below. For the un-etched surface, roughness (Ra) is approximately 0.975nm.

5.2.3.1 AFM Investigation

Fig. 5.31. AFM isometric surface profile for a 4H-SiC electrochemically (3 mA/cm$^2$) etched in a HF/H$_2$O solution for 30 minutes

Fig. 5.31 shows the result of AFM surface inspection for the HF/H$_2$O etched sample.

Through inspection of results, the observation is that etching in both HF acid/ethyl glycol and HF/H$_2$O are both shown to have significantly increased surface roughness. As shown by Figs 5.32 and 5.33, inspection by XPS shows higher carbon peaks on some etched surfaces.
Fig. 5.32. XPS spectrum of a 4H-SiC sample electrochemically (3 mA/cm²) etched in a HF/H₂O solution.

Fig. 5.33. XPS spectrum of an un-etched 4H-SiC sample.

Fig. 5.32 shows an XPS spectrum of a sample etched in 0.5% HF/H₂O solution and Fig. 5.33 shows the spectrum of the unetched sample.
In comparing these two figures, it can be seen that there is an increase in the relative height difference between the two spectra which clearly demonstrates an increase in the concentration of carbon at the surface.

5.2.3.3 Raman Spectroscopy Investigation
Raman spectroscopy results are presented in Fig. 5.34.

![Raman Spectra](image)

**Fig.5.34.** Raman spectrum of the HF/H$_2$O etched sample. A is the reference SiC sample. B, C and D are spectra for samples anodically etched in HF/H$_2$O (with 0.5 and 5 mA/cm$^2$ current densities, respectively) and soaked in HF. E is for the sample anodically etched in HF/Ethylglycol and soaked in HF. F is for the sample soaked in HF only.

The analysis shows that by taking the Raman spectrum of the sample etched in 0.5% HF/H$_2$O solution and performing subtraction of the Raman spectrum of the unetched sample, there is an emergence of a weak peak of carbon (G band, at 1598 cm$^{-1}$). The observation noted that the spectra for XPS analysis indicate more clearly the relative increase in carbon at the etched surface.

5.2.3.4 Electrical characterisation
Electrical characterisation was carried out on the etched samples by means of depositing Ni with a thickness of 50nm on the treated surface. Fig.5.35 shows the schematic of the test set-up. Results showed the surface to be significantly more conductive than that for the unetched samples.
By applying probes on the surface to two Ni contacts, the current–voltage test across each sample showed that when comparing the resultant current for the etched, compared to the unetched sample, the current is approximately two times greater in the HF/EG etched sample and approximately twenty times greater in the HF/H₂O etched sample. When samples were tested as Schottky diodes (with the bottom of the samples having an Ohmic contact as previously described) the samples did show a slightly lower turn-on voltage for all etched samples compared to the unetched sample. One of the Ni contacts in Fig 5.35 was the Schottky contact and the turn-on voltage had a voltage range of 0.7 to 0.9 Volts: lower than the 0.8 to 1.0 Volts range of the unetched Ni-SiC diodes.

5.2.4 Summary for Section 5.2
The experiment shows that selective etching has been shown to alter surface electrical conductivity, surface roughness and to selectively remove silicon atoms leaving a carbon-rich surface. The effect was to give a higher surface conductivity and Schottky diodes with lower turn-on voltage.

5.3 Silicon Carbide Substrate Effects on the Behaviour of Ohmic Contacts for Schottky Diodes

5.3.1 Brief introduction to the experiment
The main defect reported for SiC is called the micropipe defect and this, as the name suggests, is a vacancy type defect in the crystal that can extend as a micropipe for many-latticed spacing. Note that other semiconductors have their characteristic-type
defects and an example is gallium arsenide where the major defect listed in GaAs specification sheets is a point defect characterised using an etch of the surface to reveal the point defects and is reported in number per unit area. In SiC the specification sheets for it include a parameter called MPD (Micropipe Density (cm$^{-2}$)) and the lower the MPD the better the SiC crystal quality.

5.3.2 Experiments and results
The Ohmic metal is deposited first and then subjected to a heat treatment of 1000$^\circ$ C in a vacuum furnace for 10 minutes. The effect of heat treatment was investigated by examining several samples of large pairs of Ni pads on samples of 4H-SiC. A test structure for determining the specific contact resistance (SCR) of Ni to SiC Ohmic contacts was also used to compare the SCR of contacts after different process steps and for SiC with different defect densities. A test structure was designed and simulated using the FEM software used previously in this research project. The test structure called the Circular Cross Kelvin Resistor test structure is shown in the Appendix. However, the test structure reported by Collins et al [70], for contacts to bulk semiconductor, was more suitable in this case. Results show that the higher MPD SiC actually gave a lower average SCR value of $2 \times 10^{-6}$ $\Omega$cm$^2$, and low MPD SiC had a SCR of $8.5 \times 10^{-5}$ $\Omega$cm$^2$, for SiC of similar low resistivity of approximately 0.05 $\Omega$cm. The resistivity of the SiC substrates used were determined using Van der Pauw structures. Of the 4H-SiC substrates investigated there was a problem with the high resistivity, low MPD samples in that an Ohmic contact could not be formed with the resources available. These include a variety of metal depositions and low pressure heat treatment up to 1150$^\circ$ C. 4H-SiC substrates investigated included high and low resistivity SiC with high MPD values and low resistivity SiC with low MPD.
In this experiment, it was found that high MPD has more influence on electrical breakdown than Schottky electrode geometry. It is only when MPD of the SiC substrate is low that the optimisation of the Schottky electrode shows beneficial effects. This was observed to be more significant at reverse bias. In forward bias, the optimum Schottky electrode geometry was always necessary irrespective of the level of defects (MPD value). This is most likely due to the fact that in forward bias, breakdown of the diode is due to breakdown of the SiC material where the incidence of highest current density occurs: and this is always near the corner of the electrode. In a perfectly square Schottky electrode where the electrode is smaller than the ‘slab’ of substrate (as typically occurs for fabrication reasons), the highest current density is always at the corner point just below the metal of the electrode and within the SiC material. In reverse bias this is also the likely position for breakdown but as mentioned previously, when the MPD level of the SiC is high, there was no observable trend of breakdown with variation in the Schottky electrode from a square to a circle with varying shaped ‘corners’ in between. When MPD is relatively low, breakdown in forward and reverse bias varied according to Schottky electrode geometry. Tables 5.1 to 5.4 illustrate the relationship between different geometries with MPD and resistivity. The Schottky electrodes in this experiment are all Tungsten (W=2mm x 2mm, D=1mm (electrode width (or diameter in the circle case)), d=0.5mm, t=0.3mm) – R is variable. The geometry for Schottky electrodes in this experiment are illustrated by Figs 5.37, 5.38 and 5.39. W and d are constant for all samples.
Table 5.1. Average I-V characteristics for W-SiC Schottky diodes with different resistivity and associated MPD for the optimised geometry. (R=0.2 mm, d=0.5 mm. D=1mm, t=0.3mm, W=2 mm)

<table>
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<th>Low Resistivity–Low MPD</th>
<th>Low Resistivity–High MPD</th>
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<tr>
<td>$V_{BD}$ (V)</td>
<td>-105</td>
<td>-63</td>
</tr>
<tr>
<td>$V_{TO}$ (V)</td>
<td>(\sim 0.6)</td>
<td>(\sim 0.6)</td>
</tr>
<tr>
<td>$I_{\text{max}}$ (A)</td>
<td>35</td>
<td>31</td>
</tr>
</tbody>
</table>
Table 5.2. Average I-V characteristics for W-SiC Schottky diodes with different resistivity and associated MPD for the optimised geometry. (R=0 mm, d=0.5 mm. D=1mm, t=0.3mm, W=2 mm)

– Square electrode

<table>
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<th>Low Resistivity–High MPD</th>
</tr>
</thead>
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<td>$V_{BD}$ (V)</td>
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<td>-65</td>
</tr>
<tr>
<td>$V_{TO}$ (V)</td>
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<td>0.6</td>
</tr>
<tr>
<td>$I_{max}$ (A)</td>
<td>23</td>
<td>22</td>
</tr>
</tbody>
</table>

Table 5.3. Average I-V characteristics for W-SiC Schottky diodes with different resistivity and associated MPD for the optimised geometry (R=0.5 mm, d=0.5 mm. D=1mm, t=0.3mm, W=2 mm)

