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Introduction
1.1 Introduction

In the last few decades, we have witnessed tremendous improvements/change in our life style. One of the contributing factors to this is the developments in the field of semiconductor technology. Ever since the invention of the first semiconductor transistor in 1957 and integrated circuit a decade later, microelectronics technology has transformed the way people work and live. Today electronics is being used in the areas as diverse as computers, communication, entertainment, military, aerospace, automobiles, healthcare, information storage and retrieval, industrial production, scientific research etc. Electronics industry has proved to be an imperative part of economical development of many countries.

The basic semiconductor material used for most of the applications is silicon (Si). This technology is the oldest and the most refined. However, the recent research and development in semiconductor technology has brought this traditional semiconductor to its theoretical limit. Si-based technologies for power application have difficulties to deliver powers of the order 10 W and more at frequencies above 3 GHz. The power device requirements for many utility applications of power electronics are at a point where the present Si based power devices cannot handle. The requirements include higher blocking voltages, switching frequencies, efficiency, and reliability.

Due to these limitations and to meet the ever increasing high-power-high-frequency requirements, a new breed of semiconductors called wide band gap (WBG) semiconductors such as silicon carbide (SiC), zinc oxide (ZnO) and group III-Nitride semiconductors like gallium nitride (GaN), aluminum nitride (AlN), and indium nitride (InN) and their alloys
are currently being developed and are receiving intense research effort. These new semiconductors possess several striking material properties that make them suitable for the applications for which Si and other semiconductors cannot be used [1]. Apart from being chemically stable and physically hard, they offer tremendous advantages in terms of power capability (DC and microwave), radiation insensitivity, high operating temperature, high frequency operation, better linearity, optical properties and low noise capability [2,3].

These large bandgap materials allow commercialization in the environments such as pressure vessels, combustion engines, and near nuclear reactors, where Si and GaAs cannot be used due to smaller bandgap.

1.2 Advantages of Gallium Nitride Material System

Gallium nitride (GaN) is regarded, by many, as the most important new semiconductor material since silicon, and it is generating a huge international interest. GaN is a III-V compound semiconductor (gallium in group III and nitrogen in group V of periodic table) with a wide direct band gap (E_g) of 3.4 eV. Other interesting physical properties of GaN include high thermal conductivity, high melting temperature, low dielectric constant and high breakdown voltage. These properties make GaN suitable for high power RF transmission applications. GaN transistors withstand extreme heat and are capable of handling frequencies and power levels well beyond those possible with silicon, gallium arsenide, silicon carbide, or essentially any other semiconductor yet fabricated. GaN can manage both high speeds and high signal purity at high power. It is believed as “The Toughest Transistor Yet” [4]. For instance, today’s state-of-the-art GaN based high electron mobility
transistor devices (AlGaN/GaN HEMTs) exhibit a total output power over 100 W. They also show high efficiency and boast improved device robustness [5]. GaN devices are insensitive to high operating temperatures and hence their performance does not degrade significantly from thermal-based device breakdown. Delivering complete improvements in RF transmission signal processing, GaN is the quintessential semiconductor material for enabling 2.5G and 3G communication services and applications [6-8].

Together with the other direct band gap nitride semiconductors like AlN (Eg=6.2 eV) and InN (Eg=1.89 eV) [figure 1.1] [9], GaN can be alloyed to engineer its electronic and physical properties suitable for a specific device design rather than designing a device around a semiconductor. For example, by varying InN and GaN proportions, the band gap of the resulting InGaN can possibly be orchestrated between 1.89 and 3.4 eV, which is the energy range for infrared, visible, and ultraviolet light. Such materials can produce light of any color. The GaN-InN system has proved itself as a successful technology for optoelectronic devices such as light emitting diodes (LEDs), laser diodes (LDs) and photo-detectors. High bright and more efficient red, green and blue LEDs have already been demonstrated and commercialized [10]. With the recent invention of white LEDs and with improved performance figures of 66% of external quantum efficiency (equivalent to luminous efficiency of 116 lm/W, i.e. over eight times more efficient than incandescent lamps) [11], the future of solid-state lighting looks bright. GaN is expected to bring in new revolutions in the areas of solid-state lighting, optoelectronics and high-power electronics.
1.3 Research Background and Motivation for the Present Work

An absolutely key element for fabricating electronic devices is the metal-semiconductor contact. There are two types of metal-semiconductor contacts, viz., ohmic and Schottky or rectifying. Ohmic contacts have linear or quasi linear current-voltage characteristics and display symmetric current flow during forward and reverse bias. They conduct the same for both polarities and obey Ohm's law. The voltage drop across the metal-semiconductor contact must be small compared to the voltage drop across the active device region. In addition, the ohmic contact should have resistance that is much smaller compared to that of the substrate material [12, 13].

In contrast with ohmic contacts, Schottky contacts exhibit asymmetric current flow during forward and reverse bias. In forward bias,
the Schottky contact allows larger current to flow with respect to the magnitude of the bias. The increase in forward bias voltage consequentially increases current flow. In reverse bias, an increase in the bias voltage results in negligible change in the current flow. In general, the forward and reverse bias currents in Schottky contacts differ by many orders of magnitude.

