Electrical Properties of Group III Nitrides

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Abstract

Using temperature dependent Hall measurements, electron transport in \textit{n}-type GaN films grown on sapphire by MOCVD and MBE has been analysed assuming the presence of impurity band conduction. No dependence on growth method or dopant type was observed, but other trends were apparent: (i) the activation energy for the impurity band fell with increased doping; (ii) the temperature of the minimum in the Hall carrier density versus temperature curves increased with doping, but did not depend strongly on the absolute value of mobility; (iii) the ratio of the mobility in the GaN conduction band to that in the impurity band also showed systematic behaviour, possibly arising from structure-related scattering process.

Carrier transport in a set of AlGaN/GaN samples from different sources with a range of electron densities and mobilities has been investigated at low temperatures and high magnetic fields. The Shubnikov-de Haas (SdH) oscillations have been analysed to extract the quantum scattering time, and this is compared with the transport lifetime, derived from the low-field mobility. From the relationship between these parameters, it can be concluded that the effects of large-angle scattering, arising from defects such as dislocations and background impurities, dominate most samples, though one sample seems to point to grain boundary scattering.

Phonon emission process in an AlGaN/GaN heterostructure with mobility in excess of 25 000 cm$^2$ V$^{-1}$ s$^{-1}$ have also been investigated at low temperatures, where the amplitude of the SdH oscillations has been used as a thermometer for the electron temperature, and has shown that the power input per electron follows a $T^{4.4}$ dependence. Comparison with numerical modelling indicates that in this sample, electron-acoustic phonon scattering via the screened piezoelectric interaction is the dominant energy-loss mechanism.
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Vita

In a chronological order:


Chapter 1

Introduction

Since the advent of the transistor in the late 1940's, semiconductor materials and device research have enjoyed a well-deserved golden age reflecting the economic impact of semiconductor and derivative technologies. Until now, silicon formed the backbone of the semiconductor industry for device fabrication and large-scale integration. Meanwhile, the study of group III-V compounds such as gallium arsenide (GaAs) in various academic research institutions, coincided with the development of advanced epitaxial techniques, has led to the successful fabrication of structures and devices that are capable of high speed operation. This reflects the current trend in semiconductor industry where specialised compounds such as mentioned above are competing for a share of the market, which is still dominated by silicon.

It has been suggested by Strite (1996) that the group III nitrides may represent the last semiconductor material system to be developed, and judging from the current excitement generated by the recent developments of the gallium nitride (GaN) laser technology, one is inclined to agree with it. So far, there has been a flurry of activity in extensive investigations of the nitride behaviour for their opto-electronic applications, including light emitting diodes (LEDs) and lasers operating in the green to ultraviolet (UV) wavelength range. LEDs are key elements for full colour displays and lasers are necessary in high-density optical storage. Currently, because of their excellent electrical and thermal properties, they are also expected to play a major role in high temperature, high power applications. The nitrides are not without rivals in
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these applications though. The competition exists in the form of a blue laser based on group II–VI compounds, which still needs to reduce the number of stacking faults and related threading dislocations for better performance, and the silicon carbide (SiC) technology, albeit expensive, has been studied for a number of years and poses a possible threat in continued research on commercial nitride-based electronic power devices. Nevertheless, the growth and characterisation of group III nitrides is an essential part primarily in understanding their fundamental properties, and ultimately instrumental in assessing the optimum design conditions of the material growth and device fabrication. Therefore, it is important to provide feedback to the grower the information he/she needs for improving the quality of the material, and this thesis aims to carry out and present such work, where the main part of the work is concentrated on the electrical characterisation of n-type GaN epilayers and AlGaN/GaN heterostructures (transport properties in particular).

GaN was first synthesized by Juza and Hahn (1940) by passing ammonia over hot gallium, but it was only for the routine study of the crystal structure and lattice constants of various III–V compounds. Serious interest in GaN started from about 1969 when various laboratories tried to grow reasonably high quality GaN films on sapphire substrates (Maruska and Tietjen 1969). Halide vapour phase epitaxy (HVPE) was notably employed by Ileagem and Montgomery (1973), where Ga transported by gallium chloride, and N supplied by ammonia, formed GaN films in thicknesses of up to 100 μm. They found that with increasing thickness, the effect of strain in the crystal was reduced, and they then proceeded to measure transport parameters such as mobility and carrier concentration. Even though doping was not introduced, the films exhibited strong n-type conduction with electron concentrations in the region $10^{18} - 10^{20}$ cm$^{-3}$ which indicated great difficulty in p-type doping. Initially, the donors were believed to be N-vacancies (Jenkins and Dow 1989) but later, this model was questioned by Neugebauer and van der Walle (1994) on the grounds that the N-vacancy’s formation energy was too large ($\sim 4$ eV). Silicon (Si) and oxygen (O) impurities were proposed as the donors, which could have been introduced externally into the deposition system (Seifert et al. 1983). Si was actually used as the most common shallow donor atom, with activation energies in the range 10 – 40 meV, and many workers (Koide et al.
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1991; Rowland et al. 1995) have succeeded in producing n-doped GaN with electron concentrations between $10^{17} - 10^{20}$ cm$^{-3}$. However, p-type doping proved to be a much greater challenge, mainly because of the deep ionisation energy associated with the acceptors (e.g., approximately 250 meV for magnesium, Mg).

Successful p-type doping was eventually achieved by Amano et al. (1989), though only when GaN, doped with Mg acceptors, grown by metal organic chemical vapour deposition (MOCVD), was subjected to the low energy electron beam irradiation (LEEBI) treatment. Soon thereafter, Nakamura et al. (1992) reported that thermally annealing GaN:Mg above 750 °C in N$_2$ atmosphere also converted the material to conducting p-type. This progress launched a massive effort around the world on devices based on GaN p-n junctions and related ternary materials such as aluminum gallium nitride (AlGaN) and indium gallium nitride (InGaN). The enormous development of nitride device technology over the last decade can be summarised as follows:

- **Light emitting diodes** — the first bright blue GaN p-n junction LED using an AlN buffer layer was developed by Akasaki et al. (1989). However, it was Shuji Nakamura and co-workers of Nichia Chemical Industries in Japan who were the front runners in producing high-power (brightness > 1000 mcd), high efficiency (6 – 9%), commercially successful blue (≈ 430 nm) and blue-green (≈ 500 nm) LEDs (Nakamura and Senoh 1992; Nakamura et al. 1995). They employed not only the GaN p-n junction, but also other structures such as the Si-doped InGaN/GaN double heterostructure (DH), InGaN/AlGaN DH and quantum well (QW) LEDs.

- **Laser diodes** — the first room temperature pulsed short wavelength lasing (417 nm) from nitride materials was also reported by Nichia (Nakamura et al. 1996). The development was rapid and within 12 months they succeeded in continuous-wave (CW) operation for 35 hours. The structure was a continuation of their LED work on In$_{0.2}$Ga$_{0.8}$N/In$_{0.05}$Ga$_{0.95}$N multi-QWs on sapphire substrates with Al$_{0.15}$Ga$_{0.85}$N cladding layers. Problems such as high p-type contact resistance and dislocations meant that much work still needed to be done in improving the crystal quality and waveguide designs. Growth using ELOG (lateral epit
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taxial over-growth) method was utilised to tackle such problems with marked improvements (Nakamura et al. 1998).

- **Ultraviolet photodetectors** — various photodetector structures based on the $n$-type GaN Schottky barrier, have been grown by several groups (Binet et al. 1997; Chen et al. 1997). High speed, low noise $p$-$\pi$-$n$ GaN UV photodetectors (Xu et al. 1997) exhibited a peak responsivity greater than 0.1 A W$^{-1}$ at 363 nm. Also, GaN devices using the metal-semiconductor-metal (M-S-M) principle (Carrano et al. 1997) where the metal contacts take the form of an interdigitated finger structure deposited on the semiconductor surface, have reported photoconductive gains as high as 30000.

- **Electronic devices** — this family of devices stems from a range of field effect transistors (FET) such as metal semiconductor (MESFET), heterojunction (HFET), and modulation doped (MODFET) field effect transistors. Utilizing the wide band-gap nature of nitrides, the applications include high power, high temperature microwave devices. Since this thesis is concerned mainly with the electrical properties of GaN and AlGaN systems, special attention will be focused on the electronic devices, and an account of selected device examples will be given later in Section 2.4.

The recent developments mentioned above have been only possible due to the steady improvement of material quality. However, in spite of the remarkable progress that has been witnessed, a number of problems remains to be solved. Problems, such as the scarcity of suitable substrates and the lack of knowledge of the physics behind the nitrides, need to be tackled in order to ensure further progress. Precise investigations on ever-improving materials are crucial in providing reliable data for the structural and electronic parameters of nitrides, and a brief review of such investigations will be presented in Chapter 2. It should be pointed out here that the theoretical contents of this thesis are concentrated on aspects that are relevant to the results, and thus they are presented at the beginning of each corresponding result chapter.

Chapter 3 provides a general description of the experimental apparatus and techniques employed in obtaining the temperature dependent Hall and low temperature
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magneto-transport data. In addition, details of the samples studied (e.g., layer structure and preparation methods) are given.

The results are divided into three parts; transport investigation of GaN layers, transport properties of AlGaN/GaN heterostructures, and the energy loss mechanism of hot electrons in 2DEG samples. Chapter 4 includes the temperature dependent Hall measurements, which are mainly used in characterising n-GaN samples to investigate the scattering processes limiting the electron mobility, the activation energy of dopants, and the level of compensation. The role of a secondary conduction channel has also been studied in samples that are heavily affected by an impurity band conduction.

Low temperature magneto-transport studies on AlGaN/GaN heterostructures are mainly presented in Chapter 5, from which the material parameters such as electron effective mass and relaxation times are determined. By investigating the relationship between the quantum and classical lifetimes, the type of dominant scattering mechanism present at low temperatures is also predicted.

The oscillations of magneto-resistivity at various temperatures and currents of AlGaN/GaN 2DEG samples have been investigated, and the interpretation of the results are discussed in Chapter 6. The amplitude of the Shubnikov-de Haas oscillations has been used as a thermometer for the electron temperature, and from the resulting temperature dependence of the power per electron, the dominant energy-loss mechanism of hot electrons at low temperatures is determined.

Finally, Chapter 7 presents the overall conclusions of the results, and a list of suggestions for future work is also included.
Chapter 2

Physical Properties: Review

This chapter presents a brief overview of the progress made in nitride technology, including an outline of major issues such as growth, doping, device optimisation, etc., that have challenged researchers recently. The physical properties of nitrides, which have not by any means yet been fully understood, will occupy the bulk of this chapter, where the emphasis will be on transport properties of GaN and AlGaN/GaN systems.

2.1 Material properties of nitrides

This section discusses the basic material parameters and characteristics of nitrides as an introductory guide to the sections that follow, which are the growth techniques, transport properties and electronic devices. Note that there have already been several review articles and books on various aspects of group III nitrides (Monefar 1999; Orton and Foxon 1998) and the material presented here mostly consists of summarised extracts from those reviews.

2.1.1 Structural properties

GaN differs from most other III–V compounds (Madelung 1991) in that there is a very large difference between covalent radii of the two host atoms (Ga: 1.26 Å, N: 0.75 Å). This results in much reduced lattice parameters for the nitrides, and its large bonding energy (2.2 eV) implies high melting temperatures (Porowski and Grzegory 1994). Also, the electro-negativities of the constituent elements are very different: 1.8 for Ga.
and 3.0 for N. This difference induces a large ionic character and can cause problems when attempting to theoretically study the effect of charged defects (Neugebauer and van der Walle 1995).

Group III nitrides commonly exist in the thermodynamically stable hexagonal wurtzite (WZ) structure, and although GaN can grow into the cubic zinc blende (ZB) structure, most of the work on GaN has concentrated on the hexagonal form, which has a hexagonal unit cell with two lattice parameters \(a\) and \(c\). The atomic arrangement of the ZB and WZ structure of GaN is shown in Fig. 2.1 (Stampfl and van der Walle 1999). The WZ nitrides possess inherent macroscopic polarisations, comprised of a spontaneous and a piezoelectric component. The former can be explained when considering the unit wurtzite cell. Measurements of the dimensions of the unit cell have shown that it departs from the expected \(c : a\) ratio of 1.633 for perfectly packed atoms, and has a value of 1.626 (Leszczynski et al. 1996). Because of the ionic nature of Ga–N bond, and the lack of inversion symmetry, this results in a net dipole moment across the cell. The effect of this is to introduce an internal crystal field, and polarisation charges at opposite surfaces of the crystal; recent calculations of this field for the group III nitrides are in the range \(1 - 3 \text{ MV cm}^{-1}\), which, by Gauss’s law, corresponds to surface charge densities of over \(10^{13}\) electronic charges \(\text{cm}^{-2}\) (Bernardini et al. 1997). Piezoelectric polarisation appears due to strain, caused by the lattice
mismatch between the nitride layer and substrate. When an epitaxial layer is sufficiently thin, then the lattice mismatch can be accommodated by internal strain, rather than by the formation of misfit dislocations (Bykhovski et al. 1993). The piezoelectric coefficient of GaN is about three times larger than in GaAs (Shur et al. 1996), and combined with spontaneous polarisation, these effects become particularly important when considering the growth of AlGaN/GaN heterostructures. These effects will be discussed further in Section 5.1.1.

Lattice parameters and inter-planar distances are important indices because of their relevance to epitaxy and the effect of lattice mismatch with various substrates. Table 2.1 summarises the crystalline properties (e.g., lattice parameters, thermal expansion coefficient, lattice mismatch, band-gap energy, etc.) of the group III nitrides and the two main substrate candidates, sapphire (α-Al₂O₃) and hexagonal silicon carbide (6H-SiC). The values are liable to small errors when considering the effects of strain, growth conditions and experimental uncertainties. However, the spread in values is very small and perhaps this can be put into context by comparing the lattice constant values in Table 2.1 with those of presented by Leszczynski et al. (1996). They reported highly accurate measurements on a range of bulk and epitaxial GaN samples using high-resolution X-ray diffraction, and suggested values of \( a = 3.1879 \pm 0.0002 \) Å and \( c = 5.1851 \pm 0.0002 \) Å.

### Table 2.1. Summary of the structural properties of group III nitrides, sapphire and silicon carbide (Madelung 1991).

<table>
<thead>
<tr>
<th>Crystalline properties</th>
<th>GaN</th>
<th>AlN</th>
<th>InN</th>
<th>α-Al₂O₃</th>
<th>6H-SiC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice parameter (Å)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( a )</td>
<td>3.186</td>
<td>3.114</td>
<td>3.5446</td>
<td>4.758</td>
<td>3.081</td>
</tr>
<tr>
<td>( c )</td>
<td>5.178</td>
<td>4.9792</td>
<td>5.7034</td>
<td>12.991</td>
<td>15.092</td>
</tr>
<tr>
<td>( c/a )</td>
<td>1.6252</td>
<td>1.6003</td>
<td>1.6090</td>
<td>2.730</td>
<td>4.899</td>
</tr>
<tr>
<td>Thermal expansion coefficient ( (x10^{-6} \text{ C}^{-1}) )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( a )</td>
<td>5.6</td>
<td>4.2</td>
<td>5.7</td>
<td>7.5</td>
<td>4.2</td>
</tr>
<tr>
<td>( c )</td>
<td>3.17</td>
<td>5.3</td>
<td>3.7</td>
<td>8.5</td>
<td>4.7</td>
</tr>
<tr>
<td>Interplanar distance (Å)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Basal</td>
<td>2.59</td>
<td>2.49</td>
<td>2.85</td>
<td>2.165</td>
<td>2.516</td>
</tr>
<tr>
<td>(1100)</td>
<td>2.760</td>
<td>2.695</td>
<td>3.070</td>
<td>1.374</td>
<td>2.669</td>
</tr>
<tr>
<td>(1120)</td>
<td>1.593</td>
<td>1.556</td>
<td>1.772</td>
<td>2.379</td>
<td>1.541</td>
</tr>
<tr>
<td>Lattice mismatch (%)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \alpha-Al_2O_3 )</td>
<td>14.8</td>
<td>12.5</td>
<td>25.4</td>
<td>—</td>
<td>11.5</td>
</tr>
<tr>
<td>with</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SiC</td>
<td>3.3</td>
<td>1.0</td>
<td>14.0</td>
<td>-11.5</td>
<td>—</td>
</tr>
<tr>
<td>GaN</td>
<td>—</td>
<td>-2.4</td>
<td>10.6</td>
<td>-14.8</td>
<td>-3.3</td>
</tr>
<tr>
<td>Band-gap (eV) at 200 K</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.39</td>
<td>6.20</td>
<td>1.89</td>
<td>—</td>
<td>3.30</td>
</tr>
</tbody>
</table>
2. Physical Properties: Review

Many groups (Lambrecht and Segall 1994; Suzuki and Uenoyama 1996; Remediakis and Kaxiras 1999) have calculated the band structure of GaN and an example is illustrated in Fig. 2.2. GaN has a direct band gap at the Γ point, and as shown in Table 2.1, the group III nitrides span the range 1.95 – 6.2 eV in energy which includes the whole of the visible spectrum and extends into the UV region. The ability to form a complete series of ternary alloys with potential optical capabilities has been the main reason for the recent work on luminescence devices. The wide band-gaps demonstrate potential applications in electronic devices too, especially in the development of high power transistors.

2.1.2 Substrates

The choice of substrate is one of the primary factors which determine the crystallinity of an epitaxial layer, and thus its properties. One of the major difficulties, which have hindered GaN research, is the lack of a substrate material that is lattice matched and thermally compatible with GaN. Many candidates have been investigated, including GaAs and Si but there have been two main substrate materials that have been used extensively so far, which are sapphire and SiC.
• **Sapphire**: All the samples investigated in this thesis have been grown on sapphire substrates. This is a common trend, where, because of its good thermal stability and hexagonal crystal structure, not to mention the material's cheapness and wide availability, sapphire has been the preferred choice of substrate for GaN growth for many years. In addition, its transparency in the visible makes it ideal for some detector applications. Wurtzite GaN grown on sapphire is usually oriented in the c-plane [0001], and the mismatch in this configuration turns out to be 25% and thus responsible for the presence of high concentration of dislocations (Lester et al. 1995). The substantial lattice mismatch, coupled with a lower thermal expansion coefficient compared to the nitrides, presents problems when considering high power, high temperature electronic applications of GaN. Although buffer layers have been introduced to minimise dislocation effects, residual strain does exist, resulting in high piezoelectric polarisation in GaN epilayers.

• **Silicon carbide**: [0001] oriented 6H-SiC has also been tried as a substrate both because of the closer match between its hexagonal structure and that of GaN (lattice mismatch of 3.5%), and because its semiconducting and good thermal properties make it an attractive candidate for the possible fabrication of high power heterojunction devices (Sun et al. 1994). However, the material is costly, and the price needs to be reduced much further before it can compete with sapphire substrates.

Of course, it should be noted that the best substrate material would be to employ GaN itself. Homoepitaxy is an ideal situation where it is possible to minimise problems associated with difference in lattice structure, and differences in thermal expansion between the substrate and the film. Bulk single crystal technology has been developed to a production of crystalline platelets with lateral dimensions of the order of 3 – 6 mm, and thicknesses of about 100 μm (Grzegory et al. 1999). The crystals are grown in a gallium melt saturated with molecular nitrogen, at 1400 – 1600 °C and at nitrogen pressures of about 10 – 15 kbar. Other methods have been used such as MOCVD (Teisseyre et al. 1996) and HVPE (Melnik et al. 1997), all grown under similar
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temperature and pressure conditions. An important feature of these crystals is the morphology differences between the N-terminated rough surface and the Ga-terminated smooth surface (Dimitrov et al. 2000). Ga-terminated films show high degree of perfection, often with dislocation densities as low as $10^8 \text{ cm}^{-2}$. The promise of GaN substrates has not yet been fulfilled due to the platelet’s small dimensions but there are indications that larger size crystals can be grown (for example, Porowski et al. (1997) reported 1 cm GaN wafers).

2.2 Growth of nitrides

It is well known that growth techniques such as metal-organic chemical vapour deposition (MOCVD) and molecular beam epitaxy (MBE) have revolutionised the III–V compound semiconductor industry, and not surprisingly these methods also have been instrumental in much of the increased GaN activity that has occurred recently. Research has been extensive, and to present detailed accounts of the growth technology would be beyond the scope of this thesis. Instead, a general development of the nitride growth methods and the relative merits of the two techniques will be briefly discussed in the following section.