– Circle electrode

<table>
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<th></th>
<th>Low Resistivity-Low MPD</th>
<th>Low Resistivity–High MPD</th>
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<tbody>
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<td>$V_{BD}$ (V)</td>
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<td>-68</td>
</tr>
<tr>
<td>$V_{TO}$ (V)</td>
<td>0.6</td>
<td>0.6</td>
</tr>
<tr>
<td>$I_{max}$ (A)</td>
<td>25</td>
<td>25</td>
</tr>
</tbody>
</table>

Table 5.4. Same as Table 5.1 but with carbon-rich surface by selective etching

<table>
<thead>
<tr>
<th></th>
<th>Low Resistivity–Low MPD</th>
<th>Low Resistivity–High MPD</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{BD}$ (V)</td>
<td>-104</td>
<td>-63</td>
</tr>
<tr>
<td>$V_{TO}$ (V)</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>$I_{max}$ (A)</td>
<td>34</td>
<td>29</td>
</tr>
</tbody>
</table>

The MPD and the resistivity of the SiC used also affected the Ohmic contact. Ideally the Ohmic contact has no effect on the current–voltage characteristics. It was observed that once an Ohmic contact could be formed it indeed had little effect on the I-V curves obtained. Even if the value of the specific contact resistance varied considerably, this was not enough to affect the SiC SBD current–voltage characteristics (which obviously must have been dominated by other factors: the
series resistance of the substrate being the main factor competing with contact resistance).

5.3.3 Summary for Section 5.3
The best performing substrate in regard to reverse bias breakdown being at its highest value was the low resistivity SiC/low MPD. It was noted that the slightly poorer SCR value of the low MPD SiC had no effect on the current–voltage characteristics. The breakdown voltage for the low resistivity SiC/low MPD diode was closely related to the Schottky electrode geometry and this was also shown using diodes of similar geometry made using silicon as the substrate. The Ohmic contact for the silicon diodes was aluminium and the Schottky electrode was tungsten.

The specifications of the SiC obtained for this investigation did not give accurate values of resistivity, only ranges were given. Therefore, once Ohmic contacts process steps were established, it was possible (and necessary) to form Van der Pauw test structures to determine resistivity. The low resistivity samples had values that were between 0.03 and 0.09 $\Omega$cm. The high resistivity samples were approximately between $2 \times 10^2$ and $3.5 \times 10^2$ $\Omega$cm.

5.4 Further Experiment with Schottky Electrode Geometry

Investigations of the relationship between Schottky contact geometry and the maximum current a particular Schottky contact can take before it gets destroyed, were carried out.

5.4.1 Fabrication process
There are two parts in the fabrication process: the fabrication of the Ohmic contact and the fabrication of the Schottky contact. Numerous samples were fabricated and laser ablation was used to define trenched regions around some of the samples. Characterisation of the laser ablation process required extensive investigation and was optimised for silicon Schottky diodes. Trenching of SiC was possible but required further characterisation to be as good as for the silicon diodes. Since this experiment is only concerned with geometry versus maximum density, silicon was used in the
fabrication of the Schottky diodes because the trench geometry could be accurately formed.

5.4.1.1 Ohmic contact fabrication
The Ohmic contact was fabricated first, due to the need to anneal the metal electrode to form the Ohmic contact. This would not be possible after Schottky contact formation. The cleaning process was handled similarly to how the previous Schottky diode fabrication processes were handled.

5.4.1.1.1 Metal deposition
The deposition was done with PRO Line PVD 75 – thin film deposition system (e-beam evaporator) from the Kurt J. Lesker Company. The PRO Line PVD 75 is a modular design that can be configured for a variety of thin film deposition applications. See Appendix 3, Section A3.1 for further technical features and detailed information.

Fig. 5.40. PRO Line PVD 75 thin film deposition machine
The metal deposited was Ni which had a thickness of 100 nm. After Ni was deposited onto the silicon substrates for fabrication of an Ohmic contact, the samples were loaded into a furnace for annealing to form a nickel silicide Ohmic contact.

5.4.1.1.2 Annealing
Ni coated silicon wafers are loaded into the VBF-1200X-H8 (1100° C Liter Vacuum Chamber Furnace). See Appendix 3, Section A3.2 for further technical features and detailed information.

Table 5.5 (adapted from [71]) provides brief features for VBF-1200X-H8.
Table 5.5. Features for VBF-1200X-H8

<table>
<thead>
<tr>
<th>Feature</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power</td>
<td>3 KW max</td>
</tr>
<tr>
<td>Voltage</td>
<td>Single phase 208 – 240 VAC / 50/60Hz, (25 A breaker installed)</td>
</tr>
<tr>
<td>Working Temperature</td>
<td>• &lt;= 1000 °C continuously</td>
</tr>
<tr>
<td></td>
<td>• Max. 1100 °C, &lt; 30 minutes</td>
</tr>
<tr>
<td></td>
<td>• Temperature Uniformity: +/- 2°C</td>
</tr>
<tr>
<td>Heating Rate</td>
<td>• Max. 20°C/ min</td>
</tr>
<tr>
<td></td>
<td>• Recommended. 10°C/ min</td>
</tr>
<tr>
<td>Heating Elements</td>
<td>High-quality Ni-Cr-Al resistance wire as heating elements and can be heated up to 1200°C.</td>
</tr>
</tbody>
</table>

Fig. 5.42. Vacuum oven – VBF-1200X-H8
Fig. 5.43. Ni deposited on silicon substrates arranged on a tray before being inserted into the furnace (VBF-1200X-H8)

The annealing of the Ni deposited silicon samples was done in a vacuum chamber (connected to a turbomolecular pump. The process for the annealing was as follows:

- Load samples and pump down the chamber
- Start from room temperature: the ramping up rate is 30°C per minute until the temperature reaches 400°C
- Keep anneal at 400°C for 20 minutes
- Ramp down at 38°C per minute (maximum rate) until reaching room temperature
- Remove annealed samples and store for testing.

5.4.1.1.3 Ohmic contact test

All the annealed wafers were etched at a corner into 2 small islands (on the Ni Ohmic contact) to test the quality of the Ohmic contact. The results for the test confirmed that the Ni to Si (NiSi after heat treatment) on all wafers formed a good Ohmic contact.

5.4.1.2 Schottky contact fabrication

5.4.1.2.1 Surface cleaning

The cleaning process was done similarly to the cleaning process used in the Schottky diode fabrication process.
5.4.1.2.2 Photoresist deposition

The process was done with a SPS Spin 150 spin coater. See Appendix 3, Section A3.3 for further technical features and detailed information.

Fig. 5.44. SPIN150i spin coater used for photoresist deposition for patterning Schottky electrodes

The samples were deposited with photoresist AZ1512.

The settings for the deposition are as follows:

- Speed: 3,000 rpm
- Acceleration: 1000 rpm/s
- Time: 30 seconds.

After the spinning was finished, the thickness for the deposited photoresist was around 2 µm. The samples were immediately removed from the spinner and put onto the hot plate for the soft-bake process.

5.4.1.2.3 Soft-bake

The samples were soft-baked on a hot plate for 2 minutes at 110°C. Fig.5.45 shows the actual hot plate that was used for the soft-bake process.
5.4.1.2.4 Photolithography

The following pattern (Fig. 5.46) is used for patterning an array of Schottky electrode geometry.

![Mask pattern used for defining Schottky electrode geometry. The 'width' (D) of every diode is 1 mm](image)

The pattern was aligned with the sample in the contact mask aligner. The exposure time was 60 seconds.

5.4.1.2.5 Development

The development process and timing was similar to the development process for previous batches of samples in Section 5.1.
5.4.1.2.6 Schottky metal deposition

After development, the samples were arranged onto a dedicated platen to prepare for the metal deposition process.

The deposition was done with the PRO Line PVD 75 – a thin film deposition system platform from the Kurt J. Lesker Company. It was the same machine that was used for deposited Ni to fabricate Ohmic contacts for the diodes. However, for forming a Schottky electrode, three metals were deposited. They were Ni, Cr and Au with the following thickness: 50nm/20nm/20nm (a standard metalisation recipe run at RMIT). Fig. 5.47 illustrates the arrangement of these metals in forming a Schottky electrode.