The realization of high performance optoelectronic and high-power electronic devices requires low resistance, thermally stable and reproducible high quality ohmic contacts [14]. High quality ohmic contacts with low-resistance are still relatively difficult to obtain for p-type GaN, because of the difficulty in achieving high carrier concentrations and the absence of suitable metals with high work function. Also in the case of wide-band gap n-type GaN, realization of ohmic contacts with low specific contact resistance as well as thermal stability is still a challenge [15, 16]. Many schemes have been tried by the researchers in an effort to achieve low resistance and thermally stable ohmic contacts to III-nitride semiconductors. These include (i) rapid thermal annealing (RTA) process for alloyed ohmic contacts, (ii) increasing of carrier concentration, by ion implantation, for non-alloyed ohmic contacts and (iii) selection of thermally stable diffusion barrier [17-19]. RTA process is widely used to obtain alloyed ohmic contacts on n-type III-nitrides because the formation of metal-nitride phases contribute to the reduction of effective Schottky barrier height (SBH) and an increase in the carrier concentration near the surface by causing nitrogen vacancies, which act as shallow donors in n-type III-nitrides [17]. On the contrary, ion implantation process, with post annealing to recover from the ion-implanted damages, is widely employed to achieve non-alloyed ohmic contacts by increasing carrier
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concentration of the semiconductor. It has been known that this technique may be effective in n-type ohmic contacts [18].

Pretty good ohmic contacts to n-type GaN, with low specific contact resistivity (ρc), have been reported. The small work function of n-type GaN (≈ 3.2 eV) makes it easy to fabricate good ohmic contacts. Titanium (Ti) based ohmic contacts to n-GaN have exhibited specific contact resistances ranging from 8×10^{-5} to 9×10^{-8} Ωcm^2, which are good enough for optoelectronic and electronic devices [19, 20-29].

As for p-type GaN, there are two major obstacles that hamper the formation of good quality low resistance ohmic contacts. These are: (i) the difficulty in increasing the carrier concentration near p-type surface, and (ii) the absence of suitable metals with work function bigger than that of p-GaN (≈6.5 eV) [30]. The reported values of specific contact resistivity are around 10^{-3} Ωcm^2, which is quite high for the fabrication of good quality high performance electronic and optoelectronic devices. This calls for a thorough knowledge of the mechanism through which ohmic behavior is achieved. Hence the effects on ohmic behavior of contacts due to metal interlayer thickness, surface preparation, annealing temperature and interfacial reaction products need to be investigated.

Schottky contacts are of particular interest because of their rectifying properties. Schottky contacts have applications as gate contacts in photo-detectors, high power diodes and many high-power transistor designs. The devices with Schottky contacts have high switching speeds because they do not rely on minority carriers to generate the active regions of the device, as in the case of p-n junctions and MOS devices. An important aspect of the potential application of GaN based HEMTs to advanced microwave power amplifiers, and for radar and communication
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systems is the development of more reliable and thermally stable Schottky contacts [31-33]. The anticipated operation of these amplifiers under uncooled, high temperature conditions emphasizes that the thermal stability of the contact metallurgy is paramount [34]. Hence, to explore the real applications of GaN-based devices, some important research must be carried out regarding the properties of its surface and the metal-semiconductor interfaces.

1.4 Evolution of Growth and Properties of Gallium Nitride

1.4.1 Growth of GaN

The first reports on the synthesis of GaN dates back to the early 1930s. Johnson et al [35], in 1932, could successfully synthesize small needles of GaN by passing ammonia over hot gallium. Later in 1938, Juza and Hahn [36] reported the first synthesis of wurtzite (hexagonal) crystal structure of GaN with lattice constants \( a=3.189 \, \text{Å} \) and \( c= 5.185 \, \text{Å} \). Maruska and Tietjen [37] successfully deposited the first large area GaN layers on sapphire in 1969. They used the chemical vapor deposition method. The resulting films were highly n-type.

The beginning of the growth of good quality epilayers was made by Yoshida et al [38]. They showed in 1983 that if an AlN buffer layer is grown between the GaN film and the sapphire substrate, the quality of the layers improves. The two-step method was investigated and perfected by Akasaki, Amano and co-workers in 1988/1989 [39, 40]. In the first step a thin buffer layer of AlN is grown on the sapphire substrate at a low temperature of 500 °C. The GaN layer is grown on the buffer layer. The temperature at which the GaN layer is grown is much higher.
Techniques for growing p-type GaN were evolved by Amano and Akasaki [41] using Mg as the acceptor impurity. At present there are various techniques for growing both n- and p-type GaN thin films. The most widely used techniques are metalorganic chemical vapor deposition (MOCVD), hydride vapor phase epitaxy (HVPE) and molecular beam epitaxy (MBE). The GaN films synthesized using these techniques are of very good quality for device and research purpose.

1.4.2 Substrates

The worth of GaN’s attributes has long been recognized in the industry; however, the same attributes making GaN a valuable semiconductor for high power, high frequency applications also make it extremely difficult to manufacture. GaN has not, to date, been successfully grown in bulk format in commercially viable wafer diameters – anything beyond 25mm – due to the extreme environmental conditions required to achieve bulk growth. As a result, manufacturing GaN semiconductors requires a substrate material on which a film of GaN crystals can be grown to a thickness sufficient to support semiconductor device performance. The physical properties of GaN crystal structure have historically limited the choice of substrates to a few materials – most commonly, sapphire (Al₂O₃) and silicon carbide (SiC). In particular, GaN crystal structure and thermal expansion properties are sufficiently similar to those of sapphire and SiC to make GaN crystal growth feasible on those substrates. Hexagonal wurtzite GaN is most commonly grown on sapphire and SiC. Figure 1.2 illustrates wurtzite structure looking down the basal plane (0001).
Figure 1.2: Illustration of the wurtzite crystal structure. The dark spheres represent the gallium atoms and the light spheres represent the nitrogen atoms.