2.2.1 MOCVD

As far as the growth of GaN is concerned, MOCVD has been the most widely used and the most successful in preparing commercial high-quality devices. The general popularity of the MOCVD process stems from its ability to produce high quality multi-layer heterostructures in large volumes. Ammonia (NH$_3$) is used as the readily-available source of nitrogen. Ammonia becomes reactive at about 1000 °C, and hence GaN growth usually occurs at temperatures in the region 1000–1100 °C at atmospheric or low pressure, where Ga is supplied as trimethylgallium (TMG). The III/V injection ratio is very small which imposes some difficulty in controlling the reactant gases, and thus a customised system needs to be built, as reported by various groups (Nakamura 1991; Wang et al. 1999).

As mentioned previously in Chapter 1, unintentionally doped films exhibited n-
type conduction with carrier densities often greater than $10^{18}$ cm$^{-3}$. This is in part attributed to the high growth temperature used in the MOCVD process, making it difficult to accurately predict and control the growth (as a comparison, GaAs growth only requires around 700 °C). Additional problem of the lattice mismatch, causing the presence of numerous dislocations (of the order $10^{10}$ cm$^{-3}$), indicated the need to develop new, low temperature decomposition methods.

An important breakthrough came with the introduction of AlN or GaN thin buffer layers between the GaN film and sapphire substrate. The role of the buffer layer is to relax the effect of strain and defects in the heteroepitaxial growth of GaN, caused by the heavy build-up of dislocations within the buffer. It also provides copious amounts of nucleation sites having the same orientation as the substrate, and this leads to the promotion of lateral film growth due to the decrease in inter-facial energy between the epilayer and the substrate. The GaN and AlN layers are deposited at about 500 and 600 °C respectively, prior to the growth of GaN films at a temperature of 1040 °C (Amano et al. 1988). Film quality was found to be improved, as proved by the reduction in X-ray rocking curve full width half maximum (FWHM) from 8.2 to 1.9 arcmin, and also by the maximum Hall mobility of 900 cm$^2$ V$^{-1}$ s$^{-1}$. Comparison between the AlN and GaN buffers has been carried out by Kuznia et al. (1993) who found that film quality depended strongly on buffer thickness. They reported optimal thicknesses of 25 nm for GaN and 50 nm for AlN. Also, investigations on the quality of GaN epilayers under various growth conditions (Doverspike et al. 1995) suggested the best growth temperature to be about 1040 °C, with AlN as the preferred buffer material (because of its thermal stability).

2.2.2 MBE

Although the majority of the GaN devices are grown by the MOCVD method, the MBE process offers inherent advantages when attempting to grow abrupt heterostructures. The growth is carried out under a high purity ambient where the stainless-steel ultrahigh vacuum system can provide background pressure of less than $10^{-11}$ torr. Also, the growth temperatures are typically in the range 400 – 800 °C which is much lower than MOCVD, thus ensuring better control of heterostructure growth on a scale
of monolayers (e.g., AlGaN/GaN growth). However, these properties do present some experimental challenges that need to be overcome.

In such a low-pressure environment, the GaN deposition suffers heavy nitrogen loss arising from the high vapour pressure of nitrogen (Cho et al. 1995). This nitrogen loss leads to the formation of native defects such as nitrogen vacancies, and hence it was desirable to prepare nitrogen source that could supply an abundance of activated nitrogen ions. Various sources have been introduced; reactive-ion MBE (Powell et al. 1993), electron cyclotron resonance (ECR) plasma assisted MBE (Lin et al. 1993), radio frequency (RF) discharged MBE (Kim et al. 1994), and MBE involving the thermal cracking of NH₃ gas (Webb et al. 1999). These variants of MBE are handicapped by the slow growth rates of about 1 μm/hr, except for the MBE process using ammonia, which can achieve the growth rate of greater than 1 μm/hr. However, the thermally stable nature of NH₃ can be problematic in cases where lower growth temperatures are needed, such as when growing nucleation buffer layers or growth containing In, is carried out.

Among the gas sources, the ECR source is the most commonly used, not only because it provides the lowest plasma energies, but also it supplies high concentrations of radicals arriving at the substrate (Molnar and Moustakas 1994). However, the plasma sources still create large concentrations of energetic ions that damage the growing films. Hence a balance needs to be struck between the competing aspects of trying to reduce nitrogen vacancies and to minimise crystal damage, thereby customising and optimising for each experimental conditions. There is great potential in MBE growth for nitrides, and materials that possess comparable quality to MOCVD grown layers have already begun to appear.

2.3 Transport properties of GaN

Control of intrinsic electrical properties plays an important role in any device application. All the more so for the case of GaN, where the fundamental issue of self-compensation affects the material to a great extent. Key factors such as structural quality, doping level and presence of defects need to be studied thoroughly in order
to understand the transport characteristics of GaN. In addition, samples described in Chapter 4 seem to show a form of multiple carrier conduction, and various investigations into GaN films with similar problems have been carried out by several groups. This issue will be duly addressed in the next section, followed by device assessments on AlGaN/GaN heterostructures.

2.3.1 General issues

Often a figure of merit, the mobility (and carrier concentration) at low electric fields, measured by Hall effect, provides information on the quality of a semiconducting material. As mentioned before, early undoped GaN samples exhibited $n$-type behaviour with carrier densities in the range $10^{18} - 10^{20}$ cm$^{-3}$. The situation has not changed a great deal, although some 20% increase in mobility has been achieved (Orton and Foxon 1997). Rode and Gaskill (1995) compiled room temperature GaN mobility data from various sources, which is shown in Fig. 2.3. Experimentally, the electron mobility ranges from around 500 cm$^2$V$^{-1}$s$^{-1}$ at $\sim 10^{17}$ cm$^{-3}$ to 100 cm$^2$V$^{-1}$s$^{-1}$ at $\sim 10^{20}$ cm$^{-3}$ for the WZ GaN. From Fig. 2.3, it is apparent that all experimental results remain about a factor of two below the theoretical maximum mobility, suggesting the presence of compensation in these samples. Orton and Foxon (1998) came to similar conclusions, and further observed that recent samples appeared to be compensated to nearly the same extent as the earlier ones grown by Ilegems and Montgomery (1973), and reported compensation ratios in the region 0.5 - 0.7.

Compensation occurs when native defects counteract attempts at intentional doping of the material. Contrary to the accepted belief that assigned nitrogen vacancies as the main culprit for high $n$-type conductivity in undoped GaN samples (Jenkins and Dow 1989), Neugebauer and van der Walle (1994) stated that N vacancies turned out to be energetically unfavourable, and therefore ruled them out as the native donors. However, they reported that in $p$-type GaN the N-vacancy (a donor), and in $n$-type GaN the Ga-vacancy (an acceptor), are preferentially formed. Boguslawski et al. (1995) described a similar picture for $n$- and $p$-type cases, although in unintentionally doped GaN, they supported the conventional view of the N-vacancy being responsible for the $n$-type conductivity. Although there have been many other theoretical and experimen-
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FIG. 2.3. A collection of 300 K GaN electron mobility results, as reported from various sources. The top curve represents a theoretical mobility limit for zero compensation. Samples are grown by MBE and MOCVD, with and without buffer layers, and are undoped (open symbols) and Si doped (closed symbols). Mobility is plotted against electron concentration (Rode and Gaskill 1995).

tal studies of defects and their effects on transport properties, this issue has not yet been settled, and complicated compensation mechanisms still need to be investigated further before any firm conclusions are drawn.

Chin et al. (1994) considered various scattering mechanisms in undoped $n$-type GaN, and plotted its electron mobility as a function of temperature for electron concentrations of $10^{16}$, $10^{17}$, and $10^{18}$ cm$^{-3}$, and for compensation ratios of 0, 0.15, 0.3, 0.45 and 0.6 (shown in Fig. 2.4). They reported that scattering by optical phonons increases rapidly with temperature; it becomes the dominant mobility limiting process above about 200 K. At lower temperatures (below 100 K), ionised impurity scattering due to the presence of shallow donors and deep compensators, provides the most significant scattering of electrons. They also observed that the experimental mobility decreases at a higher rate than the calculated values, both below 80 K and above 500 K. Chin et al. attributed these findings to lattice strain and/or dislocation effects. As will be evident from Chapter 4, our own experimental results also exhibit different characteristics from Fig. 2.4, showing a rapid decline of Hall mobility at low temperatures,
much faster than predicted for impurity scattering process. This effect, together with
the absence of carrier freeze-out, means that an additional conducting mechanism such
as impurity band conduction could be present. Hence the following section discusses
the various aspects of multiple carrier conduction and presents selected examples of
published results.

\[ \text{mobility (cm}^2\text{V}^{-1}\text{s}^{-1}) \]

\[ \text{Temperature (K)} \]

**FIG. 2.4.** The electron mobility in n-GaN plotted against temperature, for (a) \(10^{16}\), (b) \(10^{17}\) and (c) \(10^{18}\) cm\(^{-3}\) with compensation ratios of 0, 0.15, 0.3, 0.45 and 0.6 (Chin et al. 1994).
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2.3.2 Multiple carrier conduction

Multiple carrier effects occur because of the presence of light and heavy holes, electrons and holes in near intrinsic semiconductors, or because of degenerate conduction band minima such as in silicon and germanium. Parallel conduction in a layered system is also an example of conduction involving multiple carrier types (Stradling 1990). In this section, impurity band conduction, conduction via a degenerate layer at GaN/sapphire interface and transport affected by grain boundaries, are considered.

Molnar et al. (1993) investigated the electron transport mechanism in unintentionally doped GaN films grown by ECR-MBE by studying the temperature dependence of the Hall coefficient, \( R_H \), and resistivity, \( \rho \), on samples with various concentrations of autodoping centres. They observed the Hall coefficients going through a maximum as the temperature is lowered from 300 K and then saturating at lower temperatures. The temperature at which this maximum occurs is found to be higher for samples with lower \( \rho \). They attributed these observations to the mixed electron transport in the conduction and impurity bands, and concluded that conduction through the impurity band becomes dominant at temperatures below 40 K. Similar behaviour was first explained by Hung and Gleissman (1954) who proposed a model involving transport in both the defect centres and the conduction band of germanium. The secondary conduction could be either diffusive or via hopping, and thus its mobility is expected to be much smaller than that of the conduction band.

Molnar et al. analysed their results using a simple two-band model, and a portion of such analysis will be given later in Section 4.1.4. They extracted the net total carrier concentration \( N_T = 5.8 \times 10^{17} \text{ cm}^{-3} \) and a donor activation energy \( \epsilon_d = 19 \text{ meV} \) from their analysis. Also, Fig. 2.5 shows their calculated values of conduction band mobility \( \mu_c \) and concentration \( n_c \), and of defect band mobility \( \mu_d \) and concentration \( n_d \), compared with the measured values of mobility \( \mu_{meas} \) and concentration \( n_{meas} \). Look and Molnar (1997) also conducted similar temperature dependent Hall measurements in HVPE epitaxial GaN grown on sapphire, and also reported the presence of another conducting layer. However, instead of conduction by impurity band, they assumed a thin (2000 – 3000 Å) degenerate n-type region at the GaN/sapphire interface as the secondary conduction channel. They employed a two-layer Hall model and the
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![Graphs showing temperature dependence of (a) \(\mu_{\text{meas}}, \mu_c\) and \(\mu_d\); and (b) \(n_{\text{meas}}, n_c\) and \(n_d\) (Molnar et al. 1993).]

FIG. 2.5. Temperature dependence of (a) \(\mu_{\text{meas}}, \mu_c\) and \(\mu_d\); and (b) \(n_{\text{meas}}, n_c\) and \(n_d\) (Molnar et al. 1993).

analysis carried out closely fitted carrier concentration and mobility values over the temperature range 10 – 400 K.

Götz et al. (1998) extended the two-layer concept regarding the distribution of defects by varying the thickness of the GaN films. They tested HVPE GaN films grown on zinc oxide (ZnO) or gallium chloride (GaCl) pre-treated sapphire which acts as the film nucleation layer. The temperature variation of electron concentration and mobility are shown in Fig. 2.6 for the case of ZnO pre-treated GaN. The room temperature mobility values decrease with decreasing thickness. This can be explained by the fact that thicker films allow more freedom for stacking faults and dislocations to appear, thereby relaxing strain and thus improving the material quality. For the thin film of thickness of 4.5 \(\mu m\), multiple carrier conduction is observed. They derived equations based on depth distributions for \(n(x)\) and \(\mu(x)\) and demonstrated that for ZnO pre-treated sapphire the Hall effect data clearly indicated a continuous reduction of the defect density with increasing film thickness. In contrast, GaCl pre-treated sapphire can be described as two carrier conduction in two distinct layers with an abrupt transition between them.

Wurtzite GaN exhibits a columnar microstructure, with dislocations propagating normal to the substrate and can be regarded as a poly-crystalline material. This could strongly affect the electron transport, and Fehrler et al. (1998) have proposed the
existence of potential barriers caused by electron traps at grain boundaries. These traps become charged, thus effectively producing band bending and reducing mobility. They have studied highly resistive GaN epilayers grown by MBE, and developed a theoretical model, where both the mobility and the carrier concentration follow an exponential dependence. Similarly, Salzman et al. (1999) irradiated GaN with H\(^+\) and He\(^+\) ions, and as a result of ion damage, they observed drastic and non-linear sample resistance increase with increasing dose. They also attributed these findings to transport over grain boundaries and found that the resistivity is dominated by potential barrier height, which, in turn, is inversely proportional to carrier density. Although most of the samples characterised in this thesis have much higher carrier densities than those of Salzman et al. (1999), the effect of grain boundary scattering cannot be ruled out. Grain sizes vary depending on growth methods and conditions, and understanding these properties are hampered due to characterisation being very much sample dependent.
2.4 AlGaN/GaN heterostructures

Much of the drive behind group III nitrides research has been due to the development of optical devices. However, the advantages regarding the electronic applications have also been recognized with major advances in the growth technologies such as MOCVD and MBE, and significant improvement in electronic device technology is envisaged. The nitrides will have only a niche position in the electronics market though; they have neither the intrinsic properties needed to challenge GaAs, nor the production compatibility to compete with Si. Still, the progress that has been made on the development of high power, high temperature and high frequency devices has been sufficient to show that there will be a sizeable market for the nitrides in future. Thus, a list of properties that make the nitrides so attractive, and a description of recent device development, is given in the next section.

2.4.1 Advantages of nitrides

There are four main attractive properties of wide band gap materials for solid state electronics, and from comparing various electronic properties of GaN, Si, GaAs and SiC (as shown in Table 2.2), a number of justifications for the recent interest in employing AlGaN/GaN systems can be made:

<table>
<thead>
<tr>
<th>Band-gap energy (eV)</th>
<th>1.1</th>
<th>1.4</th>
<th>3.3</th>
<th>3.4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Breakdown field (×10^5 V cm^-1)</td>
<td>2</td>
<td>4</td>
<td>30</td>
<td>30</td>
</tr>
<tr>
<td>Electron mobility (cm² V^-1 s^-1)</td>
<td>1400</td>
<td>8500</td>
<td>800</td>
<td>900</td>
</tr>
<tr>
<td>Maximum velocity (×10^7 cm s^-1)</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>Thermal conductivity (W cm^-1 K^-1)</td>
<td>1.5</td>
<td>0.5</td>
<td>4.9</td>
<td>1.6</td>
</tr>
</tbody>
</table>

(i) **Wide band gap** – the intrinsic carrier concentration (nᵢ) at any given temperature decreases exponentially with band-gap which means that GaN becomes intrinsic at higher temperatures than other materials (nᵢ of Si reaches 10^15 cm^-3 at around 300 °C, GaAs at about 500 °C, and GaN at about 1300 °C). Hence the
high temperature applications are clear for all to see, and with less cooling and fewer processing steps necessary in heat extraction, manufacturing cost would be greatly reduced.

(ii) **High breakdown fields** – Chow and Tyagi (1994) discussed high power operation as a result of high breakdown fields, and comparisons can be made with GaN’s breakdown fields of about $3 \times 10^8$ V cm$^{-1}$, and with that of Si ($2 \times 10^5$ V cm$^{-1}$) and GaAs ($4 \times 10^5$ V cm$^{-1}$), corresponding to the difference of approximately an order of magnitude.

(iii) **High electron velocity-field characteristics** – Monte Carlo simulations indicate the peak electron velocity of GaN to be $3 \times 10^7$ cm s$^{-1}$, and also a high saturation drift velocity of $1.5 \times 10^7$ cm s$^{-1}$ (Gelmont et al. 1993). The velocity-field curves for GaN, 6H-SiC (Shur et al. 1994), and for Si and GaAs (Sze 1981) are compared in Fig. 2.7. The electron mobility of $n$-GaN is high enough for the application of microwave devices (speed operation greater than 10 GHz), which has been reported by Asif Khan et al. (1993) for an AlGaN/GaN MODFET structure.

(iv) **Heterojunction capabilities** – in many ways, the developments in heterojunction group III nitrides mirror that of the AlGaAs/InGaAs system which has set the modern benchmark for microwave device performance through the advent of *band gap engineering* (Capasso et al. 1985; Döhler 1986). It is important to maximise the conduction band discontinuity ($\Delta E_c$) at the heterointerface between GaN and its ternary alloys. This allows improved charge confinement, higher sheet carrier densities and better mobilities (Sze 1981). AlGaN/GaN systems benefit from the inherent polarisation effects, inducing 2DEG densities in excess of $10^{13}$ cm$^{-2}$ without intentional doping. This aspect is of great importance in group III nitrides, and thus special attention will be given further in Section 5.1.1. Simply increasing the Al composition for the largest $\Delta E_c$ (2.8 eV) will not guarantee better performance. Constraints such as the lattice mismatch (strain) or deep level defects could adversely affect the system. In fact, Asif Khan et al. (1991) reported that in the AlGaN/GaN structure, the electron mobility...
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has a maximum for an Al composition in the range 0.13 – 0.15.

![Graph showing electron drift velocity as a function of electric field for Si, GaAs, SiC and GaN at 300 K, and electron drift velocity in GaN at 300, 500 and 750 K (Asif Khan et al. 1997).]

It should be pointed out that GaN based systems, albeit with all their attractive features, do possess some shortcomings too, mainly in high temperature applications. As can be seen from Table 2.2, the thermal conductivity of GaN is inferior to that of SiC. This problem of heat removal is accentuated by the fact that the GaN related devices are grown on sapphire which has an even lower thermal conductivity. An alternative would be to employ SiC as a substrate itself, although as stated in Section 2.1.2, the high cost makes SiC less desirable than sapphire from a manufacturing point of view. Although the majority of research on nitrides has concentrated on producing opto-electronic devices, the FET developments have also been ongoing for a number of years, and microwave power FETs of real commercial promise are beginning to appear, and the next section briefly reviews such developments.

2.4.2 Electronic devices

The first GaN MESFET was fabricated by APA Optics in the early 1990’s (Asif Khan et al. 1993). Unintentionally doped, n-type GaN was grown on a sapphire substrate using a thin AlN nucleation layer. The GaN layer was 6000 Å thick and had room temperature mobility of 350 cm²V⁻¹s⁻¹. It had many desirable characteristics; good pinch-off, reasonable transconductance (g_m) of 23 mS/mm, and a relatively high breakdown voltage (120 V). However, this device demonstrated where improvements needed
2. Physical Properties: Review

to come from. The material was unintentionally doped, making it difficult to control the optimisation process. The active channel extended to the substrate, and a low-mobility region at the interface was observed. However, recent improvements in the area of epitaxial growth have meant that GaN layers with intentional and controlled doping can now be achieved. Also, Binari et al. (1994) proposed that using a thick high resistivity GaN layer (~3 μm) above the nucleation layer could solve the problem of channel/substrate overlap.

Progress has also been made in the development of group III nitride heterojunction devices. Asif Khan et al. (1992) first observed the presence of a two-dimensional electron gas (2DEG) using an AlGaN/GaN structure grown on sapphire. Since then, several groups have succeeded in producing AlGaN/GaN MODFETs (Fan et al. 1996; Eastman et al. 1997) and they have managed to demonstrate various advantages of the group III nitride ternary-based devices. For example, Wu et al. (1996) recorded 300 K mobility of 1500 cm²V⁻¹s⁻¹ and a large $g_m$ of 140 mS/mm, using a Si-doped GaN channel. The 2DEG carrier concentration was $7.9 \times 10^{12}$ cm⁻² and the breakdown voltage of 230 V was realised for a 1 μm gate length. Fig. 2.8 shows the cross-section of the first reported MODFET, grown by MOCVD (Asif Khan et al. 1993). It consists of 1000 Å, n-type Al₀.₁₄Ga₀.₈₆N layer on top of a 0.6 μm, n-type GaN layer. The layers were unintentionally doped, and the 2DEG exhibited a 300 K Hall mobility of 560 cm²V⁻¹s⁻¹ and a $g_m$ of 28 mS/mm.