![Fig. 5.47. Arrangement of metals for Schottky electrode](image)

Normally, this process took around 3 hours to complete. The lift-off process was done with acetone and isopropanol. The samples were put into a container of acetone and to boost up the process, the container was agitated in an ultrasonic bath. After photoresist was lifted off, isopropanol was used to rinse the samples and they were rinsed again under running DI water for around 15 seconds. The final product was ready for testing and data acquisition. Fig. 5.48 shows one of the completed wafers from this fabrication batch.
Fig. 5.48. Schottky diodes with different geometry after lift-off. The diameter of the substrate is 3 inches.

5.4.1.2.7 Substrate dicing

Before conducting electrical tests, the diodes were separated from each other by trenches having similar width and depth in order to separate all the diodes from each other. This was done by using a DAD 321 automatic dicing saw from Disco. A brief list of the features of the DAD 321 dicing saw are as below (adapted from [72]).

- Wafers up to 6 inches in diameter
- Non-contact setup
- 1.5kW synchro spindle
- Dual objective microscope with eyepiece
- Exhaust fan
- Deep cut nozzle.

Fig. 5.49. DAD 321 dicing saw
After loading the stabiliser plate, which secured the sample onto the dicing saw and pulled the cover shield down, the machine automatically diced the sample following the pre-set program. The distance between adjacent diodes was 4000 µm. The depth of the trench was set at 50 µm and the width was the saw’s width, which was 20 µm.

After the sawing operation was completed, the sample was removed from the machine and loaded into a UV heater which helped to remove the plastic sheet which had adhered on top of the sample when the sample was being secured onto the stabiliser plate. The UV heater used was the Benchtop UV Transilluminator, from UVP.
5.4.2 Experimental results

In this experiment the electrode geometry of the Schottky diodes changed in shape from a square to a circle through different extents of rounding of the four corners for each iteration. This experiment was based on the study in Chapter 3 which observed that different geometry will provide different ability to withstand different maximum current: the optimum Schottky electrode geometry is neither a square nor a circle.
In this experiment, there were eleven different Schottky electrode shapes, with shapes transitioning from square to circle. The design of different geometry was based on the concept of D which is the width of the Schottky electrode versus R, which is the normalised corner (see Table 5.6) of the Schottky electrode. R determines the Schottky electrode shape. As the values of R change, the Schottky electrode shape will change accordingly. The geometry shapes for various shapes ranging from square to circle are named from R0 to R10 (R0 is a square and R10 is a circle) as illustrated in Fig. 5.54. In this experiment, the value of D is 1 mm. The dimension and normalised corner radius (Table 5.6) for the fabricated diodes is listed in Table 5.6.

![Diagram of Schottky electrode shapes](image)

**Fig. 5.54. Geometry shapes for various shapes ranging from square to circle are named from R0 to R10. Refer to Table 5.6 for the dimension and normalised corner radius**

| Table 5.6. Dimension and normalised corner radius for the fabricated Schottky diodes |
|---------------------------------|---------------------------------|
| **D (mm)** | **D/2=** | 0.5 | **Square** | **Circle** |
| 1 | | | 0 | 1 | |
| **R** | 0 | 0.05 | 0.1 | 0.15 | 0.2 | 0.25 | 0.3 | 0.35 | 0.4 | 0.45 | 0.5 | |
| **R value** | **(mm)** | 0 | 0.05 | 0.1 | 0.15 | 0.2 | 0.25 | 0.3 | 0.35 | 0.4 | 0.45 | 0.5 | |
| **Normalised Corner Radius (R)** | | 0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1 | |

The test set-up required two probes, one probe connected to the Ohmic contact (adhered to a copper board by silver paste which is electrically conductive), and one probe connected to the Schottky contact.
Fig. 5.55. Schematic for the set-up for testing Schottky diodes with different geometry

The power supply for this test is the PAN60-10A from the Kikusui Company. This unit can generate up to 10A and 60V. Hence the total power output is 600W. This test focused only on the maximum current which a Schottky contact geometry can take before it gets destroyed, hence the ability to generate up to 10A in current is very important.

Fig. 5.56. PAN60-10A regulator DC power supply
The tests resulted in damage to all the Schottky diodes that were tested. Their Schottky contacts were destroyed in some cases.
Table 5.7 shows the acquired data for maximum ON-current (A) for each of the Schottky contact geometry diodes. Refer to Fig. 5.54 and Table 5.6 for details of R0 to R10. The diodes were fabricated with Si substrate: Ni was deposited as the Schottky electrode metal. The constant characteristic dimension for the diodes was 1 mm across (edge centre to edge centre or the diameter in the case of the circle electrode).

<table>
<thead>
<tr>
<th>Contact Geometry</th>
<th>R0</th>
<th>R1</th>
<th>R2</th>
<th>R3</th>
<th>R4</th>
<th>R5</th>
<th>R6</th>
<th>R7</th>
<th>R8</th>
<th>R9</th>
<th>R10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum current</td>
<td>1.15</td>
<td>1.23</td>
<td>1.35</td>
<td>1.5</td>
<td>1.72</td>
<td>2.35</td>
<td>2.52</td>
<td>2.13</td>
<td>1.85</td>
<td>1.67</td>
<td>1.55</td>
</tr>
</tbody>
</table>

Fig. 5.60 shows the relationship between the Schottky electrode geometry versus the maximum ON-current determined for the different diodes. As has been shown in the graph, the ability to take on current increased with the changing of the geometry (starting from the square shape and slowly transforming into a circle). However, this ability is not linear, it will reach a point (a specific geometry) where the ability to withstand current is maximised; then it will decline.
Fig. 5.60. Relationship between Schottky contact geometry and maximum diode current for diodes with varying geometry. The diodes were fabricated with n-type Si substrates and Ni was deposited as the Schottky electrode metal (see note on geometry in Table 5.7)

5.4.3 Summary of Section 5.4
The results from the experiments show that there is a relationship between Schottky contact geometry and the maximum amount of current that a Schottky contact can handle before it gets destroyed. This also conforms to the finding from Chapter 3 that the optimum geometry which can withstand the most current is neither square nor circle but a shape in between.

5.5 Novel Design to Improve Schottky Electrode Current-Taking Ability

The study in Chapter 4 regarding simulation with FEM (NASTRAN) found that there is a way to improve the Schottky contact’s optimum geometry for taking more current. It is done via trenching around the Schottky contact. This experiment explored the possibility through the fabrication of real diodes. A preliminary experiment was done with the help of the Advanced Multidisciplinary MEMS-Based Integrated Electronics NCER Centre of Excellence (AMBIENCE) – Universiti Malaysia Perlis. In this experiment, a laser ablation method was undertaken to create trenches surrounding
the Schottky contact. The experiment was to confirm that it was viable to use laser ablation for the trenching. Figs 5.61 and 5.62 show successful trenching via laser ablation on sample diodes.

**Fig. 5.61.** Laser ablation trenched square Schottky contact with a dimension of 1 mm x 1mm. The substrate was n-type silicon and Ni was deposited as the Schottky electrode metal. (These initial laser ablation tests were conducted on rough polished silicon.)

**Fig. 5.62.** Laser ablation trenched rounded corner Schottky contact with a dimension of 1 mm x 1mm. The substrate was n-type silicon and Ni was deposited as the Schottky electrode metal

After successful preliminary study, it was decided that laser ablation would be used to create trench isolation due to its speed, accuracy and efficiency: it only takes a few seconds for each diode. In comparison, the traditional method for creating a trench surrounding a Schottky contact will take as much as seven steps which range from deposition to multiple masks involved in multiple photolithography processes, etching, growing of silicon dioxide (SiO₂) etc.
5.5.1 Fabrication process
Schottky diodes had to be fabricated as described previously and then the Schottky electrodes were defined by laser ablation. There are two parts to the fabrication process: the fabrication of the Ohmic contact and the fabrication of the Schottky contact. Since SiC is very expensive and difficult to ablate, and as this experiment is only concerned with geometry versus maximum density, silicon was used in the fabrication of the Schottky diodes.

5.5.1.1 Ohmic contact fabrication
The fabrication of Schottky diodes for this study was exactly like the fabrication process in Section 5.4.

5.5.1.2 Laser ablation
The trenching for Schottky contacts were completed at the Advanced Multidisciplinary MEMS-Based Integrated Electronics NCER Centre of Excellence (AMBIENCE) – Universiti Malaysia Perlis (the author had completed the task with the assistance of AMBIENCE’s engineering staff). Resonetics Micromachining Technology Rapid X 250 (Rapid X 250) was used for trenching samples in this experiment. Following, are some features of the Resonetics Micromachining Technology Rapid X 250 (adapted from [73]).