Sapphire is an insulator available as single crystal wafers. It possesses hexagonal corundum crystal structure. The atomic spacing in the (0001) plane is not close to that of GaN. The lattice mismatch between the GaN and sapphire, and the difference between the lattice parameters of the two materials at the closest distance is about 15%, which is very large [42]. The sapphire is transparent to visible light and costs much less as compared to the other popular substrate, silicon carbide.

Silicon carbide is a hexagonal semiconductor that exists in a number of polytypes or stacking arrangements along the c-axis of which 6H is the most commercially common. The arrangement of atoms on the (0001) basal plane on which GaN is grown is similar to that of the III-nitrides. The lattice mismatch between the GaN and 6H-SiC is about 3% [42]. Unlike the case of sapphire, SiC can be doped n and p-type. These
attributes of SiC make it the most suitable substrate for applications in high-power, high frequency and high-temperature devices.

1.4.3 Properties of Gallium Nitride

Tables 1.1 and 1.2 list some of the basic physical and electronic properties of GaN. Physical properties including thermal conductivity, lattice parameters, and density are listed in table 1.1. Electronic properties including the band gap energy, dielectric constant, mobility and effective mass are tabulated in table 1.2. The tables also furnish a comparison of GaN with Si, AlN, InN, GaAs and SiC.

Table 1.1: Physical properties of some common semiconductors. Data compiled from references. [42, 43]

<table>
<thead>
<tr>
<th>Physical Properties</th>
<th>GaN</th>
<th>AlN</th>
<th>InN</th>
<th>6H-Sic</th>
<th>Si</th>
<th>GaAs</th>
<th>Sapphire</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystal structure</td>
<td>Wurtzite</td>
<td>Wurtzite</td>
<td>Wurtzite</td>
<td>Wurtzite</td>
<td>Diamond</td>
<td>Zincblende</td>
<td>Corundum</td>
</tr>
<tr>
<td>Lattice constants (Å)</td>
<td>a</td>
<td></td>
<td></td>
<td>a</td>
<td>c</td>
<td></td>
<td></td>
</tr>
<tr>
<td>a</td>
<td>3.189</td>
<td>3.112</td>
<td>3.548</td>
<td>3.081</td>
<td>5.431</td>
<td>5.653</td>
<td>4.758</td>
</tr>
<tr>
<td>c</td>
<td>5.185</td>
<td>4.982</td>
<td>5.760</td>
<td>15.117</td>
<td>...</td>
<td>...</td>
<td>12.99</td>
</tr>
<tr>
<td>Thermal conductivity (W/cmK)</td>
<td></td>
<td></td>
<td></td>
<td>1.3 – 1.7</td>
<td>2.0</td>
<td>0.45–0.8</td>
<td>3.0-3.8</td>
</tr>
<tr>
<td>Thermal expansion Δa/a (10⁻⁶/K)</td>
<td>5.59</td>
<td>4.2</td>
<td>3.6</td>
<td>4.2</td>
<td>2.6</td>
<td>6.9</td>
<td>9.2</td>
</tr>
<tr>
<td>Thermal expansion Δc/c (10⁻⁶/K)</td>
<td>3.17</td>
<td>5.3</td>
<td>2.6</td>
<td>4</td>
<td>...</td>
<td>...</td>
<td>9.3</td>
</tr>
<tr>
<td>Melting temp (°C)</td>
<td>&gt;1700</td>
<td>3000</td>
<td>1100</td>
<td>2830</td>
<td>1414</td>
<td>1238</td>
<td>2050</td>
</tr>
<tr>
<td>Index of refraction</td>
<td>2.33</td>
<td>2.2</td>
<td>2.85-3.0</td>
<td>2.6-2.7</td>
<td>...</td>
<td>...</td>
<td>1.77</td>
</tr>
</tbody>
</table>
### Table 1.2: Electronic properties of GaN and some other common semiconductors