Microwave performance of a MODFET similar to the one shown in Fig. 2.8 has
been obtained by investigating a 0.25 $\mu$m gate AlGaN/GaN structure (Asif Khan et al. 1994). A cut-off frequency ($f_T$) of 11 GHz and a maximum oscillation frequency ($f_M$) of 35 GHz were reported. The progress has been rapid, and the current state-of-the-art MODFET device exhibits a $f_T$ of 68 GHz and a $f_M$ of 140 GHz (Chu et al. 2001), for a gate length of 0.15 $\mu$m. For the device with a 0.8 $\mu$m gate length, channel currents above 1000 mA/mm and a breakdown voltage of 140 V have been achieved. Chu et al. (2001) further projected the high power, high temperature performance of the device assuming that the substrate was replaced by SiC, and their prediction includes normalised output power levels over 12 W/mm, together with power added efficiency of 70%. Large periphery AlGaN/GaN based devices have also been fabricated on SiC recently, which demonstrated power densities and total powers of 6.9 W/mm and 9.1 W at a frequency of 10 GHz, respectively (Sheppard et al. 1999).
Chapter 3

Experimental Procedures

This chapter describes experimental procedures that are utilised in acquiring the results presented in this thesis. The contents of this chapter are divided into two parts. Firstly, the basic operating principles and design features of the cryogenic systems employed including the measurement set-up associated with each system, are discussed. Secondly, details of the samples investigated in this thesis are given, with an account of the sample structure and preparation.

3.1 Experimental equipment

In this thesis, the characterisation techniques based on the Hall (described in Section 4.1.1) and Shubnikov-de Haas (SdH) effect (discussed in Section 5.1.3) have been performed on GaN bulk and AlGaN/GaN 2DEG samples. In general, the Hall measurements were performed to obtain the temperature dependence of transport properties, and the SdH experiments required the application of high magnetic fields (e.g., $B > 8$ T) in a very low temperature environment (e.g., $T < 4.1$ K). From the Hall measurements, information on scattering mechanisms limiting the mobility have been obtained as well as the role of a defect band in influencing the transport properties of bulk layers (discussed in Chapter 4). The low temperature magneto-transport measurements reveal the dimensionality of the sample system, and various parameters such as electron effective mass and relaxation times can be determined by analysing the data acquired (presented in Chapter 5). In addition, energy loss rates of hot electrons in AlGaN/GaN
heterostructures can be calculated by studying the oscillations in magneto-resistivity (described in Chapter 6).

In order to cater for all the measurements taken under different conditions, various systems have been employed, which include:

- Closed cycle cryostat (CCC) for temperature dependent Hall measurements on bulk and 2DEG samples, covering temperatures in the range $10 - 600$ K at a magnetic field of about $0.3$ T.

- Variable temperature insert (VTI) for temperature dependent SdH measurements on 2DEG structures, with a magnetic field of up to $15$ T and temperatures in the range $1.3 < T < 300$ K.

- Dilution fridge (DLF) for low temperature SdH measurements ($0.03 < T < 4.2$ K) on 2DEG specimens with a magnetic field of $15$ T.

It should be pointed out that all GaN samples have been characterised using the van der Pauw (VDP) technique, and most of the 2D samples measured were of the Hall bar structure. To point out the differences of the magnetic systems used for the measurements, the following sections present a description of each experimental equipment, followed by a summary of the data acquisition techniques.

3.1.1 Closed cycle cryostat

The temperature dependent Hall characterisation has been carried out at University College London (UCL) between $10 - 600$ K using a magnetic field strength of around $0.3$ T. A constant field is supplied by a solenoid, which is powered by a $5$ A current source. Both the bulk and 2D samples have been measured, though this system only incorporates the VDP (square or clover-leaf) structure. Each sample is bonded onto a chip carrier (TO8 header), which can then be placed on the sample holder. Strictly speaking, the CCC can only access temperatures in the range $10 - 300$ K. In order to extend the measurement temperature to $600$ K, a customised hot stage was employed. Hence, the measurement techniques for both cold and hot stages are described below.
3. Experimental Procedures

Cold stage

The closed cycle cooler system comes from Oxford Instruments, which consists of the cryostat built on an Edwards model CS2/9 cold head, a water-cooled compressor unit (Edwards cryodrive 1.5), an integral control unit, and an integrated temperature controller (ITC). Fig. 3.1 shows the overall experimental arrangement of the cold measurement system.

![Diagram of the overall cold measurement system](image)

**FIG. 3.1.** Schematic diagram of the overall cold measurement system which includes a cryostat, an ITC, a helium compressor, and a Hall measurement set-up.

General descriptions of the system units and their principal modes of operation are given as follows:

- **Cold head** — this is fitted with a stepper motor. The rotational frequency of the motor controls the frequency of the coldhead displacer cycle which, in turn, controls the cooling power of the cryopump. The low temperature refrigeration is
achieved by helium flow. Helium (He) is compressed to 16.5 bar in the compressor and expanded in a controlled manner in the coldhead for cooling.

- **ITC** — a rhodium iron temperature sensor and two wire-wound resistor heaters embedded in a copper block, attached to the coldhead, allow variable temperature operation to be possible. The ITC not only controls the heater power, but also adjusts the speed of the coldhead to ensure stable temperature control.

- **Cryostat** — the first stage of the cooler is connected to a copper radiation shield which extends upwards to protect the heat exchanger and sample holder from room temperature radiation. An outer vacuum chamber, then surrounds the radiation shield to provide vacuum insulation for the cryostat. The cryostat contains 10 pins available for the electrical wiring to connect the sample to the external Hall measurement system, of which four are used for the VDP configuration.

- **Sample holder** — customised for our measurement, a diagram of the holder is shown in Fig. 3.2. A rectangular copper block was initially considered as the sample holder, but because of the sweeping nature of our temperature variation, it was important that the temperature displayed in the ITC matched with the actual sample temperature as closely as possible. Hence, the material is further sliced and trimmed for minimum thermal lag with the sample. The sample is mounted onto a TO8 header which is then inserted into the recess created in the sample holder, and placed directly in the centre of the magnet.

**FIG. 3.2.** Customised sample holder arrangement for the cold stage.
3. Experimental Procedures

Although not revealed in Fig. 3.1, the closed cycle system needs to be evacuated first before any cooling can be carried out. A rotary pump is employed to start pumping the vacuum chamber until the pressure reaches about $10^{-2}$ torr. Then, a turbo-molecular pump is switched on to further reduce the chamber pressure to around $10^{-5}$ torr. Having pumped the system down, the system can be cooled from 300 K down to 10 K for the temperature dependent Hall measurements.

Hot stage

Because the CCC can only operate up to 300 K, a separate stage for the measurements at temperatures in the range 300 — 600 K is required. As will be evident when considering both the low and high temperature stages, the sample holder and the corresponding electrical wiring are designed so that minimum effort is required when changing samples, beneficial when maintaining the consistency and reliability of the measurements. The experimental set-up for the hot stage is schematically illustrated in Fig. 3.3.

![Diecast box heater](image)

**FIG. 3.3.** The sample holder arrangement for the hot stage and the measurement system.

Within the outer casing exists an aluminum block, placed in the middle. The metal block houses the sample/TO8 header arrangement, similar to the cold sample holder.
3. Experimental Procedures

A heater resistor and a thermocouple are also implanted in the aluminum block in close proximity to the sample mount recess for efficient temperature control. Heating is generated by a variac, and the temperature is recorded by a digital voltmeter linked to the thermocouple (40 mV K$^{-1}$). The manual temperature adjustment for the hot stage is less superior to the cold stage since the cryogenic system has an advantage of being microprocessor controlled (typical temperature fluctuation of ±0.2 K). Nevertheless, each hot reading is performed within ±1 K of the assigned temperature, and is thus satisfactory for data analysis. The VDP contact leads are connected to the Hall measurement system, which is also joined to the voltmeter for Hall data acquisition. Again, the set-up is assembled in such a way that the sample is located perpendicular to and at the centre of the magnet. Finally, note that the mounted assembly is surrounded with fibreglass to enhance thermal insulation.

3.1.2 Variable temperature insert

Low temperature magneto-transport experiments on AlGaN/GaN 2DEG samples to investigate the Shubnikov-de Haas (SdH) and quantum Hall (QHE) effects have been carried out using the Oxford Instruments system at the High Magnetic Field Laboratory in Grenoble, France. The magneto-system is depicted in Fig. 3.4, which mainly consists of a superconducting solenoid (capable of delivering a field of 15 T), a variable temperature insert and a sample chamber.

As can be seen from the diagram, the sample chamber itself is thermally insulated from the helium bath by an inner vacuum space, and is surrounded over most of its length by a radiation shield. The insert is lowered slowly to prevent rapid overheating of the sample chamber, and can take between 30 to 60 minutes to reduce the temperature from 300 to 4.2 K. The temperature is monitored by a calibrated carbon glass resistance temperature sensor. For operation below 4.2 K the needle valve allows liquid helium to flow dynamically from the main $^4$He bath into the sample chamber. Subsequent closure of the needle valve and control of the vapour pressure via a manostat gives accurate temperature control from 4.2 to 1.3 K. A comprehensive coverage of measurement temperatures is realised during warming-up of the sample chamber, where measurements from 4.2 K to room temperature are carried out. As will be
discussed in Section 5.1.3, from the temperature dependence of SdH oscillation amplitudes, important material parameters such as effective mass and quantum relaxation time can be determined.

The system utilises the top loading insert where the sample rods emerge through O-ring seals at the top of the apparatus, providing easy access to replace the samples from the sample space while the cryostat is cold. Up to four Hall bar specimens can be mounted directly at the same time onto the bottom end of the insert via an 8-pin dual-in-line socket (DIL) socket.

Consisting of a NbTi outer section and a Nb₃Sn inner section, the superconducting
solenoid supplies magnetic fields of up to 15 T at 100 A, generated by a current source precise to within 1%. To avoid excessive heating of the magnet, the average sweep time was kept about 15 minutes. More details on the actual data acquisition technique will be presented later in Section 3.1.4.

3.1.3 Dilution refrigerator

Being the most sophisticated cryogenic system, the dilution fridge (DLF) is capable of reaching temperatures below 1.3 K down to about 30 mK. As mentioned in the previous section, studying the variation of SdH oscillation amplitudes with changing temperature enables the extraction of transport parameters. When combined with the investigation of the oscillation amplitude variation with varying currents at a fixed temperature, energy loss mechanisms of hot electrons can be examined, and the dilution fridge is an ideal measurement system for such purposes. Hence, the magneto-transport data obtained from DLF experiments provide a basis for analysing the behaviour of hot electrons at very low temperatures, and the corresponding results will be discussed later in Section 6.2.

The overall system is also a part of the High Magnetic Field Laboratory in Grenoble, and retains a number of similar features to the VTI system, such as the top loading sample insert (though in this case, the insert houses only two samples) and the superconducting solenoid magnet supply (15 T). However, there are differences when considering the principle of cooling mechanism, and can be explained by considering the phase diagram of a $^3$He/$^4$He mixture (Taconis and de Bruyn Ouboter 1964), which is shown in Fig. 3.5.

As can be seen from the figure, the two liquids are miscible in all proportions above the tricritical point at 0.87 K. Since both He isotopes become superfluid at different temperatures ($^3$He at 2.17 K and $^4$He at just below 1 mK), the transition temperature between superfluid and normal liquid state is dependent on the $^3$He concentration in the mixture. Below the tricritical temperature, liquid $^3$He and $^4$He are immiscible over a wide composition range, thus separating the mixture into two phases, the concentrated $^3$He phase and the dilute $^4$He phase. Hence, a mixture with composition in the unstable regime will decompose into two separate phases whose compositions are given by the
two branches of the $\lambda$-curve. As the temperature approaches 0 K the concentrated phase becomes essentially pure $^3$He, whereas the $^4$He concentration of the dilute phase drops to about 6.3%. The concentrated phase of the mixture can be regarded as liquid $^3$He and the dilute phase as a quasi-gas of $^3$He atoms dissolved in liquid $^4$He. For mixtures with a $^3$He concentration exceeding 6.3%, the excess condenses into concentrated liquid $^3$He, liberating latent heat. By evaporating $^3$He across the phase boundary from the concentrated to the dilute phase latent heat is consumed. This process constitutes the basic principle of a helium dilution refrigerator.

The schematic diagram of such a refrigerator, shown in Fig. 3.6, illustrates the working operation of the cooling process. In the still, $^3$He is selectively distilled from the $^3$He/$^4$He mixture due to a high vapour pressure, and pumped off. To obtain a useful $^3$He evaporation rate, the temperature of the still has to be raised to about 0.6 K, still guaranteeing a distinctly smaller $^4$He vapour pressure. The lower concentration of $^3$He in the still causes $^3$He atoms from the $^3$He/$^4$He mixture in the mixing chamber to diffuse through a counterflow heat exchanger into the still, thus decreasing the $^3$He concentration in the dilute phase. In order to restore the equilibrium concentration, quasi-evaporation of $^3$He atoms from the concentrated phase to the dilute phase will take place under consumption of latent heat, cooling down the mixture. The pumped-
off $^3$He is returned to the system through a condenser that is cooled to about 1 K by contact with a pumped $^4$He bath. A narrow capillary tube creates a flow impedance to maintain a high enough pressure in the condenser for the gas to condense. Before re-entering the mixing chamber, the liquefied $^3$He is further cooled, first in the still, then in the counterflow heat exchanger. The high throughput of the fridge allows cooling from room temperature to 50 mK in less than 3 hours, and further cooling to the ultimate base temperature of about 30 mK is typically done overnight.

3.1.4 Measurement techniques

The temperature dependent Hall measurement data using the CCC system have been obtained using a digital voltmeter (DVM). A typical input current was 1 mA, although in some high resistivity samples, 0.1 mA was employed. The DVM’s filtering option was utilised to improve the signal-to-noise ratio, and was found to be particularly useful at low temperatures. A weak magnetic field of 0.31 T was applied during the Hall voltage acquisition. Due to the long temperature settling time of the system during the cooling process, performing these measurements can take a long time and can become too impractical if too many temperature points are taken. In addition,
3. Experimental Procedures

the hot stage experiments needed to be completed soon after the cold measurements in order to ensure continuity of the results. Hence, readings were taken at temperature intervals in the range 10 – 20 K, resulting in a typical time taken to complete the measurement per sample of approximately 7 hours.

A more sophisticated approach has to be taken for the low temperature magneto-transport measurements using the VTI and DLF systems, and different components of the measuring set-up are shown in Fig. 3.7. The sample is of a Hall bar structure and positioned perpendicular to the magnet. A Hall probe is used to determine the magnetic field of the solenoid during a sweep, and the resulting voltage is fed via analogue/digital converter into a computer for data analysis. The sweep of the solenoid itself is controlled by a programmable power supply which acts as a ramped current source.

![Schematic diagram of experimental set-up for low temperature magneto-transport results.](image)

**FIG. 3.7.** Schematic diagram of experimental set-up for low temperature magneto-transport (using VTI and DLF systems) results.

At such low temperatures, electron heating effects can occur where the electrons might not be able to absorb all of the dissipated input power, leaving the rest to be absorbed by the lattice. This leads to an increase of the electron temperature above that of the lattice, and false interpretation of the experimental results is inevitable. Since the power is proportional to the square of the injected current, the level of cur-
3. Experimental Procedures

Current needs to be very low, and in low temperature measurements, a typical value of the driving current was chosen to be about 100 nA. Note that in cases where phonon emission processes of hot electrons are investigated (Chapter 6), the input current was deliberately increased spanning several orders of magnitude, so that the amplitudes of the dampened SdH oscillations can be used as a thermometer for the electron temperature. Another source of electron heating is eddy currents induced during a magnet sweep, where the rate of heat production is proportional to the field sweep rate. In the measurements, sweep rates are kept low (below 0.1 T/min), and temperatures measured for analysis are averaged between the temperature reading at the start and at the end of the sweep to minimise error.

A consequence of using small currents is a relative increase in the noise level of the signal when measuring the transverse and longitudinal voltages of the Hall bar. Therefore, a lock-in amplifier was employed to increase the signal-to-noise ratio. In addition, the signal was pre-amplified before being fed back into the lock-in amplifier to achieve the best resolution of the recorded data. The obtained signals are read by the DVM which are then sent to a computer through an IEEE-488 link.

3.2 Sample preparation

The characterised samples are divided into two types; wurtzite $n$-GaN layers and AlGaN/GaN 2DEG heterostructures, both of which are grown on sapphire. Growth of group III nitrides using processes such as MBE and MOCVD have already been described in Section 2.2 and thus in the following sections, the details of structure and preparation techniques of specimens studied will be mainly discussed.

3.2.1 GaN samples

The $n$-type GaN layers have been grown on sapphire substrates by various methods, RF-MBE (from Nottingham University), MBE using NH$_3$ (from National Research Council, Canada), and both atmospheric- and low pressure (100 torr) MOCVD (from Gent University, Belgium), and a variety of growth details for all GaN samples are listed in Table 3.1.
TABLE 3.1. Growth and characterisation details of WZ $n$-GaN samples.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Growth</th>
<th>Doping</th>
<th>Thickness ($\mu$m)</th>
<th>Buffer</th>
<th>VDP shape</th>
<th>Contacts</th>
</tr>
</thead>
<tbody>
<tr>
<td>MG622</td>
<td>RF-MBE</td>
<td>Undoped</td>
<td>4.6</td>
<td>None</td>
<td>clover-leaf</td>
<td>Aluminum</td>
</tr>
<tr>
<td>MG657</td>
<td>RF-MBE</td>
<td>Silicon</td>
<td>2.0</td>
<td>None</td>
<td>clover-leaf</td>
<td>Aluminum</td>
</tr>
<tr>
<td>MG676</td>
<td>RF-MBE</td>
<td>Undoped</td>
<td>2.0</td>
<td>None</td>
<td>clover-leaf</td>
<td>Aluminum</td>
</tr>
<tr>
<td>C190299</td>
<td>NH$_3$-MBE</td>
<td>Silicon</td>
<td>2.0</td>
<td>AlN</td>
<td>square</td>
<td>Indium</td>
</tr>
<tr>
<td>G50</td>
<td>AP-MOCVD</td>
<td>Undoped</td>
<td>1.0</td>
<td>GaN</td>
<td>square</td>
<td>Indium</td>
</tr>
<tr>
<td>G165</td>
<td>AP-MOCVD</td>
<td>Undoped</td>
<td>1.0</td>
<td>GaN</td>
<td>clover-leaf</td>
<td>Aluminum</td>
</tr>
<tr>
<td>G138</td>
<td>AP-MOCVD</td>
<td>Undoped</td>
<td>1.0</td>
<td>GaN</td>
<td>clover-leaf</td>
<td>Aluminum</td>
</tr>
<tr>
<td>G595</td>
<td>LP-MOCVD</td>
<td>Silicon</td>
<td>1.6</td>
<td>GaN</td>
<td>square</td>
<td>Indium</td>
</tr>
<tr>
<td>G613</td>
<td>LP-MOCVD</td>
<td>Undoped</td>
<td>2.6</td>
<td>GaN</td>
<td>square</td>
<td>Indium</td>
</tr>
<tr>
<td>G617</td>
<td>LP-MOCVD</td>
<td>Silicon</td>
<td>2.6</td>
<td>GaN</td>
<td>square</td>
<td>Indium</td>
</tr>
<tr>
<td>G649</td>
<td>LP-MOCVD</td>
<td>Silicon</td>
<td>2.5</td>
<td>GaN</td>
<td>square</td>
<td>Indium</td>
</tr>
</tbody>
</table>

The Nottingham samples were deposited using activated nitrogen from an Oxford Applied Research HD25 RF source, and did not include a buffer layer during growth. The sample grown by National Research Council (NRC) bears similar features to the samples grown by RF-MBE, though there are a couple of crucial differences. Nitrogen was delivered by ammonia instead of a RF source, and an AlN buffer layer (< 300 Å) was deposited using magnetron sputter epitaxy (MSE). A detailed description of NH$_3$-MBE growth is given by Tang and Webb (1999). The MOCVD layers were grown from TMG and NH$_3$ in a Thomas Swan reactor using a two-temperature technique (van der Stricht et al. 1995). All the MOCVD samples have the same basic structure; a 430 $\mu$m sapphire substrate, a 20 – 40 nm GaN buffer layer grown at about 550 °C, and a GaN layer grown at approximately 1100 °C.