Physical Properties:
- Wavelength: ArF193 nm and KrF 248 nm
- Maximum pulse energy: 120 mJ
- Repetition rate: 500 max (Hz)
- Pulse duration: 20 ns
- Resolution, down to 5 µm or less.

Micromachining materials: silicon, plastics, ceramics, glass, sapphire, other inorganic materials and metals. Refer to Appendix 3, Section A3.5 for further technical features and detailed information.
Laser micromachining provides important aspects such as good quality at high resolution, it is precise, has high process speeds and has low thermal damage. Furthermore, it can be used with many materials in comparison to traditional methods [74]. Rapid X 250 provides highly flexible computer numerical control (CNC) programming depending on prototype shapes. It requires few processing steps and smaller space in a cleanroom facility and has fewer substances which are harmful to humans. The machine used in this experiment consists of mechanical parts and X-Y stages orientation for the laser beam delivery system. They are controlled by a user-friendly GUI (Graphical User Interface) [73].

5.5.1.2.1 Sample Preparation

5.5.1.2.1.1 CAD input for laser ablation
Rapid X 250 can automate the trenching of multiple diodes. For accuracy, the machine requires the input file from AutoCAD (dwg format). All the dimensions and the distance between Schottky electrodes in the file must represent the exact location of all diodes on the sample substrate.

Thus, in this experiment, the mask for fabrication was designed with AutoCAD and the exact same file was fed into the Rapid X 250 console for operation.
5.5.1.2.1.2 Preparation of samples before ablation

The most difficult part of this experiment was the alignment of the laser beam operation and sample diodes. For Rapid X 250 to work effortlessly, the alignment must be accurate and the operator has to make sure that the laser beam will focus on the exact location on the Schottky contact, otherwise, the beam will miss the intended trench region and damage the diodes. Unfortunately, the alignment process must be carried out manually. It was tedious work as it took repeated attempts to align the first Schottky diode in the batch with the laser beam. This a step that could be automated later for rapid manufacturing.

Fig. 5.64. Inside the chamber where samples were loaded for laser ablation (Rapid X 250)

Fig. 5.65. Manual alignment of one of the Schottky diodes with the laser beam
Fig. 5.66. Alignment was observed and adjusted by hand via a monitor attached to the Rapid X 250 X250

Fig. 5.67 illustrates manual alignment of the sample.

Fig. 5.67. Manually aligning the samples with laser beam via a monitor

5.5.1.2.2 Ablation process

When all preparations and alignment steps were completed, the chamber door was closed for operator protection. The next step was to input the operational parameters for the ablation process. The following shows the settings determined (after initial trial and error using best estimate parameters) as being optimised for this experiment.

- Repetitive rate was set to 100 Hz
- HV was set to 0.83 kV
- Energy level was set to 15.0 mJ
- Pressure was set to 5996 mBar.
248nm wavelength is commonly used in the semiconductor industry for laser patterning [73]. The Rectangular Variable Aperture (RVA) parameter in units of millimetres (mm) controls the laser beam size and it affects the design pattern depth and width. Rapid X 250 can provide a maximum of up to 300 pulses and the number of pulses will determine either a coarse or smooth laser line pattern [74]. In this experiment, a laser energy level of 15 mJ was used due to its suitability for silicon material [74] and through experimental observation that more laser repetition actually reduces trench depth. This was explained in [74] which described the observation that existing debris from the ablation process will cover the trench pattern, and thus reduce the ability of the laser beam energy to trench deeper and in fact reduce the depth. Hence, to trench to different depths, for the two batches of diodes, this experiment resorted to using RVA as an influencing parameter for getting deeper trenches (in the process obtaining wider trench-width as RVA increases) and no laser repetition. The first batch was run with a RVA setting of 1.5 mm while the second batch was run with the higher RVA setting of 2.5 mm to obtain a deeper trench depth.

5.5.1.2.3 Trench depth and width checking
After the ablation processes were completed the trench depth and width were determined using a DektakXT stylus profiling machine.

The trench depths and widths obtained for different RVA settings are provided in Table 5.8.

<table>
<thead>
<tr>
<th>RVA setting (mm)</th>
<th>Trench depth (µm)</th>
<th>Trench width (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5</td>
<td>1.1</td>
<td>8</td>
</tr>
<tr>
<td>2.5</td>
<td>2</td>
<td>14</td>
</tr>
</tbody>
</table>

5.5.2 Laser ablation results
All Schottky diode samples were put in a secure container after profiling by the candidate and transported back to Melbourne for image acquiring and electrical testing. The candidate worked at Universiti Malaysia Perlis – Advanced
Multidisciplinary MEMS Based Integrated Electronics NCER Centre of Excellence (AMBIENCE) on several occasions during the project and fabricated samples where brought back each time to RMIT Melbourne for electrical characterisation.

Fig. 5.68 continued on next page.
Fig. 5.68. Captured images of trenched diodes with RVA setting of 1.5 mm (a) R0 to R3, (b) R4 to R7, (c) R8 to R10. Diodes were fabricated with Si, and Ni was deposited as the Schottky electrode metal. The dimension of the diodes was 1 mm in orthogonal direction across the centre (consistent for all diodes and realistic as a constant parameter as it being constant corresponds with constant alignment placement tolerance)

Fig. 5.69 continued on next page.
Fig. 5.69. Captured images of trenched diodes with RVA setting of 2.5 mm (a) R0 to R3, (b) R4 to R7, (c) R8 to R10. Diodes were fabricated with Si, and Ni was deposited as the Schottky electrode metal. The dimension of the diodes was 1 mm in orthogonal direction across the centre (consistent for all diodes and realistic as a constant parameter as it being constant corresponds with constant alignment placement tolerance)

Observations confirm that with different RVA settings, the trench depth and width is also different. In this experiment, when RVA increases, trench depth and width increase accordingly (see Table 5.8).
In this Schottky electrode trenching experiment, there were eleven settings from the AutoCAD file, each of them with a different electrode geometry which is changing from square to circle. Different geometry design was based on the concepts of D which is the width of the Schottky electrode versus R which is the normalised corner radius of the Schottky electrode. R determines the Schottky electrode shape. With the changing values of R, the Schottky electrode shape will change accordingly. The geometry shapes for various shapes ranging from square to circle are named from R0 to R10 (where R0 is square and R10 is circle) as illustrated in Fig. 5.70. In this experiment, the value D is 1 mm. The dimension and normalised corner radius for the fabricated diodes is listed in Table 5.9.

![AutoCAD design with different geometry shapes for Schottky electrode trenching operation ranging from square to circle (R0 to R10)](image)

**Table 5.9. Dimension and normalised corner radius for the trenched diodes**

<table>
<thead>
<tr>
<th>R value (mm)</th>
<th>0</th>
<th>0.05</th>
<th>0.1</th>
<th>0.15</th>
<th>0.2</th>
<th>0.25</th>
<th>0.3</th>
<th>0.35</th>
<th>0.4</th>
<th>0.45</th>
<th>0.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normalised Corner Radius (R)</td>
<td>0</td>
<td>0.1</td>
<td>0.2</td>
<td>0.3</td>
<td>0.4</td>
<td>0.5</td>
<td>0.6</td>
<td>0.7</td>
<td>0.8</td>
<td>0.9</td>
<td>1</td>
</tr>
<tr>
<td>D (mm)</td>
<td>1</td>
<td>D/2= 0.5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Square</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Circle</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

This experiment was based on the study in Chapter 4 which observed that in terms of taking more current, the performance of the Schottky diode will improve by trenching the surrounding of the Schottky electrode. Also, this experiment attempted to compare
the effect of different trench depths versus the ability of Schottky electrode to handle maximum currents with different geometry. The set-up for the test was exactly the same as the test set-up in Section 5.4.2.

Fig. 5.71. Close observation of the trenched diodes electrical test

Maximum current tests were done with all trenched Schottky diodes with different depths and their associated widths (for RVA setting of 1.5 mm and 2.5 mm – see Table 5.8). All the Schottky diodes used in the tests were destroyed.

Fig. 5.72. Destroyed Schottky diode with trench depth from RVA setting of 1.5 mm. Diodes were fabricated with Si, and Ni was deposited as the Schottky electrode metal. The dimension of the diodes was 1 mm x 1mm
Based on data acquired during the test, the two following tables present the maximum current for each Schottky contact geometry with RVS setting of 1.5 mm (refer to Table 5.10) and 2.5 mm (see Table 5.11).