<table>
<thead>
<tr>
<th>Electrical Properties</th>
<th>GaN</th>
<th>AlN</th>
<th>InN</th>
<th>6H-Sic</th>
<th>Si</th>
<th>GaAs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Band Gap Energy (eV)</td>
<td>3.4</td>
<td>6.2</td>
<td>1.89</td>
<td>3.03</td>
<td>1.12</td>
<td>1.42</td>
</tr>
<tr>
<td>Band Gap Transition</td>
<td>Direct</td>
<td>Direct</td>
<td>Direct</td>
<td>Indirect</td>
<td>Indirect</td>
<td>Indirect</td>
</tr>
<tr>
<td>Dielectric constant $\varepsilon_r$</td>
<td>9.5</td>
<td>8.5</td>
<td>15.3</td>
<td>9.66</td>
<td>11.9</td>
<td>13.1</td>
</tr>
<tr>
<td>Dielectric constant $\varepsilon_{oo}$</td>
<td>5.35</td>
<td>4.77</td>
<td>8.4</td>
<td>6.7</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>Electron Effective Mass $m_e$ ($m_0$)</td>
<td>0.22</td>
<td>0.33</td>
<td>0.11</td>
<td>0.45</td>
<td>0.98</td>
<td>0.067</td>
</tr>
<tr>
<td>Hole Effective Mass $m_h$ ($m_0$)</td>
<td>0.8</td>
<td>---</td>
<td>---</td>
<td>1.2</td>
<td>0.49</td>
<td>0.45</td>
</tr>
<tr>
<td>Electron Mobility $\mu_e$ (cm$^2$/Vs)</td>
<td>900</td>
<td>300</td>
<td>4400</td>
<td>500</td>
<td>1500</td>
<td>8500</td>
</tr>
<tr>
<td>Hole Mobility $\mu_h$ (cm$^2$/Vs)</td>
<td>15</td>
<td>14</td>
<td>---</td>
<td>50</td>
<td>450</td>
<td>400</td>
</tr>
<tr>
<td>Sat. drift Velocity ($\times 10^7$cm/s)</td>
<td>2.5</td>
<td>---</td>
<td>2.5</td>
<td>2.0</td>
<td>1.0</td>
<td>2.0</td>
</tr>
<tr>
<td>Breakdown Field ($\times 10^6$ V/cm)</td>
<td>&gt;3</td>
<td>---</td>
<td>---</td>
<td>3</td>
<td>0.3</td>
<td>0.4</td>
</tr>
<tr>
<td>Electron Affinity $\chi$ (eV)</td>
<td>3.0-4.2</td>
<td>0.2-1.1</td>
<td>---</td>
<td>---</td>
<td>1.12</td>
<td>1.42</td>
</tr>
</tbody>
</table>

### 1.5 Metal-Semiconductor Contacts

#### 1.5.1 Basic Electrical Properties of Metals and Semiconductors

According to the band theory of solids [44, 45], as atoms are brought together, the outermost energy levels of the individual atoms start to split into discrete closely spaced energy levels. These split levels begin to overlap with the split levels of the other atoms. As more and more atoms are added and their atomic distances decrease, the split levels recombine to form an energy band. This energy band contains energy states that electrons can occupy. As the atoms are brought even closer, this band eventually starts to split into separate bands. Ultimately, when atomic spacing distance reaches equilibrium, conduction and valence bands are formed. Usually, for a metal, the conduction and valence bands overlap. In the case of a semiconductor, the conduction and valence bands are
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separated by an energy gap generally referred to as the band gap. This resulting band gap in a perfect crystal of semiconductor is characteristically forbidden from containing any states for electrons to occupy; only the valence and conduction bands can contain available states.

The band diagram of a metal is depicted in figures 1.3 (a) and 1.3 (b). The energy bands of the metal tend to overlap and this is usually described by stating that the conduction band minimum is at or below the valence band maximum of the metal. A metal is usually defined in terms of Fermi level or Fermi energy ($E_{\text{fm}}$) and work function ($\phi_m$). The Fermi level is that energy at which there is a probability of $\frac{1}{2}$ for a state at that level to be occupied by an electron. For metals, the Fermi level can also be described as the highest occupied state at absolute zero temperature [44]. The work function of the metal is the difference in energy between the vacuum level and the Fermi level, where the vacuum level is the bottom of the free electron band. For most metals the value of the work function is in the range of 3.0 eV to 5.5 eV [45]. Table 1.3 contains the values of work function and electronegativity for some common metals. Electron affinity values of some common semiconductors are listed in table 1.4.

Semiconductors have conduction and valence bands separated by a band gap as depicted in figures 1.3 (a) and 1.3 (b). At room temperature of about 300 K the conduction band of an intrinsic (undoped) semiconductor is usually meagerly populated with electrons while the valence band is essentially filled. Like in the case of the metals, Fermi level ($E_{\text{fsc}}$) can also be defined for a semiconductors. However, the Fermi level in semiconductors is not in a fixed position, rather its position is anywhere within the band gap depending on the dopants or impurities.
**Table 1.3:** Values of work function and electronegativity for some common metals

<table>
<thead>
<tr>
<th>Element</th>
<th>Work Function (eV)</th>
<th>Electronegativity (eV)</th>
<th>Element</th>
<th>Work Function (eV)</th>
<th>Electronegativity (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ag</td>
<td>4.52-4.74</td>
<td>1.93</td>
<td>Ni</td>
<td>5.04-5.35</td>
<td>1.91</td>
</tr>
<tr>
<td>Al</td>
<td>4.06-4.26</td>
<td>1.61</td>
<td>Pd</td>
<td>5.22-5.6</td>
<td>2.2</td>
</tr>
<tr>
<td>Au</td>
<td>5.31-5.47</td>
<td>2.4</td>
<td>Pt</td>
<td>5.12-5.93</td>
<td>2.2</td>
</tr>
<tr>
<td>Co</td>
<td>5.00</td>
<td>1.88</td>
<td>Re</td>
<td>4.72</td>
<td>1.9</td>
</tr>
<tr>
<td>Cr</td>
<td>4.5</td>
<td>1.66</td>
<td>Sc</td>
<td>3.5</td>
<td>1.36</td>
</tr>
<tr>
<td>Cu</td>
<td>4.48-5.1</td>
<td>1.9</td>
<td>Si</td>
<td>4.6-4.9</td>
<td>1.9</td>
</tr>
<tr>
<td>Fe</td>
<td>4.67-4.81</td>
<td>1.83</td>
<td>Ta</td>
<td>4.0-4.8</td>
<td>1.5</td>
</tr>
<tr>
<td>Ga</td>
<td>4.32</td>
<td>1.81</td>
<td>Ti</td>
<td>4.33</td>
<td>1.54</td>
</tr>
<tr>
<td>Hg</td>
<td>4.48</td>
<td>1.9</td>
<td>W</td>
<td>4.32-5.22</td>
<td>1.7</td>
</tr>
<tr>
<td>In</td>
<td>4.09</td>
<td>1.78</td>
<td>Y</td>
<td>3.1</td>
<td>1.22</td>
</tr>
<tr>
<td>Ir</td>
<td>5.0-5.76</td>
<td>2.2</td>
<td>Zn</td>
<td>3.6-4.9</td>
<td>1.65</td>
</tr>
<tr>
<td>Mg</td>
<td>3.66</td>
<td>1.31</td>
<td>Zr</td>
<td>4.05</td>
<td>1.33</td>
</tr>
<tr>
<td>Mo</td>
<td>4.36-4.95</td>
<td>2.16</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Table 1.4:** The electron affinity for some common semiconductors