Doping was achieved using Si as the donor, and samples which have not been deliberately doped all exhibited $n$-type conductivity. As shown in Table 3.1, Al and In have been used as the ohmic contacts. In was melted at the four corner edges of a VDP specimen, and Al was thermally evaporated and then annealed in a tube furnace under nitrogen environment at 550 °C for 10 minutes. Square VDP specimens were about $5 \times 5$ mm$^2$ in size, and samples with the clover-leaf pattern were obtained by using sandblasting technique. The bulk samples described in this section are characterised by temperature dependent Hall measurements ranging from 10 to 600 K. The CCC system (refer to Section 3.1.1) was employed in the measurements and the data obtained are
analysed and discussed later in Section 4.2.

3.2.2 2DEG samples

The AlGaN/GaN 2DEG structures were examined by both the temperature dependent Hall (using the CCC) and the low-temperature magneto-transport measurements (using the VTI and DLF). The Hall measurements have been carried out initially on VDP squares to investigate the electron concentration and mobility of the selected samples (discussed in Section 5.2.1). All the samples are further investigated at lower temperatures (< 4.1 K) and under higher magnetic fields (15 T) for quantum effects (refer to Section 5.2.2 for a theoretical account) whose obtained data provide the main results of Chapter 5.

\[
\begin{align*}
\text{AlGaN} & \quad \longrightarrow \quad \text{Si-doped layer} \\
\hline
\text{GaN} & \\
\hline
\text{GaN or AlN Buffer layer} &
\end{align*}
\]

\text{Sapphire substrate}

FIG. 3.8. Schematic diagram of the layer structure for a AlGaN/GaN heterostructure. Modulation-doping is achieved by an introduction of a thin Si-doped layer within the AlGaN.

The 2D samples grown on sapphire substrates have been supplied by various sources; NRC employing NH₃–MBE, Gent University using LP–MOCVD, Defence Evaluation and Research Agency (DERA) of United Kingdom using MOCVD, and Tokushima University in Japan also utilising MOCVD. A typical sample structure is illustrated in Fig. 3.8. It consists of sapphire as the substrate, a GaN or AlN buffer layer, an undoped GaN layer, and an AlGaN layer which may or may not be intentionally doped with Si. Growth details of the samples are listed in Table 3.2 including different layer thicknesses \( t \) and the Al composition \( x \).

Three of the samples (J401, C251199 and D952) studied are undoped AlGaN/GaN
heterostructures in which the 2DEG arises in response to the internal piezoelectric and spontaneous polarisation fields (refer to Section 5.1.1 for a theoretical account). Layers G91 and G99 contain a Si modulation-doped AlGaN supply layer. These samples and D952 are designed specifically for room temperature MODFET operation, which requires a thin AlGaN layer in order to obtain effective capacitative coupling between the gate electrode and the 2DEG channel. Samples J401 and C251199 have a relatively thick AlGaN region, and are better suited for low temperature measurements. Nevertheless, as will be evident later in Section 5.2.2, all of the layers showed clear SdH oscillations indicative of good quality 2DEGs, and the variation in low temperature transport properties has been studied to determine the relationship between quantum and classical lifetimes ($\tau_q$ and $\tau_t$, respectively) over a useful range of values.

With the exception of C251199, the layers were photolithographically patterned into Hall bars using reactive ion etching. For C251199, the sample was a VDP square. All the samples were contacted with Ti/Al, which displayed ohmic behaviour over a wide range of currents, and throughout the measurement temperature range.

**TABLE 3.2. Summary of layer structure of Al$_x$Ga$_{1-x}$N/GaN heterostructure samples.**

<table>
<thead>
<tr>
<th></th>
<th>D952$^a$</th>
<th>G91$^b$</th>
<th>G99$^b$</th>
<th>C251199$^c$</th>
<th>J401$^d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Growth method</td>
<td>MOCVD</td>
<td>LP-MOCVD</td>
<td>LP-MOCVD</td>
<td>NH$_3$-MBE</td>
<td>MOCVD</td>
</tr>
<tr>
<td>Source</td>
<td>DERA</td>
<td>Gent</td>
<td>Gent</td>
<td>NRC</td>
<td>Tokushima</td>
</tr>
<tr>
<td>$x$ (%)</td>
<td>23</td>
<td>20</td>
<td>10</td>
<td>~ 5 (average)</td>
<td>18</td>
</tr>
<tr>
<td>$t_{\text{AlGaN}}$ (nm)</td>
<td>35</td>
<td>12$^f$</td>
<td>32$^f$</td>
<td>200$^f$</td>
<td>120</td>
</tr>
<tr>
<td>$t_{\text{GaN}}$ ($\mu$m)</td>
<td>1.0</td>
<td>1.4</td>
<td>1.4</td>
<td>0.18 (undoped)</td>
<td>2.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1.4 (C doped)</td>
<td></td>
</tr>
<tr>
<td>$t_{\text{Buffer}}$ (nm)</td>
<td>~ 40</td>
<td>50</td>
<td>50</td>
<td>20</td>
<td>25</td>
</tr>
<tr>
<td>Buffer layer</td>
<td>GaN</td>
<td>GaN</td>
<td>GaN</td>
<td>AlN</td>
<td>GaN</td>
</tr>
<tr>
<td>Substrate</td>
<td>sapphire</td>
<td>sapphire</td>
<td>sapphire</td>
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</tr>
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</table>

$^a$ Hughes et al. (1999).
$^b$ Bougrioua (2001).
$^c$ Webb et al. (1999).
$^d$ Wang et al. (1999).
$^f$ Includes 5.5 nm Si-doped region 2 nm from the interface.
$^f$ Includes 12 nm Si-doped region 10 nm from the interface.
$^f$ Ten-period superlattice [AlGaN (71 Å): GaN (128 Å)].
Chapter 4

Transport in GaN Epilayers

Many researchers currently working on nitrides have previous experience on GaAs and related materials, and their expertise has been readily transferred onto the development of GaN based devices. Although this has helped in achieving rapid progress in nitride technology, there exist other problems that are special to nitrides. One such problem is the presence of another conducting layer in \( n \)-type GaN epilayers, mainly thought to be an impurity band. There have been many reports of this phenomenon, which has been observed irrespective of different growth and processing techniques, and various investigations have been carried out to model such behaviour. In this chapter, the effect of a secondary conducting channel in GaN films has also been studied, and the experimental findings and their comparisons with theoretical analysis will be discussed later in Section 4.2.

4.1 Theoretical considerations

Before presenting analysis and results of the transport investigations on GaN layers, the relevant theory must be discussed. The theory is broadly divided into three parts; (a) basic aspects of semiconductor transport, such as the Hall effect, free carrier statistics and scattering mechanisms, providing background material that would be used to characterise non-degenerate GaN bulk samples, (b) impurity band conduction, and (c) theoretical modelling, which presents a set of equations employed to fit the behaviour of both the non-degenerate samples and specimens that exhibit impurity band conduction.
(IBC). Finally, note that the GaN parameters that will be used in the analysis are listed in Section 4.1.5.

4.1.1 Basic transport theory

Probably the most common measurement made of the properties of a semiconductor is the electrical conductivity. Consider the weak-field conductivity arising from transport in an n-type semiconductor which at equilibrium has $n$ mobile electrons per unit volume. The conductivity is defined as the proportionality constant between the applied electric field $E$ and the induced current density $J$,

$$J = \sigma E \ . \ (4.1)$$

If $n$ electrons all move with velocity $v$, then the current density they give rise to will be parallel to $v$. Hence $J$ can also be defined as

$$J = -nev \ , \quad (4.2)$$

where $e$ is the electronic charge. The motion of an electron in a semiconductor crystal can be described by adopting the relaxation time approximation (Ashcroft and Mermin 1976). This approach assumes that the effect of interactions experienced by free carriers is small, i.e., elastic collisions. The free electron mass is replaced by an effective mass $m^*$ to take into account of the periodic potential of the crystal with spherical constant energy surface, and a notion of a drift velocity is introduced, reflecting the randomly averaged motion of the carriers by various scattering processes. Then, the equation of motion for an electron is as follows;

$$m^* \frac{dv}{dt} + \frac{m^*v}{\langle \tau \rangle} = -eE \ , \quad (4.3)$$

where $\langle \tau \rangle$ denotes the average relaxation time. For low carrier density materials, this average is over the non-degenerate Maxwell-Boltzmann distribution function, i.e.,

$$\langle \tau \rangle = \int \frac{4 u^{3/2} \exp(-u)}{3\sqrt{\pi}} \, du \quad \text{where} \quad u = \frac{E}{k_B T} \ , \quad (4.4)$$

where $k_B$ is the Boltzmann's constant and $T$ is the temperature. The steady state solution of Eq. 4.3 is then given by

$$v = -\frac{e\langle \tau \rangle}{m^*} E \ . \quad (4.5)$$
Combining Eqs. 4.2 and 4.5 leads to

\[ \mathbf{J} = \frac{n e^2(\tau)}{m^*} \mathbf{E}, \]  

(4.6)

where the positive scalar quantity

\[ \sigma = \frac{n e^2(\tau)}{m^*} \]  

(4.7)

is the analytical expression for the electrical conductivity. The conductivity is otherwise known as the inverse of resistivity \( \rho \), and can be expressed as

\[ \sigma = \rho^{-1} = n e \mu, \]  

(4.8)

where

\[ \mu = \frac{e(\tau)}{m^*} \]  

(4.9)

is the drift mobility of electrons. The carrier concentration and drift mobility cannot be obtained from conductivity measurements alone. The Hall effect measurement can be used to find \( n \), while a combination of these measurements enables the evaluation of \( \mu \). Hence the next section presents the theoretical background on the electrical characterisation utilising the Hall effect.

**Hall characterisation**

When a current is injected in the \( x \)-direction in a sample and a magnetic field is applied along the \( z \)-direction, an electric field will build up in the \( y \)-direction due to the Lorentz force exerted on the carriers (Hall effect). This Hall voltage exactly balances the Lorentz force and can be measured externally. The Hall effect has been widely used by most laboratories around the world as an important tool in characterising electrical properties of semiconductors. Its popularity arises from the fact that the technique is simple to implement, and also because of the significance of the parameters it can measure, namely carrier concentration, mobility and resistivity.

Experimentally, the Hall measurements employ the van der Pauw (VDP) technique (van der Pauw 1958) where its square and clover-leaf structures are shown in Fig. 4.1. These shapes have many advantages compared with the conventional Hall bar configuration. The VDP configuration gives a relatively large Hall effect at the same amount
of heat dissipation, which is of importance when measuring materials of relatively low electron mobility (as in this case, GaN). Also, the influence of finite size contacts can be reduced significantly, provided the contacts are well-separated and positioned as symmetrical as possible near the edge of the sample with the resistance between any pair of contacts being less than approximately 10 MΩ.

![Diagram of Hall measurements using the van der Pauw method. Shown are the simple square geometry (left) and the clover-leaf geometry (right).](image)

The principles of the VDP method has been described by Look (1989), from which the following formalisms to calculate the transport parameters have been summarised below. As depicted in Fig. 4.1, when a current is injected using two adjacent contacts, the voltage drop is measured between the opposite two contacts. Different sets of measurements can be taken with various permutations obtained by rotation of contacts. From the measured values the resistance is determined by

\[ R_1 = \frac{V_{43}}{I_{12}} \quad \text{and} \quad R_2 = \frac{V_{32}}{I_{41}}. \]

The sheet resistivity can then be calculated by using the relation

\[ \rho_s = \frac{\pi}{2 \ln 2} \left( R_1 + R_2 \right) F_C, \quad (4.10) \]

where \( F_C \) is a correction factor for geometrical asymmetry as indicated by the two measured resistances (and not for anisotropy or inhomogeneity of the material). \( F_C \) is a function of \( Q = R_1/R_2 \), and is determined from the transcendental equation

\[ \frac{Q - 1}{Q + 1} = \frac{F_C}{\ln 2} \cosh^{-1} \left[ \frac{1}{2} \exp \left( \frac{\ln 2}{F_C} \right) \right], \quad (4.11) \]
The Hall effect is measured when the current \( I \) is injected using opposite contacts such that the Hall voltage \( V_H \) can be measured across the current flow at the two remaining opposite contacts with the magnetic field being applied to perpendicular to the sample. From the measured data the Hall coefficient \( R_H \) can be determined using

\[
R_H = \frac{V_H}{I B} = -\frac{r_H}{n_s e},
\]

where \( e \) is the electronic charge and \( r_H \) is the Hall factor. The significance of the Hall factor is discussed later in Section 4.1.1 but for current purposes the Hall factor is assumed to be unity. Once the Hall coefficient is found, the carrier sheet density and mobility of \( n \)-type samples can be extracted according to,

\[
n_s = \frac{1}{e R_H},
\]

and

\[
\mu = \frac{R_H}{\rho_s},
\]

respectively. A convenient feature of this technique is that no dimension needs be measured for the calculation of sheet resistance or sheet carrier concentration, although from knowledge of a thickness one can obtain volume resistance and concentration as well. In order to obtain the temperature dependence of the carrier concentration and mobility, VDP measurements have been conducted on both the GaN layers and AlGaN/GaN heterostructures in this work at temperatures in the range 10—600 K. For two-dimensional structures, the Hall measurements below 10 K have been carried out using the Hall bar configuration. A common Hall bar shape consists of a rectangular piece with a current contacts at either end and potential probes along both sides. To minimise errors arising from misaligned voltages, the potential probes need to be positioned perfectly opposite each other by photolithographic etching. A theoretical model to extract material parameters from the Hall bar is described in detail later in Section 5.1.2.

Information on electron transport in GaN can be obtained from the temperature dependences of \( n \) and \( \mu \), and the following sections will present formalisms to explain such dependences.
Free carrier statistics

Semiconductor statistics describes the probabilities that a set of electronic states are either vacant or populated. Classical Maxwell-Boltzmann statistics and quantum mechanical Fermi-Dirac statistics are employed to calculate the occupancy of states, and the electron states in the conduction band and their dependence on energy are described by the density of states. The total electron concentration in the conduction band is then obtained by integrating over the product of state density \( g(E) \), and the probability distribution \( f(E) \), that is

\[
n = \int_{E_c}^{\infty} g(E) f(E) \, dE .
\] (4.15)

Standard textbook treatment (Blakemore 1987) shows that for the case of single-valley, spherical (isotropic) and parabolic band with the \( E \) vs \( k \)-space dispersion relation of \( E = E_c + \frac{\hbar^2 k^2}{2m^*} \), where \( E_c \) is the conduction band energy and \( \hbar \) is the reduced Planck’s constant \((\hbar/2\pi)\), the \( g(E) \) for the 3-dimensional crystal is given by

\[
g(E) = \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_c} ,
\] (4.16)

and when applying Fermi-Dirac statistics,

\[
f(E) = \left[ 1 + \frac{1}{g} \exp \left( \frac{E - E_F}{k_B T} \right) \right]^{-1}
\] (4.17)

where \( E_F \) is the Fermi level and \( g \) is the degeneracy factor. For the occupational probability of the electrons in the extended states of the conduction band, \( g \) is equal to unity. When considering the donor impurity states, \( g_d = 2 \), and for the acceptor impurity states, \( g_a = 4 \). Incorporating Eqs. 4.16 and 4.17 into Eq. 4.15 results in

\[
n = \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right) \int_{E_c}^{\infty} \frac{(E - E_c)^{1/2} \, dE}{1 + \exp \left[ (E - E_F)/k_B T \right]} ,
\] (4.18)

for the case of electrons in the conduction band. Alternatively, by assigning dimensionless notations \( \epsilon \) and \( \eta \) as

\[
\epsilon = \frac{E - E_c}{k_B T} \quad \text{and} \quad \eta = \frac{E_F - E_c}{k_B T} ,
\]

respectively, Eq. 4.18 becomes

\[
n = N_C \, F_{1/2}(\eta) ,
\] (4.19)
where $N_C$ is the effective density of states at the bottom of the conduction band and $F_{1/2}(\eta)$ is the half-order Fermi-Dirac integral, which are described respectively as,

$$N_C = \frac{1}{\sqrt{2}} \left( \frac{m^* k_B T}{\pi \hbar^2} \right)^{3/2}$$  \hspace{1cm} (4.20)$$

and

$$F_{1/2}(\eta) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{e^{1/2} d\epsilon}{1 + \exp(\epsilon - \eta)}. \hspace{1cm} (4.21)$$

The temperature dependence of the electron concentration is related to the Fermi level by Eq. 4.19. The evaluation of the $F_{1/2}(\eta)$ is somewhat difficult, since it can only be done numerically, and hence it is more useful to employ approximations to obtain an analytical solution, or as is in our case, a polynomial fit can be made (discussed in more detail later in Section 4.1.3). Note that when the Fermi energy is about $3k_B T$ or more below the bottom of the conduction band, the function $f(E)$ can be approximated by a Boltzmann factor, $\exp([E_F - E]/k_B T)$, for all energies within the band, and Eq. 4.19 then becomes

$$n = \frac{1}{\sqrt{2}} \left( \frac{m^* k_B T}{\pi \hbar^2} \right)^{3/2} \exp \left( -\frac{E_C - E_F}{k_B T} \right) = N_C \exp(\eta). \hspace{1cm} (4.22)$$

This is called the Maxwell-Boltzmann distribution, which applies to semiconductor materials with non-degenerate (also called classical) carrier distribution, such as $n$-type GaN layers that are characterised in this chapter.

**Mobility variation**

The notion of Hall effect characterisation has been briefly introduced earlier, enabling the acquisition of parameters such as resistivity, Hall carrier concentration and Hall mobility. However, true carrier concentration and mobility in a semiconductor differ from the Hall values by a numerical factor, $r_H$ (called the Hall factor), and hence the Hall effect needs to be developed further by taking into account $r_H$, which is defined as

$$r_H = \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2}. \hspace{1cm} (4.23)$$
The true carrier concentration \( n \) and the Hall carrier concentration \( n_H \) are related by \( r_H \), according to

\[
n = r_H n_H ,
\]

and the Hall mobility \( \mu_H \) deviates from the drift mobility \( \mu \) by \( r_H \), where

\[
\mu_H = r_H \mu .
\]

The magnitude of the Hall factor for non-degenerate materials varies between 1 and 2 (Smith 1978), depending on the scattering process (e.g., \( r_H = 1.18 \) for acoustic phonon scattering and \( r_H = 1.93 \) for ionised impurity scattering), whereas for degenerately doped semiconductors, \( r_H = 1 \). For simplicity, it is assumed in the analysis that the \( r_H \) is unity.

In order to predict the temperature dependence of electron mobility in GaN, various scattering mechanisms and their effects on the limiting mobility must be calculated. An accurate calculation of the mobility variation requires a numerical iterative solution of the Boltzmann transport equation, and various groups have carried out such simulation (Look et al. 1997; Ridley et al. 1999). In this work, a simpler analytical approach, adopted by Tang et al. (1997), is employed. To a first approximation, the total mobility is obtained by combining the mobility limits associated with different scattering events according to Matthiesen's rule:

\[
\mu_T \simeq \frac{1}{\sum_i \frac{1}{\mu_i}} .
\]

Tang et al. have observed that the above method, when compared with the mobility calculated by the more accurate iterative procedure, results in less than 20% difference in mobility. Also, the error introduced by Matthiesen's rule becomes less significant since a larger error could be generated due to uncertainties in GaN parameter values.

The mobility limit due to individual scattering processes is calculated independently with the corresponding analytic expressions, usually derived using the relaxation time approximation, and the total mobility can be calculated by using Eq. 4.26. Hence the next section describes various scattering processes, presenting analytic expressions for the mobility limit in each scattering case.
4. Transport in GaN Epilayers

4.1.2 Scattering mechanisms

According to Bloch's theory, an electron in a perfectly periodic array of ions experiences no collisions at all, and under an external electric field, the momentum of a free electron increases continuously. In reality, collisions can occur from deviations from perfect periodicity (such as impurities and thermal lattice vibrations), and the overall effect of the gain and loss of momentum from these deviations leads to limiting mobility. The manner in which electron mobility behaves as a function of the temperature depends on the type of electron distribution, and what processes dominate scattering. In this section, scattering by ionised impurities, by dislocations, by deformation and piezoelectric potential of acoustic phonons, and by polar optical phonons, are identified as the main scattering mechanisms in GaN, and the temperature dependence of each mechanism will be considered in the following pages.