**Table 5.10. Acquired data in the unit of maximum current (A) for each of the Schottky contact geometry with RVA setting of 1.5 mm**

<table>
<thead>
<tr>
<th>Contact Geometry</th>
<th>R0</th>
<th>R1</th>
<th>R2</th>
<th>R3</th>
<th>R4</th>
<th>R5</th>
<th>R6</th>
<th>R7</th>
<th>R8</th>
<th>R9</th>
<th>R10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum current</td>
<td>1.27</td>
<td>1.32</td>
<td>1.43</td>
<td>1.61</td>
<td>1.92</td>
<td>2.73</td>
<td>3.35</td>
<td>3.53</td>
<td>4.41</td>
<td>3.25</td>
<td>2.97</td>
</tr>
</tbody>
</table>

**Table 5.11. Acquired data in the unit of maximum current (A) for each of the Schottky contact geometry with RVA setting of 2.5 mm**

<table>
<thead>
<tr>
<th>Contact Geometry</th>
<th>R0</th>
<th>R1</th>
<th>R2</th>
<th>R3</th>
<th>R4</th>
<th>R5</th>
<th>R6</th>
<th>R7</th>
<th>R8</th>
<th>R9</th>
<th>R10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum current</td>
<td>1.65</td>
<td>1.91</td>
<td>2.65</td>
<td>3.25</td>
<td>3.91</td>
<td>4.25</td>
<td>4.72</td>
<td>5.83</td>
<td>6.91</td>
<td>4.11</td>
<td>3.73</td>
</tr>
</tbody>
</table>
Fig. 5.74 shows that an increase in the RVA setting leads to an increase in the ability of the Schottky electrode to take more current. Also, the results conform to findings in Chapter 4 that trenching the surrounding of the Schottky electrode will lead to better performance in terms of the amount of current intake for the Schottky electrode. It is also different with different Schottky electrode geometry in which there is an optimum Schottky electrode that can take the highest amount of current. Moreover, this experiment also suggests that there is a positive association between trench depth versus the amount of current that a Schottky electrode can take, in which a deeper and wider trench improves the Schottky electrode’s ability to take more current.

Since there is a relationship between the experiment in this section (5.5 – Novel Design to Improve Schottky Electrode Current-Taking Ability) and the experiment in Section 5.4 (Further Experiment with Schottky Electrode Geometry). Thus, the data acquired from all the tests were plotted together to compare the differences between all those designs which range from pure geometry to ablation trenches with different depths and widths surrounding the Schottky electrode.
Fig. 5.75. Comparison between different Schottky electrode designs in terms of current-taking ability

Fig. 5.75 shows that the deeper trenched Schottky diodes (RVS 2.5 mm) outperform the shallower trenched Schottky diodes (RVA 1.5 mm). When comparing the three designs, the non-trenched Schottky diodes performed significantly worse.

5.5.3 Summary for Section 5.5
Through experimental work and real sample fabrication this experiment has concluded, as the study in Chapter 4 had suggested, that there is an optimum geometry for a Schottky electrode. It also suggests that there is a possibility for a novel design using a laser micromachining technique to do ablation, for trenching the surrounding of the Schottky electrode to enhance the performance of the Schottky diode. This novel design also offers a faster method and is cheaper in terms of the cost of fabrication, in comparison to the traditional method of etching the trench.
Chapter 6 – Conclusion and Future Work

6.1. Conclusion

This thesis has successfully examined aspects for enhancing the performance of the Schottky diode for high power applications in terms of the most suitable Schottky electrode metal: improving substrate surface with pre-metalisation surface treatment; the effect of micropipe density (MPD) and resistivity of the silicon carbide substrate Ohmic contact resistance of a Schottky diode; determining the optimum geometry for a Schottky electrode which can withstand maximum current; and, in conjunction with optimised Schottky electrode geometry, has devised a novel design to improve the ability for the Schottky electrode to take more current. There is still room for improvement which will be mentioned in the Future Work section.

During this PhD project, SiC Schottky diodes were fabricated with titanium (Ti) as the Schottky electrode metal and a low turn-on voltage of 0.25 V was obtained. The SiC substrate used did not have the epitaxial layer which is normally used in industrial diodes for enhancing breakdown ability. In this study, the focus was on the Schottky electrode influence on the current–voltage characteristics. Ti is the most suitable metal for a Schottky contact with SiC, and its reliability is enhanced by using a gold coating to prevent oxidation and for good probe contact. Other metals (Ni, Pt, W) gave high turn-on voltage or low breakdown voltage and high reverse current. Thus, Ti is the metal of choice for fabricating Schottky diodes and there is also room for improvement with the breakdown voltage. Ti is also good at adhering to the SiC. Pt peels off: it does not adhere well to the SiC surface, as is the case for other surfaces too.

6.1.1. A carbon rich surface can improve the Schottky behaviour of a Schottky interface. This research has shown that apart from the traditionally employed methods of depositing a carbon layer (e.g. graphene or graphitic carbon), using selective etching has been shown to alter the surface electrical conductivity, surface roughness and to selectively remove silicon atoms leaving a carbon-rich surface. By selective etching of Si atoms leaving a carbon-rich surface which is intrinsic to the substrate, the etched surface has higher electrical conductivity and leads to lower turn-on
voltages. The improvement was clearly observed in the case of 4H-SiC substrates which had low resistivity and low MPD (micropipe density). Note that the simplification of having no epitaxial layer and only a uniformly doped substrate led to increased confidence in the results.

6.1.2. Experimental results showed that the best performing substrate in regard to reverse bias breakdown being at its highest value was the low resistivity SiC/low MPD substrate. It was noted that the slightly poorer specific contact resistance values of Ohmic contacts to the low MPD SiC had no significant effect on the current–voltage characteristics. The breakdown voltage for the low resistivity SiC/low MPD diode was closely related to the Schottky electrode geometry and this was also shown using diodes of similar geometry which were made using silicon as the substrate. The Ohmic contact for the silicon diodes was aluminium and the Schottky electrode was also tungsten. The Si electrodes had laser trenching added to their fabrication steps and this showed improvement in the forward bias breakdown current and reverse bias breakdown voltage.

6.1.3. This research shows that there is a relationship between Schottky contact geometry and the maximum amount of current-taking ability for a Schottky contact before it gets destroyed. Experimental results showed that there is an optimum geometry which can withstand the most current and it is neither square nor circle but at a particular geometry in between (i.e. rounded corners of a particular radius for an otherwise square electrode).

6.1.4. A novel design was designed, modelled, fabricated and successfully tested. Experiments of real sample fabrication of the novel design, used laser micromachining machine to do ablation for trenches surrounding Schottky electrodes to enhance the performance of the Schottky diode. They lead to the conclusion that the optimum geometry for electrodes to a Schottky diode can be further enhanced by designing a trench surrounding the Schottky electrode using the laser ablation method. This novel design also offers a faster and cheaper cost in terms of fabrication in comparison to the traditional method of etching the trench.
6.2. Future Work

Due to the scope and time limits of this research, there are many aspects which are left for further work. Below is the recommendation for future work.

6.2.1. Titanium is a very good candidate to use as the Schottky electrode metal for power Schottky diodes. However, titanium is also prone to oxidation at high temperature, hence there is a need to explore ways to minimise or eliminate this weakness via better packaging or coating the titanium electrode surface. Gold was used as an overcoat in this work but the addition of a barrier layer and minimum thicknesses should be investigated to determine their effect, for example, on Mean Time to Failure (MTTF).

6.2.2. The surface treatment of SiC via selectively etching of silicon atoms was conducted manually by hand which was very dangerous due to the usage of hydrofluoric acid (HF), and was time-consuming. Thus, for use in mass production purposes, more research is needed into how to make the process safer, less time-consuming and, if possible, how to automate the process with some specialised equipment. Further investigation is required to determine the consistency in the lowering of turn-on voltage for different metals and to optimise the etching process for this.