<table>
<thead>
<tr>
<th>Semiconductor</th>
<th>Band Gap, $E_g$ (eV)</th>
<th>Electron Affinity $\chi$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>1.12</td>
<td>4.05</td>
</tr>
<tr>
<td>GaAs</td>
<td>1.42</td>
<td>4.07</td>
</tr>
<tr>
<td>Ge</td>
<td>0.66</td>
<td>4.0</td>
</tr>
<tr>
<td>GaN</td>
<td>3.45</td>
<td>3.0-4.2</td>
</tr>
<tr>
<td>AlN</td>
<td>6.2</td>
<td>0.2-1</td>
</tr>
<tr>
<td>6H-SiC</td>
<td>3.03</td>
<td>3.5</td>
</tr>
</tbody>
</table>

For n-type semiconductors the Fermi level is located between the mid gap and the conduction band minimum [figures 1.3 (a) and 1.3 (b)]. The work function ($\phi$) of a semiconductor depends on the impurity levels and hence does not accurately describe the energy relations of the bands to the vacuum energy. This can lead to problems while defining the electronic properties of the material. A more appropriate quantity is the electron affinity of the semiconductor ($\chi$). The electron affinity is defined
as the energy difference between the vacuum level and the conduction band minimum. This value is effectively independent of the Fermi level position and therefore independent of the semiconductor doping. Figures 1.3 (a) and 1.3 (b) depict the independent band structures for a metal and n-type semiconductor when (a) the work function of the metal is greater than the electron affinity of the semiconductor ($\phi_m > \chi_s$), and (b) the work function of the metal is less than the electron affinity of the semiconductor ($\phi_m < \chi_s$).

**Figure 1.3:** Energy band diagram of individual metal and semiconductor (a) with $\phi_m > \chi_s$ (b) with $\phi_m < \chi_s$
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The following sections deal with some general models, which try and predict the formation of Schottky barriers when a metal and a semiconductor are placed in contact with each other.

1.5.2 Schottky-Mott Model

The Schottky-Mott model deals with the formation of an energy barrier that forms when a metal and a semiconductor are placed in intimate contact. According to Schottky-Mott model, the resulting energy barrier \((\phi_b)\) is equal to the difference between the metal work function and electron affinity of the semiconductor, and is given by the relation

\[ \phi_b = \phi_m - \chi_s, \]

where \(\phi_m\) is the metal work function and \(\chi_s\) is the electron affinity of the semiconductor. According to equation 1.1, there are two cases. Case one arises when the metal work function is greater than the semiconductor electron affinity \((\phi_m > \chi_s)\). This is the case with a positive value of \(\phi_b\) that leads to the energy barrier formation and rectifying behavior of the metal-semiconductor contact. Case two occurs when the work function of the metal is less than the electron affinity \((\phi_m > \chi_s)\) with a negative value of \(\phi_b\), which leads to an ohmic contact. However, case two is rarely observed in the laboratory since most metal semiconductor contacts result in the formation of a barrier.

For case one, when a metal and semiconductor are brought into intimate contact, electrons from the semiconductor flow to the surface of the metal causing the Fermi level in the bulk of the semiconductor to line up with the Fermi level of the metal when equilibrium is reached. The electrons that flow from the semiconductor to the metal accumulate at the surface of the metal. Due to the electrons which left the semiconductor, a
net positive charge builds up in the surface region of the semiconductor. This surface region of positive charge in the semiconductor is referred to as the space charge or depletion region [44]. Charge neutrality of the system dictates that the negative charge \( Q_m \) on the metal surface is offset by the positive charge \( Q_{sc} \) in the depletion region of the semiconductor. As a result of the charge build up, an electric field is formed in the depletion region of the semiconductor. This field causes the Fermi levels to align and bands of the semiconductor to bend at the interface and produces a potential barrier \( \phi_b \) at the metal-semiconductor interface. This potential barrier is called Schottky barrier. For an n-type semiconductor the bands near the surface bend upwards, as depicted in figure 1.4(a). In figure 1.4(a), \( \phi_b \) is the resulting barrier height, \( V_{bi} \) is the built in potential, \( W \) is the depletion width, \( Q_{sc} \) is the semiconductor charge and \( Q_m \) is the charge at the metal surface.

The barrier height \( (\phi_b) \) limits the flow of electrons between the metal and the semiconductor. For an electron to travel from the metal to the semiconductor it must have enough energy to overcome the full barrier height, \( \phi_b \). On the other hand, electrons in the semiconductor see a potential barrier of \( qV_{bi} \). Electrons can flow from the semiconductor to the metal if \( V_{bi} \) can be overcome. When a bias is applied to the junction, it can have one of two effects: it can make the barrier appear lower from the semiconductor side, or it can make it appear higher. The bias does not change the barrier height from the metal side.