Ionised impurity scattering

This is governed by similar physical principles to Rutherford scattering, where the trajectory of a charged particle is diverted by the interaction with another charged particle. The Coulombic interaction of the two charged particles \( \propto \frac{e^2}{r} \) is strongest for a small distance between particles and a long interaction time. Such a long interaction time is given for slowly moving electrons, that is for a non-degenerate carrier gas at low temperatures. The low temperature mobility is therefore a measure of the impurity content in non-degenerately doped semiconductors. The mobility limited by ionised impurities has been formulated by Brooks and Herring (Brooks 1955) after taking into account the screening effect due to free carriers and impurity ions, and has the following expressions:

\[
\mu_{ii} = \frac{128 \sqrt{2\pi} \varepsilon^2_s (k_BT)^{3/2}}{e^3 \sqrt{m^*} (n + 2N_A)} \left[ \ln(1 + y) - \frac{y}{1 + y} \right]^{-1}
\]

with

\[
y = \frac{24m^* \varepsilon_s (k_BT)^2}{e^2 k^2 n'};
\]

\[
n' = n + \frac{(N_D - N_A - n) (n + N_A)}{N_D},
\]
where \( \varepsilon_s \) is the low frequency (static) dielectric constant, \( N_D \) and \( N_A \) are donor and acceptor concentrations, respectively, and \( n \) is the free carrier concentration. When only the screening by free carriers is considered, \( n \) instead of \( n' \) is used for calculation.

**Dislocation scattering**

GaN is known to contain a large number of dislocations in the range \( 10^8 - 10^{11} \) cm\(^{-3} \), arising from the lattice mismatch between the epilayer and the substrate. Weimann et al. (1998) have reported that the lateral mobility of low to moderately \( n \)-type doped films is significantly lower than predicted by ionised impurity scattering, and attributed its cause to the effect of dislocations. Their model proposed that threading dislocations with an edge component act as Coulombic scattering centres, where acceptor centres along the dislocation line are introduced, thereby capturing electrons. The dislocation line becomes negatively charged and the Coulomb field that forms around it scatters travelling electrons, thus reducing the mobility. This scattering mechanism becomes more dominant as the dislocation induced trap concentration exceeds the doping level.

Pödör (1966) has solved the Poisson equation analytically for cylindrical symmetry, assuming a continuously charged negative line and screening by ionised impurities and free carriers, and has obtained the electron mobility due to scattering by dislocations, which is given by the expression:

\[
\mu_{\text{disl}} = \frac{30\sqrt{2\pi\varepsilon_s^2d_L^2(k_BT)^{3/2}}}{{N_{\text{disl}}e^2f\lambda_D}\sqrt{m^*}}
\]

(4.28)

where \( d_L \) is the distance between acceptor centres along the dislocation line (\( 5.1 \times 10^{-10} \) m), \( f \) is the occupation rate of the acceptor centres, \( N_{\text{disl}} \) is the density of dislocations, and \( \lambda_D \) is the Debye screening length,

\[
\lambda_D = \left( \frac{\varepsilon_s k_B T}{e^2 n'} \right)^{1/2}
\]

Weimann et al. have assumed that all the neutral dangling bonds in the dislocation line trap electrons and become fully charged, i.e., \( f = 1 \), thereby lowering their energy of states. However, this is unlikely to be the case since as more dangling bonds get charged, there is also an increase in the repulsive force due to the neighbouring Coulomb potential. Hence the occupation rate is expected to be much lower than unity, though it remains unclear as to the exact value of \( f \).
FIG. 4.2. Electron mobility vs free carrier concentration of n-GaN films at room temperature. The dotted lines are theoretical curves fitted to Eq. 4.28 with the indicated dislocation densities (Ng et al. 1998). The circles that lie on near the solid line correspond to samples whose transport is dominated by ionised impurity scattering.

Based on the dislocation model using Eq. 4.28, Ng et al. (1998) have investigated transport in n-GaN films grown by ECR-MBE with concentrations in the range $10^{15} - 10^{20}$ cm$^{-3}$. They found that the 300 K mobility versus carrier concentration followed a family of bell-shaped curves as shown in Fig. 4.2, where for the samples with lower $N_{\text{disl}}$, transport is mainly controlled by ionised impurity scattering. For a given carrier concentration, much lower mobilities are observed for the samples with higher dislocation densities. It should be noted that most of the samples studied in this thesis have mobilities that correspond to transport dominated by ionised impurity scattering, and thus dislocation scattering is not expected to play a major role (this issue will be explained more fully in Section 4.2.1). There are a few samples with very low mobilities, thus pointing towards dominant dislocation scattering. Unfortunately, transmission electron microscopy (TEM) studies have not been carried out on the samples that have been characterised in this thesis, and the exact level of dislocation density of the samples is unknown, thus making the incorporation of
dislocation scattering in the analysis difficult. Hence, the mobility limited by dislocation scattering is excluded in the calculations, and is theoretically presented here for completeness.

**Deformation potential scattering**

Free carriers can be subjected to scattering by thermal vibrations of the lattice atoms, represented by quasi-particles as acoustic phonons, which can propagate through the crystal by longitudinal and transverse waves. During propagation, an additional periodic potential is superimposed on the periodic field of the internal crystal field. This alters the energy structure of the crystal, and the equivalent alternating potential energy of the carriers is known as the deformation potential. The mobility limited by acoustic-mode deformation potential scattering is (Anderson and Aspley 1989):

$$
\mu_{dp} = \frac{2(2\pi)^{1/2} q v_s^2 \hbar^2 e}{3\Xi_{dp}^2 (m^*)^{3/2} (k_B T)^{3/2}}
$$

where $q$ is the density of mass, $v_s$ is the crystal sound velocity, and $\Xi_{dp}$ is the deformation potential.

**Piezoelectric scattering**

This is another form of the acoustic phonon scattering, which arises in ionic semiconductors, where the acoustic vibrations produce a piezoelectric field that perturbs the crystal. Anderson and Aspley (1989) have also given an analytical expression for the mobility limited by piezoelectric scattering, which is given by:

$$
\mu_{pz} = \frac{16(2\pi)^{1/2} q s^2 \hbar^2 e}{3(e h_{pz} / \varepsilon_s)^2 (m^*)^{3/2} (k_B T)^{1/2}}
$$

where $h_{pz}$ is the piezoelectric constant.

**Polar optical scattering**

Polar semiconductors such as GaN possess a high degree of ionicity, thus the interaction between carriers and the optical vibrations of the lattice atoms is likely to be strong. This type of scattering is different from acoustic phonon scattering, where the energy exchange during the absorption and the emission of acoustic phonons is small, and
the scattering is regarded as elastic. However, judging from the high polar optical phonon energy (91.2 meV), the scattering by polar optical phonon is grossly inelastic, and becomes effective mainly at high temperatures. As a result, it is not suitable to treat optical scattering with the relaxation time approximation. Instead, Gelmont et al. (1995) have developed an analytical theory to describe optical phonon scattering, where the mobility limited by polar optical phonons is given by:

\[ \mu_{\text{op}} = \frac{4\pi \kappa \varepsilon_0 \hbar^2}{e F_p m^*} \left[ \frac{1 - 5V_{th}/E_g}{\sqrt{2m^*\varepsilon_{\text{op}}(1 + \Phi_{\text{op}}/E_g)}} \right] \]  

(4.31)

where \( \kappa = (1/\kappa_\infty - 1/\kappa_0)^{-1} \) is the coupling constant, \( \kappa_\infty = \varepsilon_\infty/\varepsilon_0 \) and \( \kappa_0 = \varepsilon_s/\varepsilon_0 \) are the high frequency and static dielectric constant ratios, respectively, \( \varepsilon_0 \) is the free permittivity,

\[ F_p = [\exp(\Phi_{\text{op}}/V_{th}) - 1]^{-1} \]

is the Planck function, \( V_{th} = k_B T/e \) is the thermal voltage, \( \Phi_{\text{op}} \) is the polar optical phonon energy, and \( E_g \) is the energy gap.

### 4.1.3 Impurity band conduction

Before discussing the origin of an impurity band and its implications on GaN transport, the Mott transition needs to be considered (Mott and Twose 1961). It refers to an insulator-to-metal transition occurring in semiconductors at high doping concentrations. The transition occurs when the distance between impurities becomes comparable to the Bohr radius, i.e., when the impurity concentration exceeds a critical value \( N_{\text{crit}} \), where

\[ N_{\text{crit}} = \left( \frac{0.25}{a_B^*} \right)^3. \]  

(4.32)

\( a_B^* \) is defined as the effective Bohr radius and is given by (with the donor ground state of \( j = 1 \))

\[ a_B^* = \frac{4\pi \varepsilon_s \hbar^2 j^2}{(e m^*)^2}. \]  

(4.33)

In GaN, this corresponds to about 24 Å, which consequently yields the Mott (critical) concentration of approximately \( 1 \times 10^{18} \text{ cm}^{-3} \).
The impurity band formation is graphically illustrated in Fig. 4.3. At impurity concentrations well below the critical Mott concentration, impurities can be considered as isolated, non-interacting entities. As the concentration increases but still well below the Mott concentration, impurities begin to interact. Charge transport at low temperatures occurs via thermally assisted hopping conduction. At still higher impurity concentrations, overlapping of the impurity wavefunction results in the formation of an impurity band. At low temperatures, carriers can propagate within the impurity band without entering the conduction band. At even higher doping densities, the impurity band widens and merges with the conduction band, which occurs at $N_{CB} = 1/4\pi a_B^2 \approx 6 \times 10^{18}$ cm$^{-3}$ (Matsubara and Toyozawa 1961). It should be pointed out that there is always a degree of compensation in GaN layers. Hence, the existence of acceptors means that although the free electron density falls way below the critical concentration, there still could be numerous ionised donors compensated by acceptors, and the total donor density could still be around or above the $1 \times 10^{18}$ cm$^{-3}$ level.

**FIG. 4.3.** (a) Donor impurity level/band at $N_D \ll N_{crit}$, $N_D \ll N_{crit}$ and $N_D \geq N_{crit}$ for a random impurity distribution. (b) Band diagram illustrating hopping and impurity band conduction.
The insulator-to-metal transition occurs abruptly at the critical concentration, and an impurity band is formed. Then, the widening of the impurity band is gradually evolving with increasing impurity concentration. This gradual behaviour can be expressed in terms of a continuously decreasing impurity activation energy. Screening of impurity potentials contributes to the reduction of the activation energy, since screened potentials are less capable of binding electrons. Quantitatively, experimental donor activation energy $\varepsilon_d$ have been described by the equation

$$\varepsilon_d = E_{DO} - \alpha N_D^{1/3}, \quad (4.34)$$

where $E_{DO} \approx 29$ meV is the Si-donor activation energy for $N_D \ll N_{\text{crit}}$ (Wang et al. 1996), and $\alpha \approx (2.1 \pm 0.2) \times 10^{-5}$ meV cm is the screening factor (Meyer et al. 1995).

An important distinction should be drawn between conduction of electrons in the extended states of the conduction band, and conduction of electrons which travel from one impurity to another. The mobility of conduction band electrons has already been described by Eq. 4.9, and is much higher than that of impurity band electrons, since transport involving localised impurities is characterised by a shorter mean free path (due to the close proximity of impurities) and a heavier effective mass (Schubert 1993). The competition between the high conduction band mobility and the lower impurity band mobility means that the parallel conduction effects becomes dominant at low temperatures when the free carriers are frozen out into the defect centres. This effect can drastically change the temperature dependence of the carrier concentration and mobility from the ideal case of a non-degenerate bulk layer with a single shallow donor case, and is typically displayed in Fig. 2.5 (see Section 2.3.2). The measured Hall concentration ($n_{\text{meas}}$) starts to fall with decreasing temperature, as expected from the conventional carrier freeze-out, but a further reduction in temperature results in a rise in $n_{\text{meas}}$, which finally begins to saturate at a constant value below about 40 K. In addition, the low temperature Hall mobility exhibits a steeper temperature dependence than expected for mobility limited by ionised impurity scattering ($\mu_{ii} \propto T^{1.5}$).

Hence, in order to explain the measured Hall data, two-carrier transport needs to be considered. A review of two-carrier investigations, where the secondary conducting channel is assumed to be an impurity band, a degenerate interfacial layer or grain
boundaries, has been presented in Section 2.3.2. For the case of impurity band conduction, the analysis carried out by Molnar et al. (1993) suggested that (a) the low temperature Hall density is equivalent to the net donor density \(N_D - N_A\), (b) the effect of the impurity band cannot be ignored even at room temperature, and (c) the true conduction band mobility is higher than the Hall mobility. Their analysis provided a basis for the mathematical modelling that has been carried out in this work, which has been further modified to fit the experimental data, and the next section presents such models.

### 4.1.4 Transport modelling

Electrical characterisation based on temperature dependent Hall measurements enables one to extract material parameters such as the donor concentration, the acceptor concentration and the activation energy, and to determine transport properties such as scattering mechanisms, mobility variation and the nature of parallel conduction. The experimental results will show a set of samples that behave, in common with other n-type III-V semiconductors, as non-degenerate bulk layers with electron transport in the conduction band, and another set of specimens that can be characterised by incorporating the effects of parallel conduction via an impurity band. Hence the mathematical analysis will require two different models, and the derivations for each model are given below.

**Non-degenerate bulk transport with a shallow donor**

Consider an n-type extrinsic semiconductor which is controlled by a single set of donors and by the partial compensation of these donors by acceptors, as shown in Fig. 4.4. Charge neutrality implies that

\[
n + N_A^- = N_D^+ + p ,
\]

where \(N_A^-\) is the ionised acceptor concentration, \(N_D^+\) is the ionised donor concentration, and \(p\) is the concentration of holes.

In the case of GaN, because of its wide band-gap nature, it is assumed that there are no holes created from thermal excitations (i.e., \(p = 0\)), and thus assuming Fermi-Dirac
statistics, Eq. 4.35 reduces to

$$n + N_A = \frac{N_D}{1 + g_d \exp \left( \frac{E_F - E_d}{k_B T} \right)},$$ \hspace{1cm} (4.36)

where $N_D$ is the total donor density, $N_A$ the total acceptor density, $g_d = 2$ is the degeneracy of the donors, and $E_d = E_c - \epsilon_d$ is the energy of the donor level, with $\epsilon_d$ being the donor ionisation energy. Rearranging the above equation leads to

$$\frac{(n + N_A) \exp(\eta)}{(N_D - N_A - n)} = \frac{1}{2} \exp \left( -\frac{\epsilon_d}{k_B T} \right).$$ \hspace{1cm} (4.37)

For the case of non-degenerate layers, the classical approximation can be applied (see Eq. 4.22), and the fitting equation is then given by

$$\frac{n(n + N_A)}{(N_D - N_A - n)} = \frac{N_C}{2} \exp \left( -\frac{\epsilon_d}{k_B T} \right).$$ \hspace{1cm} (4.38)

This equation, called the charge balance equation (CBE), has been mainly used for the fitting of non-degenerate bulk GaN layers, where the measured Hall concentration data provide numerous values to fit and obtain material parameters such as $N_D$, $N_A$ and $\epsilon_d$.

One method of extracting the parameters is by fitting the measured $n$ vs $T$ data using Eq. 4.38 alone. The extracted $N_D$ and $N_A$ values are then substituted into
Eqs. 4.27 and 4.28 to calculate the temperature dependence of mobility for ionised impurity and dislocation scattering, respectively. The remaining scattering limited mobilities can also be simulated using Eqs. 4.29, 4.30 and 4.31, and the temperature dependence of total mobility, calculated by using Matthiesen’s rule, can then be plotted over the experimental mobility data for comparison.

However, performing simultaneous fittings of both measured carrier concentration and mobility would enhance reliability and accuracy of extracted quantities, as demonstrated by Look et al. (1997). The \( N_A \) value obtained from fitting the low temperature mobility limited by ionised impurity scattering is unique, and the remaining parameters values calculated using the CBE equation are likely to be associated with smaller errors.

**Transport affected by an impurity band**

For GaN layers with a conduction band electron concentration \( n_c \) and mobility \( \mu_c \), and with an impurity band electron concentration \( n_d \) and mobility \( \mu_d \), a two-carrier analysis must be used. Molnar et al. (1993) have provided the starting point of the analysis, by assuming that the net total carrier concentration \( N_T \) is given by

\[
N_T = n_c + n_d = N_D - N_A .
\]  

The value of \( N_T \) can be obtained directly from the experimental data (the Hall density at the lowest temperature). In addition, by setting \( b = \mu_d/\mu_c \), the experimental Hall resistivity, carrier concentration and mobility can be described by:

\[
\rho_H = \frac{1}{n_c \mu_c + n_d \mu_d} = \frac{1}{\mu_c \left[(1 - b)n_c + N_T b\right] ,}
\]  

\[
n_H = \frac{(n_c \mu_c + n_d \mu_d)^2}{n_c \mu_c^2 + n_d \mu_d^2} = \frac{[(1 - b)n_c + N_T b]^2}{(1 - b^2)n_c + N_T b^2} ,
\]  

and

\[
\mu_H = \frac{n_c \mu_c^2 + n_d \mu_d^2}{n_c \mu_c + n_d \mu_d} = \frac{\mu_c [(1 - b^2)n_c + N_T b^2]}{(1 - b)n_c + N_T b} ,
\]  

respectively. Assuming \( b \) is not a strong function of temperature, it can be shown that \( n_H \) in Eq. 4.41 has a minimum

\[
n_{min} = \frac{4N_T b}{(1 + b)^2} ,
\]  

\[
(4.43)
\]
4. Transport in GaN Epilayers

when

\[ n_c = \frac{N_T b}{(1 + b)} \]  \hspace{1cm} (4.44)

In order to calculate the temperature dependence of \( n_c \), the activation energy \( \epsilon_d (= E_c - E_d) \) needs to be evaluated. Assuming from Eqs. 4.17 and 4.22 for non-degenerate conduction band statistics, the \( n_d \) and the \( n_c \) are described by the relations:

\[ n_d = N_D - N_D^+ = \frac{N_D}{1 + \frac{1}{2} \exp \left( -\frac{\epsilon_d}{k_B T} \right) \exp \left[ -\frac{(E_F - E_c)}{k_B T} \right]} \]  \hspace{1cm} (4.45)

\[ n_c = N_C \exp \left[ -\frac{(E_F - E_c)}{k_B T} \right] \]  \hspace{1cm} (4.46)

Combining Eq. 4.39 with Eqs. 4.45 and 4.46 results in

\[ N_T - n_c = \frac{N_D}{1 + \frac{N_C}{2n_c} \exp \left( -\frac{\epsilon_d}{k_B T} \right)} \]  \hspace{1cm} (4.47)

This equation can be solved for \( \epsilon_d \), where

\[ \epsilon_d = -k_B T \ln \left[ \frac{2n_c}{N_C} \left( \frac{N_A + n_c}{N_T - n_c} \right) \right] \]  \hspace{1cm} (4.48)

By substituting Eq. 4.44, \( \epsilon_d \) can also be expressed as

\[ \epsilon_d = -k_B T \ln \left[ \frac{2b(N_A + N_A b + N_T b)}{N_C (1 + b)} \right] \]  \hspace{1cm} (4.49)

To evaluate \( \epsilon_d \), the value of \( b \) needs to be obtained, and this can be found using Eq. 4.43, which yields a quadratic relationship between \( b \) and \( N_T/n_{\text{min}} \),

\[ b^2 + b \left( 2 - 4 \frac{N_T}{n_{\text{min}}} \right) + 1 = 0 \]  \hspace{1cm} (4.50)

Hence, the activation energy is a function of the ratio \( N_T/n_{\text{min}} \) (which can be directly obtained from the experimental \( n_H \) data), and therefore can be evaluated by initially solving Eq. 4.50 for \( b \), and then using Eq. 4.49.