6.2.3. Even though a novel improved design has been realised, there are still areas to consider such as the upper limitation of the depth and the width in which the positive effect of trenching will not outweigh the negative effect on the design (due to refilling of the trenches with the debris from ablation). Also, even though with laser micromachining it is possible to have mass production through automation, there are still aspects to improve and overcome such as manual alignment which is also timing-consuming. Further the possibility of miss-alignment needs to be determined and controlled. However, with this process, many electrode trenches can be formed after one accurate alignment. This can be done by tuning the controlling code for the machine as well as doing some fine-tuning with the input file for the automation process. Lastly, laser micromachining techniques are used in medical operations and some investigation could be done with those machines to examine whether it is
possible to use them in mass production for trenching of the Schottky electrode. The limitation of those machines is the low power that they generate because human tissue is far less tough to penetrate than the materials which are used in manufacturing the Schottky diode (e.g. metals, silicon, silicon carbide, etc.).
Appendix 1 – Circular Cross Kelvin Resistor Test Structure for Low Specific Contact Resistivity

Ohmic contacts are important for power diodes and minimising the contact resistance is a serious objective to reduce power loss. This appendix describes a technique developed as a side study for this thesis but relevant to the thesis topic. The content was reported by the candidate at an international conference and was peer reviewed.

In determining the specific contact resistance of an Ohmic contact, using conventional Cross Kelvin Resistor (CKR) test structures, it was found that the errors in doing so occur from parasitic resistances around the contact. These parasitic resistances are difficult to determine because no convenient analytical expression is available to calculate this resistance. However, electrical current entering a circular contact uniformly from all directions can be modelled using analytical expressions. Here we present a new test structure where parasitic resistance can easily be calculated because it occurs between concentric equipotentials. This resistance is then subtracted from the total resistance to give the resistance due to the contact interface and hence the specific contact resistance of that interface. Using aspects of the CKR and the Circular Transmission Line Model (CTLM), we have designed a new test structure, here called the Circular Cross Kelvin Resistor (CCKR) test structure for determining specific contact resistance.

A.1. Introduction

The Cross Kelvin Resistor (CKR) test structure has been used for more than 20 years to determine the specific contact resistance ($\rho_c$) of Ohmic contacts which are typically metal-to-semiconductor contacts. The ideal CKR [75] (see Fig. A1.1a) is not realisable because to fabricate such a structure requires perfect alignment of the two contact layer CKR features. Real CKRs obey standard design rules and the semiconductor active layer surrounding the contact adds parasitic resistance (error) to the contact interface resistance (due to $\rho_c$) determined from CKR measurements. It is the estimation of this error that has been the focus of many research papers. Here we
propose a test structure that is a modified CKR structure and has an easily determined (using an analytical model [76]), parasitic resistance.

The Circular Transmission Line Model (CTLM) [77] was developed for determining specific contact resistance using an easily fabricated test structure. However, the CTLM is not suitable for determining low values of specific contact resistance [78]. The CTLM uses the regularity of circular concentric equipotentials to determine the resistance between a circular (ring) contact and a central circular disc contact. Such resistances are easier to model than the resistance of the parasitic region surrounding a contact in a CKR test structure (Fig.1b) [79-82]. The regularity of circular concentric equipotentials was used in a previous study [77] to model the parasitic resistance around a circular contact in a CKR. The equation developed in [76] is given here (1).

\[
\rho_c' = \rho_c + \frac{R_{SH} w^2}{8} \left( \frac{d}{w} \right)^2 \left[ \frac{1}{4} - \ln \left( \frac{d}{w} \right) \right]
\]  

(1)

The parameters used in (1) are as follows:

- \( \rho_c \) is the true specific contact resistance (Ωcm2)
- \( \rho_c' \) is the specific contact resistance determined from measurements and includes the effect of parasitic resistance.
- \( R_{SH} \) is the sheet resistance of the semiconductor active layer
- \( w \) is the width of the region of the semiconductor layer around the contact
- \( d \) is the diameter of the contact.

Equation (1) assumes circular equipotentials around the contact which is not the case for the entire parasitic region around a conventional CKR contact. In the CKR, \( w \) is the width of the semiconductor arms. Therefore, in this study we present a new type of CKR test structure (the Circular Cross Kelvin Resistor (CCKR). In the CCKR, \( w \) is the diameter of the semiconductor region around the contact.
A.2. Test structure design

Fig. A1.1b shows a CKR test structure with a relatively small circular contact. Close to the contact, which is small compared to the width of the voltage tap and current arms, the equipotentials are concentric. However, away from the contact they are not because of the asymmetry due to the voltage tap in the semiconductor layer. This asymmetry is difficult to model using analytical expressions and therefore the parasitic resistance due to the region around the contact, which increases the voltage measured on the voltage tap, cannot be readily calculated. If the region around the contact was a circular region with uniform current flowing to the contact, then the parasitic resistance could readily be calculated from (1). The ideal case for (1) to be applicable is represented by the schematic of Fig. A1.2. To test (1), finite element modelling (FEM) software was used to model and simulate the test structure shown in Fig. 2 and results are compared to determine the accuracy of this equation. In effect, the voltage tap (in Fig. A1.2) is the entire circumference of the semiconductor active region but of course this is not practicable. A practical design is shown in Fig. A1.3. FEM models were made to determine if this design suitably represents the structure in Fig. A1.2.
Fig. A1.1b. CKR with a small circular contact

Fig. A1.2. Schematic of ideal test structure to be used with equation (1). Note the arrows represent current flowing into the semiconductor layer. $V_2$ is now the equipotential that is at all points on the circumference because the input current density is uniform.
Fig. A1.3. Schematic of practical test structure to be used with equation (1). Note the arrows represent current flowing into the semiconductor and $V_k$ is the voltage sensed on the voltage tap

A.3. Test structure modelling

In order to test the accuracy of (1), FEM models were made based on the schematic of Fig. A1.2. Simulations were run using these models to determine $V_k$ for different $R_{SH}$ and $\rho_c$ combinations. These steps were repeated for CCKRs with a voltage tap (shown as a schematic in Fig. A1.3) to see how accurately such a structure could be used in conjunction with (1) to determine $\rho_c$. Fig.A1.4a shows the distribution of equipotentials (obtained by FEM) that occur around a contact for uniform current flowing from all directions towards the contact. Fig.A1.4b shows the slight distortion that occurs in the equipotential distribution due to the presence of a voltage tap. Further investigation is required to determine improved designs for current input and for the positioning the voltage tap.
A.4. Results and discussion

Results of the simulations of FEM models of CCKR structures with and without voltage taps are presented in Tables A1.1 to A1.3. These tables also include results for comparing the analytical model with the FEM models for different values of $R_{SH}$ and $\rho_c$. For equation (1) to accurately model the CCKR the value of $\alpha r_0$ should be less than 2, where $\alpha$ is the attenuation factor ($\alpha = \frac{1}{L_t}$, $L_t$ is the transfer length $\left(\frac{\rho_c}{\sqrt{R_{SH}}}\right)$) and $r_0$ is the radius of the contact ($r_0 = \frac{d}{2}$).

Equation (1) accounts for parasitic error (PE) and can be written as follows:

$$\rho' = \rho + PE$$

$$PE = \frac{R_{SH} w^2}{8} \left(\frac{d}{w}\right)^2 \left[\frac{1}{4} - \ln \left(\frac{d}{w}\right)\right]$$
Using (3), we will subtract the value of PE for a particular CCKR from the value of \( \rho_{c}' \) obtained from the FEM models using \( V_{K} \), current I and contact area A. Note, \( R_{K} = \frac{V_{K}}{I} \) and \( \rho_{c}' = R_{K} \times A \).

Table A1.1. Results obtained from FEM models for \( \rho_{c}' \) and \( \rho_{c} \) for \( R_{SH} = \frac{50\Omega}{\text{SQR}} \) AND \( \rho_{c} = 10 \times 10^{-8} \Omega \text{cm}^2 \). \( W = 10 \mu m \)

<table>
<thead>
<tr>
<th>( d/W )</th>
<th>( \alpha_{c} )</th>
<th>( \rho_{c}' )-ANL</th>
<th>( \rho_{c}' )-FE1</th>
<th>( \rho_{c}' )-FE1</th>
<th>( \rho_{c}' )-FE2</th>
<th>( \rho_{c} )-FE2</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>1.1</td>
<td>25.9</td>
<td>15.9</td>
<td>26.3</td>
<td>10.4</td>
<td>24.5</td>
</tr>
<tr>
<td>0.2</td>
<td>2.2</td>
<td>55.8</td>
<td>46.5</td>
<td>56.5</td>
<td>9.32</td>
<td>51.2</td>
</tr>
<tr>
<td>0.3</td>
<td>3.3</td>
<td>91.8</td>
<td>81.8</td>
<td>88.09</td>
<td>6.29</td>
<td>84.7</td>
</tr>
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<td>0.4</td>
<td>4.4</td>
<td>126</td>
<td>116</td>
<td>117</td>
<td>1</td>
<td>120</td>
</tr>
<tr>
<td>0.5</td>
<td>5.6</td>
<td>157</td>
<td>147</td>
<td>139</td>
<td>-8</td>
<td>133</td>
</tr>
</tbody>
</table>

(NOTE: ‘ANL’ indicates the analytical model and ‘FE1’ and ‘FE2’ indicate the FEM models for the CCKRs with and without a voltage tap, respectively. PE is the parasitic error determined by the analytical model (3). Values of specific contact resistivity are given in units of \( \Omega \mu \text{m}^2 \)).
Table A1.2. Results obtained from FEM models for $\rho_c'$ and $\rho_c$ for $R_{SH} = \frac{50\Omega}{\text{SQR}}$ AND $\rho_c = 100 \times 10^{-8} \ \Omega \text{cm}^2$. $W=10\mu$m.