For case two, which occurs when the work function of the metal is less than the electron affinity of the semiconductor, also the energy bands line up according to the diagram in figure 1.4(b). In this case, contrary to case one, electrons are transferred from the metal surface into the
semiconductor when the metal and semiconductor are placed in intimate contact. The Fermi level of semiconductor is raised up to lineup with the Fermi level of the metal and the conduction and valence bands near the surface bend downwards. On reaching equilibrium, a net positive charge is built up on the metal surface and a negative charge built up in the surface and sub-surface regions of the semiconductor. The resulting Schottky barrier height for this type of contact is negative. Current can flow in either direction without being blocked by potential barriers.

Figure 1.4: Energy band diagram for intimate metal-semiconductor (a) with $\phi_m > \chi_s$ (rectifying) and (b) with $\phi_m < \chi_s$ (ohmic)

1.5.3 Interface/Surface State Model

According to Schottky-Mott model, the Schottky barrier height ($\phi_b$) varies directly as the metal work function ($\phi_m$) [equation 1.1]. However, studies have shown that for covalently bonded semiconductors such as
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silicon and germanium, there is weak dependence between the barrier height and metal work function. This discrepancy was explained in 1947 by Bardeen [46]. According to his proposition, there exist interface states (energy levels) in the classically forbidden bandgap of the semiconductor [figure 1.5]. These states can be due to the termination of the periodic lattice, surface defects in the lattice and/or contamination and impurities at the semiconductor surface. These states can assume any level in the band gap and can exist as continuous or discrete levels within the forbidden gap [46]. According to Bardeen, the Schottky barrier is given by

\[ \phi_b = E_g - \phi_0 \]  

(1.2)

where \( \phi_0 \) is the charge neutral level. Also known as the energy level at the surface, the charge neutral level (\( \phi_0 \)) coincided with the Fermi level before the metal-semiconductor was formed. It also specifies the level below which all surface states must be filled for charge neutrality at the surface. The empty interface states below \( \phi_0 \) have positive charge and behave as donors [47]. Electrons are transferred from the semiconductor to the surface states and build a negative charge at the interface and a positive charge in the semiconductor. This dipole at the semiconductor surface creates a depletion region and results in the upward bending of energy bands for an n-type semiconductor [figure 1.5].

Cowley and Sze [48] further refined this model and a general expression of barrier height was proposed based on the following assumptions: (i) with intimate contact between metal and semiconductor, an interfacial layer of atomic dimensions exists and will be transparent to electrons, and (ii) the surface states per unit area per unit eV at the interface are a property of the semiconductor alone. Their model also
combines Schottky-Mott model with the concept of the charge neutral level which was put forth by Bardeen [46]. A more detailed energy-band diagram of a metal n-type semiconductor contact is shown in figure 1.5.

According to Cowley and Sze [48], the Schottky barrier is given by

\[ \phi_b = \left( \frac{\varepsilon_i}{\varepsilon_i + q\delta D_s} \right) (\phi_m - \chi_i) + \left[ 1 - \left( \frac{\varepsilon_i}{\varepsilon_i + q\delta D_s} \right) \right] (E_g - \phi_s) - \Delta \phi', \]

where \( \delta \) is the interface thickness, \( D_s \) is the density of surface states, \( \Delta \phi' \) is the image force lowering, \( \varepsilon_i \) is the dielectric constant of the interface layer. The image force lowering (\( \Delta \phi' \)), also known as the Schottky barrier lowering, is the reduction in barrier height due to the electric field generated by the moving electrons in the semiconductor. Its value is roughly a couple of meV and therefore it has negligible effect on the barrier height.

From equation 1.3, there are three cases for the Schottky barrier height. First, when the density of states \( D_s \) is zero, the barrier height becomes completely dependent on the work function of the metal

\[ \phi_b = \phi_m - \chi_i - \Delta \phi'. \]  

This is the Schottky-Mott model of the metal-semiconductor junctions with a correction for image force lowering and represents an upper limit to the barrier height.

Second, when the density of states \( D_s \) is sufficiently large, the Fermi level is pinned and the barrier height becomes completely independent of the metal work function. The barrier height is now defined in terms of the semiconductor band gap and neutral level according to the following equation

\[ \phi_b = E_g - \phi_0 - \Delta \phi', \]  

where \( \phi_0 \) is the Fermi level in the semiconductor.
Third, when the density of surface states $D_s$ is low, the resulting barrier is partially due to the difference between the metal work function and the semiconductor electron affinity.

\[ \phi_m - \phi_b \]

Figure 1.5: Energy Band diagram for interface state model

All the models, including the above, attempt to explain the formation of the Schottky barrier height. The theory behind the formation Schottky barrier height is still unknown. While support for any model can be found, the theoretical research on the origins of the Schottky barrier height lags behind experimental investigation.

1.6 Current Transport Mechanism

The current flow in Schottky contacts is mainly due to the movement of majority carriers across the interface. Electrical properties of Schottky contacts are determined primarily by the carrier concentration and Schottky barrier height (SBH). The conduction mechanisms for a metal-n-type semiconductor are illustrated in figure 1.6. There are three
different current transport processes that can occur: (1) thermionic emission (TE) over the barrier due to thermally excited electrons, (2) thermionic-field emission (TFE) and (3) field emission (FE) or tunneling. The type of current transport process is mainly a function of Schottky barrier height and carrier concentration.