The temperature dependence of \( n_c \) could then be calculated by Eq. 4.46. However, this would not draw an accurate picture of the transport behaviour of the real situation at higher temperatures. The change of the Fermi level with temperature, can be better predicted by incorporating full Fermi-Dirac statistics (refer to Eq. 4.19). As mentioned
4. Transport in GaN Epilayers

previously, the difficulty in calculating $F_{1/2}(\eta)$ numerically has meant that a polynomial fit is employed, i.e.,

$$n_c = \frac{2}{\sqrt{\pi}} F_{1/2}^*(\eta) \approx N_C P(\eta) \exp(\eta)$$  \hspace{1cm} (4.51)

where $F_{1/2}^*$ is the Fermi-Dirac integral without the $2/\sqrt{\pi}$ factor, and $P(\eta)$ is a polynomial function $(P_0 + P_2\eta + P_3\eta^2 + \ldots)$. Fig. 4.5 plots the polynomial fit to the Fermi-Dirac integral as a function of Fermi energy for reference, from which the $P(\eta)$ function is determined using Eq. 4.51, and is given by $P(\eta) = 0.632536 - 0.123161 \eta - 0.009321 \eta^2 + 0.001333 \eta^3 + 0.000151 \eta^4 + \ldots$. The shift in the Fermi level with temperature can be incorporated when modelling the $n_c(T)$ by the following procedure.

Rearranging Eq. 4.36 gives

$$n_c + N_A = \frac{N_D}{1 + 2 \exp\left(\frac{\epsilon_d}{k_B T}\right) \exp(\eta)}.$$ \hspace{1cm} (4.52)

Let $C = \exp(\epsilon_d/k_B T)$ and $\beta = \exp(\eta)$, then equating the above equation with Eq. 4.51 leads to a quadratic equation

$$2C P(\eta)N_C \beta^2 + [P(\eta)N_C + 2CN_A] \beta - N_T = 0,$$ \hspace{1cm} (4.53)
where the solution is given by

\[
\beta \simeq -\frac{\sqrt{\left(\frac{P_{\eta}N_C + 2CN_A}{4CN_T}\right)^2 + 8CP(\eta)N_CN_T}}{4CP(\eta)N_C}.
\]

Hence the Fermi level variation with temperature can be calculated by solving the above equation iteratively, which has been programmed by Matlab. Using the acquired variation of \(\eta\), the true temperature dependence of \(n_c\) is finally obtained by calculating Eq. 4.52.

Returning to Eqs. 4.41 and 4.42, it can be seen that the parameters \(n_c\) and \(n_d(= N_T - n_c)\) are now known, which leaves the temperature dependences of \(\mu_c\) and \(\mu_d\) to be found. Eq. 4.41 can be shown to be a quadratic equation in \(b\), and has the solution

\[
b = \frac{n_c \pm \sqrt{n_H \left[ n_c \left( 1 + \frac{1}{r_n} \right) - \frac{n_H}{r_n} \right]}}{n_H - n_d},
\]

where \(r_n = n_d/n_c\). Once the ratio \(b\) is extracted, the \(\mu_c\) can be calculated for each temperature using Eq. 4.42, and since \(\mu_d = \mu_c b\), the temperature dependence of \(\mu_d\) can also be found.

Note that the calculation procedure described so far cannot be classified as a fitting process. In essence, the procedure de-convolutes the experimental \(n_H\) and \(\mu_H\) data into its constituent parts \((n_c, n_d, \mu_c\) and \(\mu_d\)). This is not the case when trying to fit the experimental data, where simultaneous fitting of both measured mobility and carrier concentration, similar to the procedure that has been described for the case of single donor non-degenerate bulk layers, makes the extraction of \(\epsilon_d, N_D\) and \(N_A\) possible (Look et al. 1997).

However, there is a problem with the de-convolution method regarding the compensation. Incorporating compensation brings the \(N_A\) into analysis, which is a parameter that cannot be solved uniquely. Hence, from the beginning of analysis, the value of \(N_A\) needs to be assigned a priori. GaN layers are known to be strongly affected by compensation; a typical compensation ratio ranges between 0.2 – 0.6. For a given \(N_A\), it is not unreasonable to assume qualitatively that the contribution of compensation effects is likely to be lower for the samples with high doping levels (\(\sim\) high \(10^{18}\) cm\(^{-3}\)) than for the samples with \(\sim\) mid \(10^{17}\) cm\(^{-3}\) doping level. To investigate the role of
compensation, the de-convolution has been carried out by using different levels of the acceptor concentration, and the corresponding calculation results are compared with the measured data for a best agreement. Although this method cannot be described as a self-consistent modelling, the ability of the de-convolution method to separate the behaviour of both the conduction band and the impurity band electrons achieves the main aims of the characterisation, which is to assess the material quality, and to provide the growers with the necessary feedback so as to improve the growth process.

4.1.5 Calculation parameters

A list of the GaN parameters that has been used in the calculations is summarised in Table 4.1. Unfortunately, many of these parameters are not well known, and a range of values has been reported. Hence, the listed parameter values are chosen on the basis that they are the most commonly used by other researchers, allowing a more direct comparison with their results to be made. Also included in Table 4.1 are common physical constants which are used throughout the thesis.

<table>
<thead>
<tr>
<th>GaN parameters and constants</th>
<th>Values</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Effective mass</td>
<td>$m^*$</td>
<td>0.22$m_0$ kg</td>
</tr>
<tr>
<td>Low freq. dielectric constant</td>
<td>$\varepsilon_s$</td>
<td>10.4$\varepsilon_0$ F m$^{-1}$</td>
</tr>
<tr>
<td>High freq. dielectric constant</td>
<td>$\varepsilon_{oo}$</td>
<td>5.47$\varepsilon_0$ F m$^{-1}$</td>
</tr>
<tr>
<td>Density of mass</td>
<td>$\rho$</td>
<td>6.1 x 10$^3$ kg m$^{-3}$</td>
</tr>
<tr>
<td>Speed of sound</td>
<td>$v_s$</td>
<td>6.6 x 10$^3$ m s$^{-1}$</td>
</tr>
<tr>
<td>Deformation potential</td>
<td>$\Xi_{dp}$</td>
<td>9.2 eV</td>
</tr>
<tr>
<td>Piezoelectric constant</td>
<td>$h_{pz}$</td>
<td>0.5 C m$^{-2}$</td>
</tr>
<tr>
<td>Polar optical phonon energy</td>
<td>$\Phi_{op}$</td>
<td>0.0912 eV</td>
</tr>
<tr>
<td>Electronic charge</td>
<td>$e$</td>
<td>1.60 x 10$^{-19}$ C</td>
</tr>
<tr>
<td>Free electron mass</td>
<td>$m_0$</td>
<td>0.91 x 10$^{-30}$ kg</td>
</tr>
<tr>
<td>Permittivity in vacuum</td>
<td>$\varepsilon_0$</td>
<td>8.85 x 10$^{-14}$ F cm$^{-1}$</td>
</tr>
<tr>
<td>Reduced Planck constant</td>
<td>$\hbar$</td>
<td>1.05 x 10$^{-34}$ J s</td>
</tr>
<tr>
<td>Boltzmann constant</td>
<td>$k_B$</td>
<td>1.38 x 10$^{-12}$ J K$^{-1}$</td>
</tr>
</tbody>
</table>
4.2 Results and discussion

This section presents the results of transport properties of GaN layers grown on sapphire by MBE and MOCVD, based on interpretations of the temperature dependent Hall measurements data. General descriptions of the resistivity, Hall carrier concentration and Hall mobility variation with temperature are given in Section 4.2.1. Systematic studies of these variations allow material parameters such as the density of impurities, their activation energies and the level of compensation to be found. Also, the role of scattering mechanisms in limiting the mobility of free carriers can be assessed, and the results of such investigations on non-degenerate bulk samples will be discussed in Section 4.2.2. Understanding the electronic properties of GaN, e.g., for high power FET applications, is complicated by (a) poor structural quality arising from lattice mismatch, (b) high background doping levels present, and (c) the existence of additional parallel conducting channels in the material. A study of these effects in samples that are either unintentionally doped or deliberately doped with Si, covering an impurity range from mid $10^{17}$ to high $10^{18}$ cm$^{-3}$, is presented in Section 4.2.3. Hall measurements from 10 to 600 K have been analysed to determine the transport properties of electrons in the conduction band and in the secondary conduction channel, from which the role of structural imperfections in limiting the mobility in this material has been investigated.

4.2.1 General Hall results

Table 4.2 lists the samples studied and includes the growth method, the nature of $n$-type doping, the epilayer thickness, $t$, and the Hall concentration and mobility values at 300 K. For further details of the sample growth and preparation techniques, refer to Section 3.2.1.

The samples cover a wide range of carrier concentration values, and the general trend in mobility and carrier density with temperature does not depend systematically on the growth technique used, layer thickness or the dopant type. This aspect will be discussed later in Section 4.2.3. Before presenting the results, an issue regarding the mobility limited by dislocation scattering needs to be addressed. As mentioned earlier
in Section 4.1.2, a characterisation technique such as TEM has not been available in this work to obtain the exact level of dislocation density. It should be also noted that although the low- and high-temperature mobilities are mainly dominated by ionised impurity and polar optical scattering respectively, the total temperature dependence of mobility will be characterised by the sum of reciprocal mobility limits of individual scattering mechanisms. Since the mobility limited by polar optical scattering (refer to Eq. 4.31) is same for all the samples, the total mobility will be influenced, even at room temperature, by $\mu_{it}$ which is a function of $N_A$ and therefore sample-dependent. Hence, when comparing the mobility values of the samples in Table 4.2 with the theoretical curves calculated by Ng et al. (1998) in Fig. 4.2, it can be seen that all the samples (except G613, G138 and G595) have room temperature mobilities which correspond to those limited by ionised impurity scattering only. Thus in this chapter, the effect of dislocation scattering has been excluded in the calculations.

For analysis, the samples have been mainly divided into two groups, non-degenerate films (G165 and C190299) without an impurity band and samples that have been affected by an impurity band. This can be put into context by looking at Fig. 4.6, which shows the temperature dependence of $n_H$ for selected samples, G165, G50 and MG622. The Hall carrier concentration of G165 increases with increasing temperature in a similar manner found in most semiconductors, where the dependence initially follows an

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**TABLE 4.2.** A list of the measured n-type GaN samples and their Hall results at room temperature.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Growth</th>
<th>Doping</th>
<th>$t$ (µm)</th>
<th>$n_H$ at 300 K (cm$^{-3}$)</th>
<th>$\mu_H$ at 300 K (cm$^2$ V$^{-1}$ s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>G165</td>
<td>AP-MOCVD</td>
<td>Undoped</td>
<td>1.0</td>
<td>$2.8 \times 10^{17}$</td>
<td>330</td>
</tr>
<tr>
<td>C190299</td>
<td>NH$_3$-MBE</td>
<td>Silicon</td>
<td>–</td>
<td>$3.8 \times 10^{17}$</td>
<td>450</td>
</tr>
<tr>
<td>G613</td>
<td>LP-MOCVD</td>
<td>Undoped</td>
<td>2.6</td>
<td>$3.0 \times 10^{17}$</td>
<td>6</td>
</tr>
<tr>
<td>G138</td>
<td>AP-MOCVD</td>
<td>Undoped</td>
<td>1.0</td>
<td>$3.6 \times 10^{17}$</td>
<td>50</td>
</tr>
<tr>
<td>MG676</td>
<td>RF-MBE</td>
<td>Undoped</td>
<td>2.0</td>
<td>$4.0 \times 10^{17}$</td>
<td>200</td>
</tr>
<tr>
<td>G50</td>
<td>AP-MOCVD</td>
<td>Undoped</td>
<td>1.0</td>
<td>$7.0 \times 10^{17}$</td>
<td>230</td>
</tr>
<tr>
<td>MG622</td>
<td>RF-MBE</td>
<td>Undoped</td>
<td>4.6</td>
<td>$2.5 \times 10^{18}$</td>
<td>160</td>
</tr>
<tr>
<td>G649</td>
<td>LP-MOCVD</td>
<td>Silicon</td>
<td>2.5</td>
<td>$4.0 \times 10^{18}$</td>
<td>210</td>
</tr>
<tr>
<td>G617</td>
<td>LP-MBE</td>
<td>Silicon</td>
<td>2.6</td>
<td>$4.3 \times 10^{18}$</td>
<td>160</td>
</tr>
<tr>
<td>MG657</td>
<td>RF-MBE</td>
<td>Silicon</td>
<td>2.0</td>
<td>$5.7 \times 10^{18}$</td>
<td>90</td>
</tr>
<tr>
<td>G595</td>
<td>LP-MOCVD</td>
<td>Silicon</td>
<td>1.6</td>
<td>$6.4 \times 10^{18}$</td>
<td>30</td>
</tr>
</tbody>
</table>
exponentially activated conduction band behaviour, eventually beginning to settle into an exhaustion region at high temperatures. However, samples G50 and MG622 show quite different characteristics. Although the carrier density initially decreases with falling temperature (similar to the non-degenerate behaviour), it then goes through a minimum, and the density rises again to a $n_H$ value comparable to the high temperature value. The temperature at which this minimum occurs is found to be higher for samples with higher $n_H$. As mentioned in Section 2.3.2, these observations can be explained by the presence of parallel conduction channel in the form of an impurity band. The non-degenerate and impurity band conduction behaviour can also be distinguished by investigating the temperature dependence of Hall mobility (Fig. 4.7).
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and resistivity (Fig. 4.8).

![Graph](image)

**FIG. 4.7.** A plot of the Hall mobility as a function of temperature for samples G165, G50 and MG622.

Fig. 4.7 shows a trend where the peak mobility occurs at a lower temperature for a sample with a higher carrier concentration. However, G165 mobility continues to decrease at low temperatures (below 50 K), whereas other samples exhibit an onset of saturation, and a similar observation can be made from the resistivity variation in Fig. 4.8. Above 300 K, the G165 mobility falls more steeply at higher temperatures (approximately $T^{-1.5}$ dependence) than the G50 and the MG622 mobility, which suggests that assuming an impurity band is present in G50 and MG622, the parallel conduction effects are strong throughout the measurement temperature range, i.e., a large portion of carriers still remain in the donor band even at high temperatures. The interpretation of the Hall results will be given in more detail next in Section 4.2.2 for non-degenerate GaN layers and in Section 4.2.3 for specimens with the impurity band.

### 4.2.2 Non-degenerate bulk samples

Quantitative analysis of the Hall data has been carried out by performing simultaneous fits of both measured mobility and carrier concentration data. The theoretical
background on the fitting equations has been already discussed in Section 4.1.4. The experimental mobility can be fitted by the calculated mobility limited by the various scattering mechanisms assuming the Matthiesen's rule. In particular, the mobility limited by ionised impurity scattering is a sensitive function of $N_A$ (described by Eq. 4.27), and its concentration can be deduced from the $\mu_H$ vs $T$ curve. Using the extracted $N_A$, the values of $N_D$ and $\epsilon_d$ are then determined from the fit of the $n_H$ vs $T$ data using the charge balance equation (refer to Eq. 4.38).

**C190299 results**

Fig. 4.9 shows the fit of the $\mu_H$ vs $T$ data of sample C190299, displaying also the mobility limit curves of the different scattering events derived from the fit. It can be clearly seen that similar to most semiconductors with conduction band electron transport, the mobility is mainly limited by the ionised impurity scattering at low temperatures whereas at high temperatures, the polar optical scattering appears to be the dominant mobility limiting mechanism. The $N_A$ value of $1.5 \times 10^{17}$ cm$^{-3}$ has been used as the fitting parameter. The temperature dependence of the mobility limited
by ionised impurity scattering follows a near linear dependence between 40 – 500 K, but a weaker dependence is observed below 40 K. This can be explained by examining the Brooks-Herring formulation (see Eq. 4.27), which is known to be valid for non-degenerate semiconductors particularly in the carrier freeze-out temperature regime, and a practical criterion for the validity of using the formulation is \( y \gg 1 \) (Brooks 1955). This means that the calculation is reliable for any carrier concentration at very high temperatures, or for sufficiently low concentrations at low temperatures. In this sample, the \( y \) value is the order of unity up to about 40 K (note that \( y > 1 \) above 40 K), and hence the calculated \( \mu_{\text{ii}} \) limit below 40 K is regarded to be less reliable. Nevertheless, the agreement between the experiment and theory is good in the temperature range 40 – 100 K. The \( \mu_{\text{ii}} \) limit has been calculated using the free carrier concentration as the effective concentration (i.e., \( n = n' \)). Introducing an added level of screening by ionised impurities could change the behaviour of the \( \mu_{\text{ii}} \) limit, and this is also included in Fig. 4.9 (represented by \( \mu_{\text{ii}}^+ \)). Comparing the \( \mu_{\text{ii}} \) and \( \mu_{\text{ii}}^+ \) limits show that the mobility is more or less equal at temperatures above 100 K. However, the effect of extra screening becomes more pronounced at lower temperatures, and the \( \mu_{\text{ii}}^+ \) limit lies at higher levels than the \( \mu_{\text{ii}} \) limit, resulting in a poorer agreement between the experimental and simulated results.

The total combined mobility limit and the experimental data are plotted in Fig. 4.10 for comparison. As expected, the contributions from \( \mu_{\text{op}}, \mu_{\text{pz}} \) and \( \mu_{dp} \) are negligible at low temperatures, and the mobility is mainly limited by ionised impurity scattering. At higher temperatures (above 200 K), polar optical scattering plays a dominant role. However, there exists about 40% discrepancy between the measured mobility and theory in these temperatures. Difficulty in fitting GaN mobility data in the high temperature range has also been reported by various authors (Look et al. 1997; Tang et al. 1997). Different material parameters have been employed by Look et al. (1997) to shift down the theoretical mobility as much as 30%, and since their experimental mobility reflected that of the high quality sample (\( \mu = 600 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1} \)), the mobility at high temperatures was fitted successfully. However, the quality of samples studied in this thesis are significantly lower, and varying the material parameter values would not affect the mobility discrepancy a great deal. Tang et al. (1997) have attributed
FIG. 4.9. The experimental $\mu_H$ of C190299 (open circles) fitted in terms of the various scattering mechanisms involved using the Matthiesen's rule. The solid curves illustrate the mobility limits associated with polar optical, piezoelectric and deformation potential scattering. The dashed curve represents the mobility limited by ionized impurity scattering without screening, and the dotted curve shows the screened $\mu_{ii}$ limit.

this disagreement to the various kinds of crystalline defects such as grain boundaries and strain induced fields. A more likely explanation could be made by considering the theory describing polar optical scattering (refer to Section 4.1.2). Due to the inelastic nature of polar optical scattering, an analytical theory has been employed instead of the relaxation time approximation to model the $\mu_{op}$. It is possible that an incomplete treatment of polar optical scattering could be the reason behind the calculated values being relatively greater than the experimental data, and further work needs to be carried out to properly evaluate the mobility limited by polar optical scattering.

Since the value of $N_A (= 1.5 \times 10^{17}$ cm$^{-3}$) has been independently determined by fitting the mobility data, the $N_D$ and $\epsilon_d$ are to be extracted from the fit of the $n_H$ vs $T$ data. This has been carried out for sample C190299 and the fit to the experimental data is shown in Fig. 4.11. A close match between experiment and theory is observed for most of the temperature range, and the $N_D$ and $\epsilon_d$ value of $7.7 \times 10^{17}$ cm$^{-3}$ and 11.3
meV have been obtained respectively. It is interesting to note that all fitting parameters can be extracted by fitting the $n_H$ vs $T$ data alone. However, this procedure resulted in fitted parameter values that were not unique, and $N_A$ was found to be an insensitive parameter in the fit. The $N_A$ value found from a single CBE fitting ($3.5 \times 10^{17}$ cm$^{-3}$) resulted in $\epsilon_d$ which was much smaller (about 3.4 meV) than obtained by using the simultaneous fitting procedure. In addition, the combined theoretical mobility at low $T$ was about half the mobility calculated by the simultaneous fitting method, and lay well below the experimental mobility, which is clearly inconsistent. This demonstrates that the reliability and uniqueness of the fitting results are significantly improved by using the simultaneous fitting procedure due to the reduced number of fitting parameters.

**G165 results**

The fitting has been also carried out on sample G165 and the results of the best fit are shown in Fig. 4.12 and 4.13. The extracted parameters include $N_A = 3.3 \times 10^{17}$ cm$^{-3}$, $N_D = 8.0 \times 10^{17}$ cm$^{-3}$ and $\epsilon_d = 8.7$ meV.