<table>
<thead>
<tr>
<th>$d/w$</th>
<th>$\alpha r_0$</th>
<th>$\rho_c'$-ANL</th>
<th>$P_E$</th>
<th>$\rho_c'$-FE1</th>
<th>$\rho_c$-FE1</th>
<th>$\rho_c'$-FE2</th>
<th>$\rho_c$-FE2</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.35</td>
<td>116</td>
<td>16</td>
<td>116</td>
<td>100</td>
<td>114</td>
<td>98</td>
</tr>
<tr>
<td>0.2</td>
<td>0.71</td>
<td>147</td>
<td>47</td>
<td>147</td>
<td>100</td>
<td>141</td>
<td>94</td>
</tr>
<tr>
<td>0.3</td>
<td>1.06</td>
<td>182</td>
<td>82</td>
<td>182</td>
<td>100</td>
<td>173</td>
<td>91</td>
</tr>
<tr>
<td>0.4</td>
<td>1.41</td>
<td>216</td>
<td>116</td>
<td>214</td>
<td>98</td>
<td>201</td>
<td>85</td>
</tr>
<tr>
<td>0.5</td>
<td>1.77</td>
<td>247</td>
<td>147</td>
<td>241</td>
<td>94</td>
<td>229</td>
<td>82</td>
</tr>
</tbody>
</table>

Table A1.3. Results obtained from FEM models for $\rho_c'$ and $\rho_c$ for $R_{SH} = \frac{50\Omega}{\text{SQR}}$ AND $\rho_c = 1 \times 10^{-9} \ \Omega \text{cm}^2$. $W=10\mu$m.

<table>
<thead>
<tr>
<th>$d/w$</th>
<th>$\alpha r_0$</th>
<th>$\rho_c'$-ANL</th>
<th>$P_E$</th>
<th>$\rho_c'$-FE1</th>
<th>$\rho_c$-FE1</th>
<th>$\rho_c'$-FE2</th>
<th>$\rho_c$-FE2</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>1.11</td>
<td>0.26</td>
<td>0.16</td>
<td>0.27</td>
<td>0.11</td>
<td>0.24</td>
<td>0.08</td>
</tr>
<tr>
<td>0.2</td>
<td>2.2</td>
<td>0.57</td>
<td>0.47</td>
<td>0.57</td>
<td>0.10</td>
<td>0.52</td>
<td>0.05</td>
</tr>
<tr>
<td>0.3</td>
<td>3.36</td>
<td>0.92</td>
<td>0.82</td>
<td>0.89</td>
<td>0.07</td>
<td>0.68</td>
<td>-0.14</td>
</tr>
<tr>
<td>0.4</td>
<td>4.48</td>
<td>2.17</td>
<td>1.17</td>
<td>2.21</td>
<td>0.04</td>
<td>0.83</td>
<td>-0.34</td>
</tr>
<tr>
<td>0.5</td>
<td>5.6</td>
<td>2.46</td>
<td>1.46</td>
<td>2.51</td>
<td>0.05</td>
<td>0.88</td>
<td>-0.57</td>
</tr>
</tbody>
</table>

For good agreement/verification (of the analytical model) there should be little difference between $\rho_c'$ for the analytical model and for FE1. Results show that this always occurs for $\alpha r_0 < ~2$. It occurs (but not always) for other values of $\alpha r_0$ too (see Table A1.1) but always for $\alpha r_0 < ~2$. For values of $\alpha r_0 > 2$ it is obvious that results obtained using FE1 are poor and with FE2 are meaningless.

If an AFM electrical probe is used to contact the centre contact (diameter d) then electrical measurements corresponding to FE1 can be made. Allowing for parasitic resistance will give an accurate determination of specific contact resistance (SCR). If
a voltage tap is used as in FE2 then an accurate value of SCR can be determined but for lower values of \( \alpha_0 \). PE values for different \( \frac{d}{w} \) can be determined without knowing SCR. By determining SCR’ then SCR can be determined and also \( \alpha_0 \) if this is done for several \( \frac{d}{w} \) and if \( \alpha_0 \) is appropriately small and the SCR is consistent, then confidence can be had in the SCR obtained.

A.5. Conclusion and further work

Results demonstrate that the presence of a small voltage tap does not significantly disturb the equipotential distribution because the allowed deviation of the measured SCR can realistically be 100% and this is much greater than the difference obtained in this work. For example, a value of \( 1 \times 10^{-8} \) \( \Omega \text{cm}^2 \) is not significantly different to \( 2 \times 10^{-8} \) \( \Omega \text{cm}^2 \). Further work suggested is to modify the shape of the active area to compensate for the effect of the voltage tap. This could be done by finite element modelling to determine what egg shape for example would be appropriate for this compensation.
Appendix 2 – Schottky Diode Area Information and Naming Convention

A2.1. Schottky diode area information

This section contains tables which provide information about the area for Schottky diodes with Schottky electrodes made from: nickel (Ni), platinum (Pt), titanium (Ti) and tungsten (W)

Table A2.1. Area for Schottky diodes with Schottky electrodes made from Ni, Pt and Ti

<table>
<thead>
<tr>
<th>Diode</th>
<th>Diameter (mm)</th>
<th>Radius (mm)</th>
<th>Area (mm²)</th>
<th>Area (cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0.5</td>
<td>0.785</td>
<td>0.00785</td>
</tr>
<tr>
<td>2</td>
<td>1.2</td>
<td>0.6</td>
<td>1.1304</td>
<td>0.011304</td>
</tr>
<tr>
<td>3</td>
<td>1.5</td>
<td>0.75</td>
<td>1.76625</td>
<td>0.0176625</td>
</tr>
<tr>
<td>4</td>
<td>1.7</td>
<td>0.85</td>
<td>2.26865</td>
<td>0.0226865</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>1</td>
<td>3.14</td>
<td>0.0314</td>
</tr>
<tr>
<td>6</td>
<td>2.4</td>
<td>1.2</td>
<td>4.5216</td>
<td>0.045216</td>
</tr>
<tr>
<td>7</td>
<td>3</td>
<td>1.5</td>
<td>7.065</td>
<td>0.07065</td>
</tr>
<tr>
<td>8</td>
<td>4.8</td>
<td>2.4</td>
<td>18.0864</td>
<td>0.180864</td>
</tr>
</tbody>
</table>
Table A2.2. Area for Schottky diodes with Schottky electrodes made with W

<table>
<thead>
<tr>
<th>Area #</th>
<th>Area (mm²)</th>
<th>Area (cm²)</th>
</tr>
</thead>
<tbody>
<tr>
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</tr>
<tr>
<td>A2</td>
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<td>0.005</td>
</tr>
<tr>
<td>A3</td>
<td>0.2</td>
<td>0.002</td>
</tr>
<tr>
<td>A4</td>
<td>0.1</td>
<td>0.001</td>
</tr>
<tr>
<td>A5</td>
<td>0.5</td>
<td>0.005</td>
</tr>
<tr>
<td>A6</td>
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<td>0.0025</td>
</tr>
<tr>
<td>A7</td>
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<td>0.001</td>
</tr>
<tr>
<td>A8</td>
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<td>0.0005</td>
</tr>
<tr>
<td>A9</td>
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<td>0.002</td>
</tr>
<tr>
<td>A10</td>
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<td>0.001</td>
</tr>
<tr>
<td>A11</td>
<td>0.04</td>
<td>0.0004</td>
</tr>
<tr>
<td>A12</td>
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<td>0.0002</td>
</tr>
<tr>
<td>A13</td>
<td>0.1</td>
<td>0.001</td>
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<tr>
<td>A14</td>
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</tr>
<tr>
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<td>0.0001</td>
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</table>
A2.2. Schottky diode naming

This section provides information regarding the naming for associated areas for nickel (Ni), platinum (Pt) and titanium (Ti).