The depletion width (space charge region) $W$ is relatively large and the built-in potential $V_{bi}$ is low in moderately doped ($N_D \leq 10^{17}\text{cm}^{-3}$) semiconductor [figure 1.6 (a)] and the dominant current transport mechanism is thermionic emission. In thermionic emission mechanism, thermally excited electrons flow across the barrier and constitute current [47]. Due to large depletion width the amount of current density is relatively low. The total current density, $J$, of an ideal metal-semiconductor contact due to thermionic emission over the barrier is given by [12]

$$J = A^* T^3 \exp \left( \frac{-q\phi_b}{kT} \right) \left[ \exp \left( \frac{qV}{kT} \right) - 1 \right],$$

and specific contact resistance ($R_{sc}$) is given by the expression

$$R_{sc} \propto \exp \left( \frac{q\phi_b}{kT} \right),$$

where $k$ is the Boltzmann's constant and $q$ is the elementary charge, $A^*$ is the Richardson constant, and $\phi_b$ is the barrier height. According to equation 1.7, $R_{sc}$ depends primarily on Schottky barrier height ($\phi_b$) and temperature ($T$).

Thermionic field emission is dominant in the intermediately doped ($10^{17}\text{cm}^{-3} < N_D < 10^{19}\text{cm}^{-3}$) semiconductors [49, 50]. The width of the space charge region is sufficiently narrow for quantum tunneling of carriers to take place [figure 1.6 (b)]. Also, carriers are thermally excited and a
fraction of them flow across the barrier. The specific contact resistance for TFE conduction is expressed as

\[ R_{sc} \propto \exp \left( \frac{q \phi_s}{E_\infty \coth \left( \frac{E_\infty}{kT} \right)} \right) \tag{1.8} \]

where \( E_\infty \) is the tunneling parameter defined as

\[ E_\infty = \frac{qh}{4\pi} \sqrt{\frac{N_d}{\varepsilon_s m^*}} \tag{1.9} \]

where \( N_d \) is the carrier concentration (or doping concentration) of the semiconductor, \( m^* \) is the effective mass of the semiconductor, \( \varepsilon_s \) is the dielectric constant of the semiconductor, \( h \) is the Plank's constant and \( q \) is the carrier charge.

In TFE mechanism, \( R_{sc} \) depends on SBH, temperature and on the tunneling parameter \( E_\infty \). The term \( E_\infty/kT \) is a measure of the ratio of the field emission or tunneling current to thermionic emission current. For lightly and moderately doped semiconductors, \( E_\infty/kT < 1 \) and thermionic emission dominates. For heavily doped semiconductors, \( E_\infty/kT > 1 \) and tunneling current dominates. For intermediately doped semiconductors, \( E_\infty/kT \approx 1 \) and current transport mechanism will be thermionic-field emission.

When the carrier concentration is high (\( N_D > 10^{19}\text{cm}^{-3} \)), the width of the barrier, and therefore the width of space charge region, decreases and becomes very thin. In addition, the built-in potential increases and becomes large as shown in figure 1.6 (c). This increases the probability of the carriers tunneling through the metal-semiconductor junction. This phenomenon is known as field emission (FE) [49]. The increased tunneling
probability leads to the formation of ohmic contact. The specific contact resistance $R_{sc}$ for FE conduction is expressed as

$$R_{sc} \propto \exp \left( \frac{q \phi_v}{E_c} \right).$$

(1.10)

In FE mechanism, as indicated in equation 1.8, $R_{sc}$ depends primarily on tunneling parameter $E_c$ which again is a function of carrier concentration [equation (1.9)].

(a) Thermionic Emission

(b) Thermionic Field Emission

(c) Field Emission

Figure 1.6: Schematics of band diagrams and carrier transport mechanism in metal-n-type semiconductor.
By taking into account the three different carrier transport mechanisms, the two methods by which contacts can be made ohmic are: (i) decrease of the SBH to increase the current due to thermionic field emission and (ii) increase of the carrier concentration of the semiconductor to increase the field emission current. These two methods are generally used for obtaining ohmic contacts. The other widely used way of achieving ohmic contacts is by decreasing the band gap of the semiconductor (i.e. by making $\phi_{sc} << \phi_m$). This is accomplished by embedding a graded semiconductor or a super-lattice between the metal and the semiconductor. In this method, the decrease in band gap decreases the width of the space charge region and therefore the current transport mechanism is largely determined by the quantum tunneling of carriers.

1.7 Measurement of Specific Contact Resistance

An important parameter that determines the quality of a metal-semiconductor is its specific contact resistance. The two methods used to measure specific contact resistance are: (1) transfer length method [14] and (2) circular-transmission line method (C-TLM).

1.7.1 Transfer Length Method (TLM)

Initially proposed by Schockley [51], the transfer length method (TLM) consists of more than three contacts with unequal spacing between contacts. This method can be used to measure the contact resistance, specific contact resistance and sheet resistance between and under the contacts. A typical arrangement used in TLM is shown in figure 1.7. In the figure, $Z$ and $L$ are the contact/pad width and length, $W$ is the width of the sheet, and $d_1$, $d_2$ etc. are the separation between the pads. For contacts with $L \geq 1.5L_T$, where, $L_T$ is the transmission length and is defined as
The total resistance between any two pads, $R_T$, is given by

$$L_T = \frac{\rho_s}{\sqrt{\rho_s}}.$$  
(1.11)

The total resistance between any two pads, $R_T$, is given by

$$R_T = \frac{\rho_s d}{Z} + 2R_c \approx \frac{\rho_s d}{Z} + 2 \frac{\rho_c L_T}{Z},$$  
(1.12)

where $\rho_s$ is the sheet resistance and $\rho_c$ is the contact resistance.