The general characteristics of the fits appear to be identical to that of the C190299
FIG. 4.11. A plot of the measured $n_H(T)$ data of C190299 (solid squares) and the fitting curve (solid curve) using CBE.

fits and therefore similar conclusions may be drawn. A closer inspection, however, reveals differences that could be crucial in interpreting the data. The high temperature $\mu_H$ data, although significantly lower than predicted by theory, follows a weaker temperature dependence than expected for the polar optical scattering limit. Also, the fit to the temperature dependence of $n_H$ matches closely only in the temperature range 120 – 600 K, whereas in C190299's case, the experimental data were successfully fitted down to about 40 K. In fact, the Hall carrier density continues to decrease up to 40 K but then rises again at a lower temperature. These observations could suggest the presence of an impurity band. This is reasonable since although the extracted donor density is lower than the Mott carrier density ($1 \times 10^{18}$ cm$^{-3}$), it could be argued that with the $8.0 \times 10^{17}$ cm$^{-3}$ donor level, some overlap of the electron wavefunction is likely to occur, thereby providing a parallel channel for electrons to conduct. Hence, the analysis of G165 based on non-degenerate carrier statistics could provide less accurate results. Nonetheless, the mixed conduction effects are thought to be significant only at very low temperatures, and at higher temperatures (above about 100 K) the
4. Transport in GaN Epilayers

Comparison of C190299 and G165 results

For comparison, the calculated and measured mobility are plotted in Fig. 4.14, and the list of extracted parameters is also given in Table 4.3. Note that the compensation ratio ($\theta = N_A/N_D$) is also included in Table 4.3.

The difference in mobilities of the samples is smaller at high temperatures than the mobilities at low temperatures. The sample with the lower $N_A$ value (C190299) has higher low temperature mobility. This correlation between the low temperature mobility and $N_A$ demonstrates that the presence of compensating acceptors in $n$-GaN layers influences very sensitively the low temperature mobility, and as mentioned previously in Section 4.1.2, analysing the low temperature data can give a good estimate of the acceptor concentration. However, the acceptors seem to have little effect on limiting the

![Graph](image-url)
high temperature mobility. An interesting feature in comparing the high temperature mobility is that although the theoretical mobility values lie closely together at high temperatures, the differences in measured values are larger than predicted by theory and become very small only at the highest temperature. As mentioned previously, this indicates that the impurity band effects are at work in sample G165; the low mobility impurity band and the high mobility conduction band compete with each other and the distribution of carriers between the two bands changes with temperature. Hence the measured mobility does not represent the true conduction mobility (i.e., $\mu_H < \mu_c$). However, raising the measurement temperature further ($T > 600$ K) should give mobility that are similar to the theoretical values, since the conduction band electron transport dominates with increasing temperature.

The various parameters of $n$-GaN samples with a single shallow donor level ($\epsilon_d, N_D, N_A$ and $\mu_H$ at 300 K) are given in Table 4.3. Both C190299 and G165 are undoped, and exhibit similar activation energies. These values are expected for hydrogenic donors with screening effect. Eq. 4.34 describes such screening effect, and substituting the
The calculated value of $N_D$ in the formula results in activation energies of 9.8 and 9.5 meV for C190299 and G165, respectively. These values are comparable to the values found from fits to the measured data. Small discrepancies may have come from the uncertainty of the $N_A$ values determined from the mobility analysis. The main difference between the samples is the mobility (C190299 being higher than G165) and this can be correlated to the difference in the compensation ratio (or the level of acceptor concentration). Larger compensation levels result in lower mobility, which is expected considering the dominant mobility limiting mechanism at low temperatures is ionised impurity scattering (described by Eq. 4.27).

**TABLE 4.3.** A list of the parameters for non-degenerate bulk samples.

<table>
<thead>
<tr>
<th>Sample</th>
<th>$\epsilon_d$ (meV)</th>
<th>$N_D$ ($\text{cm}^{-3}$)</th>
<th>$N_A$ ($\text{cm}^{-3}$)</th>
<th>$\theta$</th>
<th>$\mu_H$ at 300 K ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C190299</td>
<td>11.3</td>
<td>$7.7 \times 10^{17}$</td>
<td>$1.5 \times 10^{17}$</td>
<td>0.19</td>
<td>450</td>
</tr>
<tr>
<td>G165</td>
<td>8.7</td>
<td>$8.0 \times 10^{17}$</td>
<td>$3.3 \times 10^{17}$</td>
<td>0.41</td>
<td>330</td>
</tr>
</tbody>
</table>

Samples C190299 and G165 are unintentionally doped and this is reflected in the similar shallow activation energies, and compensation levels of about $\sim 20$ and $\sim 40\%$. 

**FIG. 4.14.** The experimental $\mu_H$ vs $T$ data (open circles and solid squares) and the calculated fit curves (solid and dotted curves) of sample C190299 and G165, respectively.
for C190299 and G165 respectively. The origin of the shallow donor cannot be directly deduced from the results, but it is possible to assume that a substitutional hydrogenic impurity is likely to be the culprit. G165 was grown by MOCVD, thus the deposition took place at very high temperatures (> 1000 °C), and contaminants such as Si or O could have been introduced during growth (Seifert et al. 1983). Contaminants could also enter during MBE growth for C190299 but since the MBE growth is expected to occur at lower temperatures and in a cleaner environment than MOCVD, the level of defect density and compensation is likely to be lower for C190299 than for G165. Si is expected to be an amphoteric impurity in III–V compounds, and Koo et al. (1999) have reported a GaAs lateral p-n junction where the p-n junction was defined by incorporating Si into GaAs in different geometric orientations. Hence, judging from the compensation levels in the measured samples, Si could be the common source of donor and acceptor concentrations.

Finally, the reason for choosing to apply the analysis based on non-degenerate GaN bulk layers on G165 must be addressed. With regards to the Mott concentration of \(1 \times 10^{18} \text{ cm}^{-3}\), the total impurity density \(N_i (= N_D + N_A)\) for C190299 and G165 are approximately \(9.2 \times 10^{17}\) and \(1.1 \times 10^{18} \text{ cm}^{-3}\) respectively, and the presence of an impurity band in G165 is supported by this. Although the difference in the concentration level between the samples is small, the sudden nature of the insulator-to-metal transition (as mentioned earlier in Section 4.1.3) implies that G165 suffers from parallel conduction effects. However, the behaviour of the G165 results indicate that the impurity band effects are not prominent at all temperatures. In fact, strong impurity band effects may exist particularly at low temperatures (below 40 K) and therefore the \(N_A\) value extracted from the low temperature mobility fit to ionised impurity scattering is expected to carry a larger error than in C190299. At higher temperatures however (above 100 K), the overall temperature dependence of \(n_H\) and \(\mu_H\) can be approximated by non-degenerate behaviour, and it is reasonable to assume that the parallel conduction via an impurity band is minimal.
4.2.3 Samples with strong impurity band conduction

The results of sample G165 in the previous section clearly demonstrated some difficulties when trying to fit non-degenerate characteristics to a sample with a small degree of impurity band effects. The samples investigated in the following section are heavily affected by impurity band conduction where its effects cannot be ignored even at high temperatures. Clearly an analysis based on two-carrier conduction needs to be employed, which has been described earlier in Section 4.1.4. In this section, the temperature dependent results of the IBC samples are given and the interpretation of their transport properties is discussed.

General remarks

As mentioned previously in Section 4.2.1, the appearance of a minimum in the temperature dependence of Hall density data is indicative of two conduction paths with different carrier mobilities (see Fig. 4.6). The nature of secondary channel could be identified as either an impurity band or a degenerate layer at the GaN/substrate interface. When assuming the presence of an accumulation layer at the interface, it would simplify the analysis since the accumulation layer would exhibit known, fixed carrier density and mobility values that are independent of temperature (obtained from the low temperature data). However, looking at the high temperature end of the results displayed in Fig. 4.6, it can be seen that there is some saturation of \( n_H \) in IBC samples. Sample MG622 in particular shows that \( n_H \) at the highest temperature is lower than the lowest temperature \( n_H \) value, and indeed these trends have been observed in all of the samples studied. In the case of an accumulation layer at the interface, the above trends would not appear. Instead, it is expected that the Hall density would continue to increase with temperature, eventually showing saturation at a value that is higher than the lowest temperature value. This is because the transport properties of the degenerate layer are approximately constant, the behaviour of \( n_H \) at high temperatures would represent a contribution of interface conduction with that of conduction band electrons from a shallow donor. Hence, assigning an impurity band as the secondary conduction channel would provide a more reasonable theoretical model to investigate the measured data. In addition, since most of the samples studied in this thesis are
close to or above the Mott density of $1 \times 10^{18}$ cm$^{-3}$, it is likely that there is a degree of parallel conduction due to impurity wave-function overlap taking place.

**FIG. 4.15.** Hall mobility plotted against the average carrier density as measured by room temperature Hall effect. The solid line is a theoretical model assuming 60% compensation (Chin et al. 1994).

The list of basic sample details and the room temperature Hall results have been already given in Table 4.2 (refer to Section 4.2.1), and Fig. 4.15 plots the 300 K Hall mobility against Hall carrier density. It can be seen that the general reduction in mobility with increasing carrier density does not depend systematically on the growth technique used, layer thickness or the dopant type. This suggests that:

- ionised impurity scattering is important, even at 300 K.
- the unintentional dopant is similar in effect to Si.
- the best material quality is comparable for MBE and MOCVD growth.

Fig. 4.16 shows the temperature of the $n_H$ minimum, $T_{\text{min}}$, plotted against the room temperature carrier density. Again, a trend is observed which displays no systematic dependence on sample preparation or on the carrier mobility. Incidentally, the mobility values correspond to theoretical compensation levels of about 60% but
because of parallel conduction band effects, these measurements do not accurately represent the conduction band properties. Hence the experimental data need to be de-convoluted to obtain the true conduction band properties.

**De-convolution assuming \( N_A = 0 \)**

Two-carrier conduction has been mathematically represented in Eqs. 4.41 and 4.42, which include various parameters such as \( n_c, n_d, \mu_c \) and \( \mu_d \). In order to obtain the temperature dependence of \( n_c \), Eq. 4.52 is employed. However, there is no direct way to extract the unique value of \( N_A \), and hence a fixed \( N_A \) value needs to be assigned. Firstly, the analysis has been carried out assuming zero compensation for simplicity. The procedure described in Section 4.1.4 can be carried out with \( N_A \) set to zero and \( N_D \) replaced by \( N_T \). The de-convoluted results of \( n_c, \mu_c \) and \( \mu_d \) for sample MG676 have been plotted in Fig. 4.17 along with the measured Hall data. It should be noted that the de-convoluted data of MG676 only is considered in this section since the calculated behaviour is typical of all samples.

The calculations show that (a) even at 300 K, most of the available electrons

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**FIG. 4.16.** Temperature of the minimum in Hall carrier density as a function of room temperature Hall density. The solid line is a guide to the eye.
FIG. 4.17. De-convoluted results of sample MG676. Solid squares and circles represent the temperature dependence of the Hall carrier mobility and concentration, respectively. The solid curve follows the calculated temperature dependence of conduction band density \( n_c \), the dotted curve shows the conduction band mobility \( \mu_c \) variation and the dashed curve represents the impurity band mobility variation.

(usually more than two-thirds) remain in the impurity band, (b) \( \mu_c \) can be much larger than \( \mu_H \) (e.g., up to about 50% greater at the peak), and (c) \( \mu_d \) is significantly lower than \( \mu_c \) and less temperature dependent. The results of de-convolution for all IBC samples are listed in Table 4.4, in terms of the net impurity band density, \( N_T \), the activation energy \( \epsilon_d \) from this band to the conduction band, and the ratio, \( \mu_c/\mu_d \) at 77 K. There is an overall reduction in \( \epsilon_d \) as \( N_T \) increases, due to broadening of the impurity band at high densities. This trend seems not to depend on dopant type or growth method, supporting the picture that deliberate and unintentional donors occupy similar positions in the energy gap (Si being the possible donor).

An interesting point can be made when considering the spread in mobility ratio values. It has been noted earlier from Fig. 4.16 that \( T_{n\text{min}} \), which is a function of the mobility ratio (Molnar et al. 1993), also only depends weakly on mobility. However, the temperature dependence of \( \mu_c \) is expected to be more strongly affected than that of
TABLE 4.4. Summary of transport parameters calculated for all IBC samples, assuming zero compensation.

<table>
<thead>
<tr>
<th>Sample</th>
<th>(N_T, (\times 10^{18} \text{ cm}^{-3}))</th>
<th>(\epsilon_d, (\text{meV}))</th>
<th>(\mu_d, \text{at 77 K (cm}^2, \text{V}^{-1}, \text{s}^{-1}))</th>
<th>(\mu_c, \text{at 77 K (cm}^2, \text{V}^{-1}, \text{s}^{-1}))</th>
<th>(\mu_c/\mu_d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>G138</td>
<td>0.43</td>
<td>41.0</td>
<td>6.8</td>
<td>86</td>
<td>12.5</td>
</tr>
<tr>
<td>G613</td>
<td>0.50</td>
<td>43.6</td>
<td>0.8</td>
<td>6</td>
<td>8.2</td>
</tr>
<tr>
<td>G50</td>
<td>0.77</td>
<td>18.8</td>
<td>57.0</td>
<td>405</td>
<td>7.1</td>
</tr>
<tr>
<td>MG676</td>
<td>0.78</td>
<td>30.0</td>
<td>15.4</td>
<td>235</td>
<td>15.2</td>
</tr>
<tr>
<td>MG622</td>
<td>3.77</td>
<td>18.1</td>
<td>41.5</td>
<td>180</td>
<td>4.3</td>
</tr>
<tr>
<td>G649</td>
<td>4.56</td>
<td>1.7</td>
<td>105.0</td>
<td>200</td>
<td>1.9</td>
</tr>
<tr>
<td>G617</td>
<td>4.76</td>
<td>1.2</td>
<td>87.0</td>
<td>172</td>
<td>2.0</td>
</tr>
<tr>
<td>MG657</td>
<td>7.40</td>
<td>6.4</td>
<td>45.5</td>
<td>106</td>
<td>2.3</td>
</tr>
<tr>
<td>G595</td>
<td>9.00</td>
<td>3.5</td>
<td>17.3</td>
<td>25</td>
<td>1.4</td>
</tr>
</tbody>
</table>

\(\mu_d\), by the variations in the combinations of scattering mechanisms present such as by ionised impurities and lattice vibrations. Hence it can be predicted that the mobility ratio varies similarly with the change in \(\mu_c\). Clearly, this is not the case in this work; samples with \(N_T\) of \(10^{18} \text{ cm}^{-3}\) or less have similar mobility ratios in the range 7 - 15, while for \(N_T > 3 \times 10^{18} \text{ cm}^{-3}\), the average is approximately 2, despite widely differing values of \(\mu_c\) within each of these sets of samples. A partial explanation may be that there are electrostatic barriers in the layers, e.g., at grain boundaries, which has been proposed by Fehrer et al. (1998) to reduce the mobility by a factor \(\exp(\phi_B/k_BT)\) where \(\phi_B\) is the barrier height. Since the effect of such barriers would be same for conduction and impurity bands, the reduction would occur by the same factor. However, there is no evidence of single thermally activated mobility changes (i.e., hopping) in the measured samples, and this could be due to a distribution of barrier heights in the samples, giving a weaker temperature dependence on conduction. Fig. 4.18 schematically illustrates various barriers arising from grain boundaries of different sizes. The size of the grain would be very much sample dependent but as far as the author is aware of, there have yet been a detailed systematic study of the grain size linking with different growth procedures and its effect on transport properties. It is possible to stipulate though, that materials with smaller grain sizes would exhibit higher barrier heights due to close proximity of neighbouring barriers, therefore making it difficult for carriers to hop over while conducting.
The evidence of barriers has been reported by Hamilton et al. (1999) where scanning tunnelling microscopy (STM) spectra were taken close to and spanning the large terraces which typically form at the point of emergence of threading dislocations. These spectra showed that the energy was varying measurably in these regions. Close to a dislocation, the gap was reduced relative to the average, over distances of about 100 nm, and was accompanied by an increase in local free electron density. Hence local energy fluctuations, driven by strain variation, result in non-uniformity of the electron density and thus give rise to potential barriers, due to a combination of band offsets and space charge (Harris et al. 2000).

Finally, the effects of dislocations and grain boundaries on electron transport can be investigated further by considering the Gent samples listed in Table 4.4. Except for G595, a striking feature is observed, where the calculated 77 K mobility is found to improve drastically from less than 90 cm$^2$ V$^{-1}$ s$^{-1}$ for the low-density samples (G138
and G613) to between 170 – 410 cm\(^2\) V\(^{-1}\) s\(^{-1}\) for the highly doped samples (G50, G649 and G617). This sudden increase in the mobility for other Gent samples have also been reported by Bougrioua et al. (1999), where the room temperature carrier density of around \(8 \times 10^{17}\) cm\(^{-3}\) was found to be the critical value which distinguishes the two different regimes of transport. Assuming similar dislocation densities present in all the samples, they observed from the TEM studies that in the highly doped films there are fewer dislocations in the grain boundaries and a larger number of isolated vertical ones located within the grains than the samples with less than \(8 \times 10^{17}\) cm\(^{-3}\) carriers. They further suggested that greater density of dislocations in the grain boundaries for the low-density layers resulted in the appearance of narrow barrier potentials which can possibly be penetrated by a tunneling process. This would impose a damping factor on the mobility, thus explaining the steep reduction in the mobility for the lightly-doped samples. Note that although G595 is highly doped, it still exhibits a low mobility of less than 30 cm\(^2\) V\(^{-1}\) s\(^{-1}\) and thus departs from the afore-mentioned trend. This is possibly explained by assuming G595 contains a much higher concentration of dislocations than the rest of the Gent samples, though the exact value of dislocation density is not known to verify this assumption.

**De-convolution assuming a fixed level of compensation**

The previous section demonstrated that the de-convolution method successfully separates the transport behaviour of conduction and impurity band, and various parameters extracted from the analysis reveal much information on the role of the impurity band in limiting the apparent mobility. However, the analysis is only complete when the compensation effects are taken into account. Although the analysis assuming zero compensation still provides valid data regarding the trends observed in the samples, the actual numerical values of the calculation are not completely accurate. Most GaN layers are known to contain large levels of acceptor concentration, and since the investigation on non-degenerate bulk samples has been treated with \(N_A\) included (refer to Section 4.2.2), this section presents de-convolution results of IBC samples assuming different levels of compensation. As mentioned earlier in theory (Section 4.1.4), different values of \(N_A\) have been chosen before the calculation, and in this work, the
acceptor concentration ranges from $3 \times 10^{17}$ to $6 \times 10^{18}$ cm$^{-3}$. The modelling has been carried out on samples MG676 and MG622, with room temperature carrier densities of $4.1 \times 10^{17}$ and $2.5 \times 10^{18}$ cm$^{-3}$, respectively.

Figs. 4.19 and 4.20 show the de-convoluted results of MG676 and MG622, respectively. For the case of MG676, the conduction band mobility has been de-convoluted from the Hall data at acceptor concentrations of $3 \times 10^{17}$, $6 \times 10^{17}$ and $1 \times 10^{18}$ cm$^{-3}$. Similar to the results assuming zero compensation (as shown in Fig. 4.17), a closer agreement is achieved between the conduction band and Hall mobility at higher temperatures. At low temperatures, the conduction band electrons are frozen out and the Hall mobility is a result of the two-carrier conduction where a large portion of it is affected by the low-mobility impurity band. Hence the de-convoluted $\mu_c$ is much bigger than $\mu_H$ below about 80 K. In addition, the $\mu_c$ values calculated by incorporating a fixed $N_A$ is lower than those obtained assuming zero compensation, and with an increasing level of $N_A$, $\mu_c$ becomes smaller.
Also included in Fig. 4.19 is the theoretical mobility limited by screened ionised impurity scattering, calculated at various acceptor concentrations. Note that in contrast to non-degenerate samples C190299 and G165 (see Section 4.2.2), screening has been taken into account in the analysis of MG676 since, in this case, the presence of an impurity band suggests a high level of compensation (this aspect will be discussed further at the end of this section). By comparing \( \mu_i^+ \) with de-convoluted \( \mu_c \) allows \( N_A \) to be estimated. The best agreement is observed for the case of \( N_A = 1 \times 10^{18} \) cm\(^{-3}\) (the dotted line), particularly in the temperature range 60 – 200 K. Polar optical scattering dominates above 200 K, and the discrepancy below 60 K is currently unclear. This may be explained by considering the effect of dislocations. Although the presence of screening enhances the low-temperature mobility, the mobility limited by dislocation scattering (described by Eq. 4.28) could play an important role in restricting the mobility at low temperatures. Currently, due to the lack of knowledge of dislocation density, it is difficult to verify such possibility. Nevertheless, the de-convolution analysis demonstrates that material quality can be assessed, where information on the compensation and the behaviour of conduction and impurity band transport is obtained.