![Fig. A2.1. Areas associated with different sizes of Schottky diodes](image)

The naming convention follows the convention shown in Tables A2.3, A2.4, A2.5 and A2.6
Table A2.3. The naming convention for the Schottky diode with the Ni Schottky electrode and their areas in fabrication: Batch 1, Sample 1

<table>
<thead>
<tr>
<th>Batch #</th>
<th>Sample #</th>
<th>Metal associated</th>
<th>Area #</th>
<th>Naming convention</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
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<td>Ni</td>
<td>1</td>
<td>B1S1N1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>Ni</td>
<td>2</td>
<td>B1S1N2</td>
</tr>
<tr>
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</tbody>
</table>

Table A2.4. The naming convention for the Schottky diode with the Ni Schottky electrode and their areas in fabrication: Batch 1, Sample 2

<table>
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<tbody>
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</table>
Table A2.5. The naming convention for the Schottky diode with the Pt Schottky electrode and their areas in fabrication: Batch 2, Sample 1

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<th>Metal associated</th>
<th>Area #</th>
<th>Naming convention</th>
</tr>
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<tbody>
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Table A2.6. The naming convention for the Schottky diode with the Ti Schottky electrode and their areas in fabrication: Batch 3, Sample 1

<table>
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<th>Sample #</th>
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</table>
Fig. A2.2 and Table A2.7 provide the naming convention and associated areas of the Schottky diodes with tungsten (W) as the Schottky electrode.
Table A2.7. The naming convention for the Schottky diode with W as the Schottky electrode and their areas in fabrication: Batch 4, Sample 1

<table>
<thead>
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<th>Area #</th>
<th>Naming convention</th>
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<td>2</td>
<td>B4S1A2</td>
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</table>
Appendix 3 – Technical Information for Equipment Used in the Research Experiments

A3.1. PRO Line PVD 75

The deposition was done with PRO Line PVD 75 – thin film deposition system (e-beam evaporator) from the Kurt J. Lesker Company. The PRO Line PVD 75 is a modular design that can be configured for a variety of thin film deposition applications [83].

- Up to four HV magnetron sputtering sources
- Up to one multi-pocket electron beam evaporation source
- Up to four thermal evaporation sources
- Up to two organic evaporation sources available (multi-technique options available)
- Wet or dry rough pumping, turbo pump, or cryogenic pump high vacuum pumping options available
- Standard configurations compatible with up to 11" OD substrates; up to 850°C heating, cooling, and biasing options available
- Single wafer, zero-footprint load lock option available for substrates up to 6"
- PRO Line series of PVD tools include KJLC's innovative eKLipse™ base control package with the ability to upgrade to the eKLipse™ advanced control package.

A3.2. VBF-1200X-H8 (1100°C Liter Vacuum Chamber Furnace)

The VBF-1200X-H8 is a UL/CSA standard vacuum furnace. It is equipped with a 7.5" ID x 13.4"L quartz tube chamber sitting horizontally. Water-cooled stainless steel vacuum flanges with valves are installed to achieve a vacuum of $10^{-2}$ to $10^{-5}$ Torr through a mechanical or molecular vacuum pump. It is designed for annealing semiconductor wafers (up to 6") under vacuum or various other gas atmospheres with a temperature up to 1100°C. It also can also be used as vacuum brazing furnace for fusing small parts. Table A3.1 (adapted from [71]) provides some brief features for VBF-1200X-H8.
### Table A3.1. Features for VBF-1200X-H8

<table>
<thead>
<tr>
<th>Feature</th>
<th>Specification</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Power</strong></td>
<td>3 KW max</td>
</tr>
<tr>
<td><strong>Voltage</strong></td>
<td>Single phase 208 - 240 VAC / 50/60Hz, (25 A breaker installed)</td>
</tr>
<tr>
<td><strong>Working Temperature</strong></td>
<td>• &lt;= 1000 °C continuously</td>
</tr>
<tr>
<td></td>
<td>• Max. 1100 °C, &lt; 30 minutes</td>
</tr>
<tr>
<td></td>
<td>• Temperature Uniformity: +/- 2°C</td>
</tr>
<tr>
<td><strong>Heating Rate</strong></td>
<td>• Max. 20°C/ min</td>
</tr>
<tr>
<td></td>
<td>• Recommended. 10°C/ min</td>
</tr>
<tr>
<td><strong>Heating Elements</strong></td>
<td>High-quality Ni-Cr-Al resistance wire as heating elements and can be heated up to 1200°C.</td>
</tr>
</tbody>
</table>

### A3.3. SPS Spin 150 Spin Coater

The following provides the features of the machine (adapter from [84, 85]).

The coater offers a vacuum secured sample holder with capabilities ranging from very small samples to up to 150 mm diameter or 101.6 mm x 101.6 mm square substrates. The programs are easy to set up with up to 99 steps per program, 0 - 2,000 rpm/sec acceleration, a max speed of 10,000 rpm and a maximum time per step of 6000 seconds.

- Affordable spin coater for universities
- Spin processor for cleaning, drying, coating, developing and/or etching of up to Ø 160 mm substrates
- Full-plastic system in natural polypropylene (NPP)
- Table-top model for manual or automated (optional) chemical dispense
- Transparent lid with syringe holder for central dispensing
- Electro-magnetic safety lid lock
- Detachable controller interface for easy integration
- N2 diffuser for N2 purge during process
- Easy, step-by-step recipe programming via large colour touchscreen
• Unlimited program storage for recipes with multiple steps / each for:
  ▪ Time 0.1-99999 sec/step
  ▪ Speed 0-12,000 rpm
  ▪ Rotation direction (CW, CCW, puddling)
  ▪ Acceleration/Deceleration 1-30,000 rpm/sec, selectable per step
  ▪ Vacuum On/Off
• 3 Programmable dry contacts: e.g. for automated control of dispense unit, nitrogen diffuser, etc.
• Structured and password protected recipe storage for easy and safe management
• Digitally controlled motor with digital incremental speed signal feedback.

A3.4. DAD 321 Automatic Dicing Saw

The brief features of the DAD 321 dicing saw are as below (adapted from [72]).
• Up to 6” wafers
• Non-contact set-up
• 1.5kW synchro spindle
• Dual objective microscope with eyepiece
• Exhaust fan
• Deep cut nozzle.

A3.5. Resonetics Micromachining Technology X 250

The Resonetics Micromachining Technology Rapid X 250 (Rapid X 250) was used for trenching samples in this experiment. Following are some features of the Resonetics Micromachining Technology X 250 (adapted from [73]).

Physical Properties:
• Wavelength: ArF193 nm and KrF 248 nm
• Maximum pulse energy: 120 mJ
• Repetition rate: 500 max (Hz)
- Pulse duration: 20 ns
- Resolution, down to 5 µm or less.

Micromaching materials: silicon, plastics, ceramics, glass, sapphire, other inorganic materials and metals

It is a tool for quick investigation of the work on the prototype with low cost in the following applications: microholes in the biomedical catheters, microfluidic channels, microlens array, plastic stent, microvias for circuit packaging, microholes for ink jet nozzles, fibre grating, etc.

**A3.6. DektakXT Stylus Profiling Machine**

The features from [86] stated that DektakXT® stylus profiler features a revolutionary design that enables unmatched repeatability of 4Å and up to 40% improved scanning speeds. This major milestone combined with its other breakthroughs, uniquely enable the DektakXT to perform the critical nanometre-level film, step and surface measurements needed to power future advances in the microelectronics, semiconductor, solar, high-brightness LED, medical, scientific and materials science markets. Moreover, DektakXT implements a single-arch design and also incorporates a true-colour HD optical camera to harness 64-bit parallel processing architecture to achieve optimal measurement and operating efficiency.
Fig. A3.1. Dektak XT stylus profiling machine

Fig. A3.2. Dektak XT moves to sample for profiling

Fig. A3.3. Dektak XT locating point for profiling
List of Publications


References