A plot of total resistance $R_T$ versus distance between the pads $d$, as shown in figure 1.8, is a straight line with slope equal to $\rho_s/Z$ and y-axis intercept, at $d=0$, equal to $2R_c$. The x-axis intercept, at $R_T=0$ gives $d=2L_T$, using which, we can calculate the specific contact resistance $\rho_c$ with $\rho_s$ known from the slope of the plot and by using equation 1.11.

![Figure 1.7: A schematic of TLM test structure.](image)

To measure the specific contact resistance, the voltage drop $\Delta V$ between the sample contacts/pads is measured by passing a constant current $I_o$, through the adjacent pairs of contact pads with different spacing. Using the measured voltage drop and the current, the total resistance $R_T$ is calculated for each pair of contacts. The specific contact resistivity $\rho_c$ is estimated using the plot of $R_T$ versus $d$ together with the equation 1.11.
1.7.2 Circular-Transmission Line Method (C-TLM)

Circular transmission line model method is relatively simple. The test pattern used in C-TLM is shown in figure 1.9. The total resistance $R_T$ measured between the circular pads is given by the expression [52, 53]

$$R_T = \frac{\rho_s}{2\pi} \left( \ln \frac{r_2}{r_1} + \frac{1}{L_T} \left( \frac{1}{r_1} + \frac{1}{r_2} \right) \right),$$  \hspace{1cm} (1.13)

where $L_T$ is the transfer length defined as $L_T = \sqrt{\frac{\rho_c}{\rho_s}}$, $r_1$ is the radius of the inner contact, $r_2$ is the radius of the outer contact, $\rho_s$ is the sheet resistance, $\rho_c$ is the specific contact resistance and $L_T$ is the transfer length. The spacing between the outer and inner contacts is given by $d = (r_2 - r_1)$. Now, a graph of total resistance $R_T$ versus spacing $d$ is plotted for calculating the specific contact resistance.
1.8 Importance of Present Study

There is currently great interest in studying wide-band gap materials for optoelectronic, high-power, high-frequency and high-temperature applications. Group III nitride semiconductors, gallium nitride (GaN) in particular, are highly attractive materials for optoelectronic devices such as photo-detectors, light emitting diodes and laser diodes operating in short wavelength region. In addition, these materials also have been recognized as prospective candidates for high-temperature and/or high power devices such as metal-semiconductor field effect transistors (MESFETs), metal-insulator field effect transistors (MISFETs) and high electron mobility transistors (HEMTs). To realize high performance, GaN based electronic and optoelectronic devices require thermally stable good quality metal-semiconductor contacts. In particular, thermally stable ohmic contacts with low contact resistivity are difficult to obtain, because of the intrinsic nature of the GaN layer. GaN-based Schottky contacts suffer from abnormal leakage current under reverse bias, which strongly degrade the gate current characteristics and increase power consumption. Therefore the development of ohmic contacts with low-resistance and thermal stability, and Schottky contacts with high
SBH, low leakage current and good thermal stability to GaN-related semiconductors is of great practical importance.

Though many attempts have been made to find ways of lowering contact resistivity, mostly using variation of metal schemes and surface treatments, there is still much work to be done to understand the means to improve the performance and efficiency of the devices. The high-temperature behavior, in particular, of many of the metal contacts to GaN is not clear and hence it is necessary to understand the physics of interface between metals and GaN at different temperatures.

The main objectives of the present work are:

1. Fabrication of ohmic and Schottky contacts on moderately doped n-type and p-type gallium nitride.

2. Study of thermal annealing effects on contacts by annealing samples at different temperatures.

3. Study of electrical properties of contacts using I-V and C-V techniques before and after annealing.

4. Investigation of structural properties of contacts by x-ray diffraction (XRD) and Auger electron microscopy (AES) before and after annealing.

5. Study of surface morphologies of ohmic contacts using atomic force microscopy (AFM) before and after annealing.

1.9 Outline of Dissertation

The results of the investigations and a detailed discussion are presented in the thesis. The thesis consists of five chapters.
The introduction to group III-nitrides (GaN), concepts of ohmic and Schottky contacts, importance of the present work, and outline of the thesis are presented in the first chapter.

The second chapter contains the experimental techniques are used for characterization of the ohmic and Schottky contacts.

The third chapter deals with the formation of thermally stable low-resistance Pt/Ag/Au ohmic contacts to p-GaN and their electrical and structural properties. The electrical and micro-structural properties of low-resistance thermally stable Ti/W/Au ohmic contacts to n-type GaN are also described in this chapter.

The fourth chapter contains the details of fabrication and study of electrical properties of Rh Schottky contacts on n-type GaN as a function of annealing temperature. The development of Rh/Au Schottky contacts to n-type GaN and their electrical and structural properties, at different annealing temperatures, are also discussed in this chapter.

The summary of the results and the conclusions drawn from the present study, and the scope for future work are presented in the fifth chapter.
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References


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References


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References