Similar conclusions to MG676 can be drawn for the de-convoluted results of MG622 which is depicted in Fig. 4.20. However, since the room temperature Hall concentration \( (n_H = 2.5 \times 10^{18} \text{ cm}^{-3}) \) is nearly an order of magnitude greater than that of MG676 \( (n_H = 4 \times 10^{17} \text{ cm}^{-3}) \), higher levels of \( N_A \) have been used in this case \( (1 \times 10^{18}, 3 \times 10^{18} \text{ and } 6 \times 10^{18} \text{ cm}^{-3}) \). An inspection of the calculated curves reveals that the acceptor concentration of about \( 3 \times 10^{18} \text{ cm}^{-3} \) is estimated to be present in MG622 (the solid line), though the agreement between \( \mu_c \) and \( \mu_i^+ \) occurs within a smaller range of temperature than MG676. As mentioned previously in theory (refer to Section 4.1.2), the mobility limited by ionised impurity scattering, given by Eq. 4.27, is a measure of the impurity content in non-degenerately doped semiconductors at low temperatures. However, MG622 exhibits a high carrier concentration and the calculated \( \mu_i^+ \) is expected to be less accurate at lower temperatures. As a result, the difference between \( \mu_c \) and \( \mu_i^+ \) becomes greater more rapidly with decreasing temperature than in the case of MG676.
Finally, the issue of compensation is addressed here. From the estimated $N_A$ values and by using the relation $N_T = N_D - N_A$ (from Eq. 4.39), the compensation ratio ($N_A/N_D$) and the total impurity concentration ($N_D + N_A$) can be obtained. The acquired values are listed in Table 4.5. An initial look at the values indicate that strong compensation is present in the samples (about 40 – 60%). Consequently, the impurity content exceeds the Mott concentration for both MG676 and MG622, which is expected for the samples heavily affected by an impurity band. In fact, the doping

![Graph showing electron mobility vs temperature for different acceptor concentrations.](image)

**FIG. 4.20.** De-convoluted results of MG622, where the symbols correspond to the experimental Hall mobility, and the curves represent the calculated conduction band mobility ($\mu_c$) and the theoretical mobility limited by ionised impurity scattering with screening ($\mu_{\text{ifs}}$). The simulation has been performed at acceptor concentrations of $1 \times 10^{18}$, $3 \times 10^{18}$ and $6 \times 10^{18}$ cm$^{-3}$.

**TABLE 4.5.** A list of parameters obtained from the study of de-convoluted results of MG676 and MG622.

<table>
<thead>
<tr>
<th>Sample</th>
<th>$N_T$ (cm$^{-3}$)</th>
<th>$N_A$ (cm$^{-3}$)</th>
<th>$N_D$ (cm$^{-3}$)</th>
<th>$N_D + N_A$ (cm$^{-3}$)</th>
<th>$N_A/N_D$ (%)</th>
<th>$\epsilon_d$ (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MG676</td>
<td>$0.78 \times 10^{18}$</td>
<td>$1 \times 10^{18}$</td>
<td>$1.78 \times 10^{18}$</td>
<td>$2.78 \times 10^{18}$</td>
<td>56</td>
<td>7.8</td>
</tr>
<tr>
<td>MG622</td>
<td>$3.77 \times 10^{18}$</td>
<td>$3 \times 10^{18}$</td>
<td>$6.77 \times 10^{18}$</td>
<td>$9.77 \times 10^{18}$</td>
<td>44</td>
<td>0</td>
</tr>
</tbody>
</table>
concentration in MG622 is greater than $6 \times 10^{18} \text{ cm}^{-3}$, which is the point at which the impurity band merges with the conduction band, and this is demonstrated by its zero activation energy. As mentioned earlier in this section, the de-convoluted $\mu_c$ has been compared with the mobility limited by screened ionised impurity scattering. Such high concentrations of impurities in these samples suggest that screening effects are likely to be strong, and thus incorporating screening in the analysis is thought to be justified.
Chapter 5

Magneto-transport in
AlGaN/GaN Structures

In this chapter, magneto-transport studies on AlGaN/GaN heterostructures will be presented, concentrating on the behaviour of carriers in strong magnetic fields at low temperatures. Section 5.1 describes theoretical concepts regarding the electrical characterisation of group III nitrides and methods of calculating parameters such as the GaN electron effective mass, $m^*$, and the quantum scattering time, $\tau_q$. Based on the obtained results an assessment of material quality in the samples investigated will then be given in Section 5.2.

5.1 Theoretical considerations

A two-dimensional electronic system can be realised when two semiconductors with different band-gaps are brought into contact with each other. In this thesis, the system is formed at the interface between the AlGaN and the GaN layers where there exist discontinuities in the conduction and valence bands. This section begins with an outline of the general properties and basic underlying physics of the two-dimensional electron gas (2DEG) systems based on AlGaN/GaN heterostructures, paying particular attention to important issues such as the spontaneous and piezoelectric polarisation effects. The transport properties of semiconductors are profoundly altered by the application of electric and magnetic fields, and magneto-transport experiments utilising
5. Magneto-transport in AlGaN/GaN Structures

the Shubnikov-de Haas (SdH) effect at low temperatures have been mainly employed in the characterisation. Thus, the theory behind the SdH characterisation technique, and various calculation procedures for extracting material parameters, will then be presented. It should be noted here that there are a wealth of theoretical information that covers the transport behaviour of 2DEG systems as a whole, and to describe all the aspects of the theory is beyond the scope of this thesis. Hence in the sections that follow, it is assumed that the reader is familiar with the basic level of transport theory, and only selected topics that are closely relevant and of importance to the results will be discussed.

5.1.1 General overview

Most modern electronic devices are built upon heterojunctions between materials with different band-gaps. A typical device structure based upon a single heterojunction is the modulation doped heterojunction field effect transistor (MODFET). Alternatively known as the high electron mobility transistor (HEMT), it utilises the modulation doping technique where ionised impurity scattering is significantly reduced by spatially separating the mobile carriers from their parent impurities through the introduction of an undoped spacer layer. As an example, Fig. 5.1 depicts the band diagram of an AlGaAs/GaAs HEMT structure. The wider band-gap material, AlGaAs, is doped n-type (e.g., using Si) whilst keeping the narrow band-gap material (GaAs) free from intentional doping. Some of the electrons introduced by the Si donors into the conduction band of the AlGaAs diffuse into the lower-lying Γ-conduction band minimum of the GaAs leaving behind ionised donors in the AlGaAs layer. The redistribution of the charge creates an electrostatic potential which bends the bands in the vicinity of the interface, until at equilibrium a constant Fermi level across the structure is established. In this system, electrons are trapped at the interface in an asymmetric, approximately triangular shaped, potential well formed by the conduction band discontinuity and the Coulomb potential of the parent ionised donors. The potential well confinement of the electrons in the growth direction (z) means that the electron movement has only 2 degrees of freedom (x and y), and the physics of the 2DEG formed at the interface is subtly different from 3-dimensional (3D) bulk materials. In particular, quantum
effects mean that the energy spectrum for motion perpendicular to the interface is no longer continuous but rather a set of discrete levels known as electronic subbands. The fundamental transport aspects of 2DEG systems will be described in more detail in Section 5.1.2.

The general principles of the 2DEG formation for the case of AlGaN/GaN heterostructure are similar to that of the AlGaAs/GaAs system. The interfaces of the AlGaN/GaN are of type I, i.e., for a double heterostructure there is a direct confinement of both electrons and holes (Fig. 5.2). The values for the band offsets are not very accurately determined (Monemar 1999), and vary with type of substrate (built-in strain), but the approximate values indicated in Fig. 5.2 seem to be consistent with the experience from AlGaN/GaN device structures (Martin et al. 1994), as well as recent theoretical estimates (van der Walle and Neugebauer 1997).

The advantages of group III nitrides for electronic device applications have been briefly introduced previously in Section 2.4.1, and in order to fully realise the potential of AlGaN/GaN structures, the key mechanisms controlling the formation of the 2DEG
at the AlGaN/GaN interface must be well known. Much work has been done on revealing the nature of the high 2DEG densities in the nominally undoped AlGaN/GaN structures. The large interface densities in this system have been correlated to the piezoelectric and spontaneous polarisation, resulting in high electric fields (≈ 5 MV cm⁻¹) in both AlGaN and GaN layers (Bernardini et al. 1997; Ambacher et al. 1999). The presence of these polarisation fields profoundly changes the interface band structure from the usually expected case for the conventional AlGaAs/GaAs systems, and the modified calculated conduction band structure of a AlGaN/GaN heterojunction due to polarisation fields is graphically illustrated in Fig. 5.3 (discussed in more detail in the next section). Several theoretical attempts have been made to pinpoint the main scattering mechanisms limiting the electron mobility in the AlGaN/GaN heterostructures (Shur et al. 1996; Smorchkova et al. 1999), and a brief review of their findings will also be given.

**Polarisation-induced 2DEG density**

Group III nitrides are heavily affected by spontaneous and piezoelectric polarisation fields, and the origin of such fields has been briefly explained earlier in Section 2.1.1. In
this section, the effects of the polarisation fields on the 2DEG formed at the interface between AlGaN and GaN will be discussed.

In the absence of external electric fields, the total macroscopic polarisation \( \mathbf{P} \) of a GaN or AlGaN layer is the sum of the spontaneous polarisation \( \mathbf{P}_{sp} \) in the equilibrium lattice and the strain-induced or piezoelectric polarisation \( \mathbf{P}_{pe} \). Considering polarisations along the [0001] axis (the growth axis), the spontaneous polarisation along the \( c \)-axis of the wurtzite crystal is \( \mathbf{P}_{sp} = P_{spz} \), and is directed opposite to the growth direction for GaN and AlN. Bernardini et al. (1997) reported that the theoretical spontaneous polarisation is very large in nitrides (comparable to zinc oxide), and also increases from GaN to InN and AlN.

Piezoelectric polarisation arises from the strain effect at the interface and the lattice constant mismatch between AlGaN and GaN. The magnitude of the piezoelectric
polarisation is given by \( \textit{Ambacher et al. }1999\)

\[
P_{\text{PE}} = 2 \frac{a - a_0}{a_0} \left( e_{31} - e_{33} \frac{C_{13}}{C_{33}} \right),
\]

(5.1)

where \(a_0\) is the equilibrium lattice constant, \(e_{33}\) and \(e_{31}\) are piezoelectric coefficients, and \(C_{13}\) and \(C_{33}\) are elastic constants. For wurtzite GaN, the positive \(z\) direction is defined along the \(c\)-axis pointing from N plane to the Ga plane. However, positive polarisation is defined as the direction from the cation (Ga) to the anion (N) along the \(c\)-axis. Incidentally, Ga-polarity means Ga on the top position of the \([0001]\) bilayer. The polarisation orientation depends on the polarity of the crystal, and must be found experimentally. Various authors have determined the polarity using methods such as ion channelling and convergent beam electron diffraction (Daudin et al. 1996), photo-electron diffraction (Seelmann-Eggebert et al. 1997), chemical etching (Weyher et al. 1997), and X-ray standing wave studies (Ambacher et al. 1999). Two common observations can be made from these studies: (a) the layers exhibiting rough morphology were found to be N-face, while smoother surfaces were associated with the Ga-face, (b) in general, MOCVD grown films tended to be of Ga-face material and N-face polarity was prominent in MBE grown films.

| TABLE 5.1. Spontaneous polarisation, lattice, piezoelectric, and elastic constants for III–V wurtzite nitrides |
|---------------------------------|--------|--------|--------|
| \(P_0\) (C m\(^{-2}\))        | AIN    | GaN    | InN    |
| ---                            | -0.081\(^a\) | -0.029\(^a\) | -0.032\(^a\) |
| \(a_0\) (Å)                    | 3.112\(^b\) | 3.189\(^b\) | 3.54\(^b\) |
| \(e_{31}\) (C m\(^{-2}\))     | -0.60\(^a\) | -0.49\(^a\) | -0.57\(^a\) |
| \(e_{33}\) (C m\(^{-2}\))     | 1.46\(^a\) | 0.73\(^a\) | 0.97\(^a\) |
| \(C_{13}\) (GPa)               | 105\(^c\) | 103\(^c\) | 92\(^c\) |
| \(C_{33}\) (GPa)               | 373\(^c\) | 405\(^c\) | 224\(^c\) |

\(^a\) Bernardini et al. (1997)  
\(^b\) Ambacher et al. (1999)  
\(^c\) Ambacher et al. (2000)

The values for spontaneous and piezoelectric polarisations are listed in Table 5.1 for III–V wurtzite nitrides. Bernardini et al. (1997) observed that the calculated piezoelectric coefficients are up to ten times larger than in GaAs based crystals, and the sign is opposite to other III–V compounds. Also, the piezoelectric polarisation
increases with strain, and similar to the spontaneous polarisation, for crystals from GaN to InN and AlN. Note that in Eq. 5.1, the condition
\[ (e_{31} - e_{33} \times \frac{C_{13}}{C_{33}}) < 0 \]
is valid for AlGaN over the whole range of compositions. Therefore, the piezoelectric polarisation is negative for tensile and positive for compressive strained AlGaN barriers. In addition, the spontaneous polarisation is negative. Consequently, in strained layers, the alignment of spontaneous and piezoelectric polarisation is parallel in tensile strain and anti-parallel in compressive strain. For heterostructures like the samples characterised in this thesis, where the AlGaN barriers are grown on GaN layers, the AlGaN layer is under tensile strain. Also, the polarisation induced charge density \( \sigma(x) \) is given as (Smorchkova et al. 1999)

\[ \sigma(x) = P_{SP}(Al_xGa_{1-x}N) + P_{PE}(Al_xGa_{1-x}N) - P_{SP}(GaN) . \] (5.2)

Fig. 5.4 illustrates the effect of polarisation fields on the formation of 2DEG at the AlGaN/GaN interface. Assuming the AlGaN/GaN structure is grown with Ga-polarity, the positive induced charge will be compensated by free electrons, and as a result, a sheet carrier density \( n_s \) is formed as a 2DEG at the AlGaN/GaN interface. For N-face AlGaN/GaN heterostructures, the polarisations have opposite directions in comparison to the Ga-face structure, and it is expected that electrons will be confined if GaN is grown on top of AlGaN, due to the formation of the positive sheet charge.

At the top of the AlGaN layer, the negative polarisation charge density will induce the formation in a Schottky barrier structure of a positive sheet charge in the metal at the metal-nitride interface, or at a free surface of a positive sheet charge that most likely arises from charging of surface states. Hence, the maximum sheet carrier concentration located at the Al\(_x\)Ga\(_{1-x}\)N/GaN interface can be calculated by a simple electrostatic analysis, which is given by Yu et al. (1997) as

\[ n_s(x) = \frac{\sigma(x)}{e} - \left( \frac{\varepsilon_0 \varepsilon(x)}{e^2 t_{AlGaN}} \right) [e\Phi_b(x) + E_F(x) - \Delta E_c(x)] , \] (5.3)

where \( \varepsilon(x) \) is the dielectric constant, \( t_{AlGaN} \) is the width of the AlGaN barrier, \( e\Phi_b \) is the Schottky barrier of a gate contact, \( E_F \) is the Fermi level with respect to the GaN
conduction band-edge energy, and $\Delta E_c$ is the conduction band offset at the interface.

Based on the theory discussed above, Ambacher et al. (1999) have calculated the polarisation induced sheet charge density $\sigma/e$ and the maximum 2DEG density $n_s$ as a function of the Al composition, and the results are shown in Fig. 5.5, focussing mainly on the Ga-face polarity case.

Ambacher et al. (2000) compared the theoretical calculations shown in Fig. 5.5 to the experimental data (using Hall effect and Capacitance–Voltage profiling measurements) obtained from various AlGaN/GaN heterostructures such as undoped and
Si-doped HEMTs, and arrived at the following conclusions:

(i) The fact that the measured sheet carrier concentration for undoped HEMTs are higher than the calculated concentrations induced only by the piezoelectric polarisation meant that spontaneous polarisation effects are significant, and has to be taken into account in the determination of the total sheet charges and electron densities.

(ii) Even with heavy doping of the barrier, the measured differences in the measured and calculated sheet carrier densities between doped and undoped AlGaN/GaN heterostructures are found to be small (less than 15%). This demonstrated that the formation of a 2DEG in HEMT structures is dominated by polarisation induced effects.
Remarkably high sheet charge and 2DEG density ($> 10^{13}$ cm$^{-2}$) for heterostructures containing AlGaN barriers with $0.15 \leq x \leq 0.4$ promise great potential in the fabrication of high power microwave devices. The agreement between experiment and theory becomes less good for $x > 0.4$, where the large lattice and thermal mismatch between the GaN and AlGaN layers causes a high density of structural defects in the AlGaN, and interface roughness scattering becomes significant in limiting the 2DEG mobility. Also, for $x < 0.15$, the conduction band offset reduces, resulting in weak confinement of the polarisation induced charges.

Further contributing to the outstanding features of AlGaN/GaN heterostructures is the ever-improving electron mobility of the 2DEGs. In order to understand and optimise the 2DEG transport characteristics, various scattering mechanisms involved in 2D structures need to be identified in a similar manner described earlier in Section 4.1.2 for the 3D bulk case, and these are discussed in the following section.

### 2DEG electron mobility

Scattering mechanisms governing the mobility in 2DEG structures can be classified into two categories; those normally present in bulk films (e.g., optical and acoustic phonon, and ionised impurity scattering), but which may be modified by the 2D nature of the carrier distribution, and processes which are specific to heterostructures (such as alloy disorder, interface roughness, inter-subband, remote impurity and residual donor scattering). A review of these processes present in AlGaAs/GaAs heterojunctions has been published by Harris et al. (1989).

Theoretical calculations of the 2D electron mobility in the AlGaN/GaN heterostructures have been made by several researchers. Shur et al. (1996) used a 3D approximation to find the mobility limited by scattering mechanisms in these structures. Zhang et al. (2000) investigated electron transport in an AlGaN/GaN HEMT by using the Kubo formula. Monte Carlo simulation of the electron mobility has also been performed (Li et al. 2000). Hsu and Walukiewicz (1997) found that the optical phonon limits the room temperature mobility to 2000 cm$^2$ V$^{-1}$ s$^{-1}$ by using a variational principle calculation, and predicted low temperature intrinsic mobilities in excess of $10^6$ cm$^2$ V$^{-1}$ s$^{-1}$ for optimised structures. However, they have not considered the effects...
of polarisation fields and surface roughness on the electron mobility. More precise calculations of the 2D electron mobility in the III-nitride heterojunction structures have been carried out by Yu and Brennan (2001). They have incorporated into their analysis the issues such as polarisation fields and surface roughness at the AlGaN/GaN interface for a comprehensive theoretical model.

Yu and Brennan presented a self-consistent calculation of the sheet charge density for the electron mobility. The numerical wave functions and sheet carrier concentration are calculated from the self-consistent calculation of the Schrödinger and Poisson equations, and then the effects of polarisation fields are included. All of the relevant scattering is included in the mobility calculation, including inelastic polar optical scattering and elastic processes such as deformation potential acoustic, piezoelectric, surface roughness, and ionised impurity scattering (remote and background). Elastic processes have been treated using the relaxation time approximation (refer to Section 4.1.1). This cannot be applied to optical phonon scattering due to its inelastic nature, and hence for better theoretical modelling, the linearised Boltzmann equation is solved numerically using an iterative technique (Kawamura and Das Sarma 1992).

The calculated results of Yu and Brennan are displayed in Fig. 5.6 in the temperature range 10 – 300 K, which includes the experimental data for a MOCVD grown HEMT (Wu et al. 1996). As can be seen from the figure, the polar optical scattering begins to dominate at temperatures above 200 K. At low temperature the surface roughness scattering is the dominant mobility limiting scattering process. The interface roughness has been generally described in terms of a Gaussian distribution of the correlation length $L$ and the amplitude of the roughness $\Delta$. By adjusting these parameters to fit the measured data, $L$ and $\Delta$ were chosen to be 1.5 and 0.1 nm, respectively. The mobility limited by interface roughness scattering is found to be a sensitive function of interface parameters (Sakaki et al. 1984), where the momentum relaxation rate for electrons being scattered from interface roughness is given to be proportional to $L^2\Delta^2$. However, Ridley et al. (1999) reported that the assumption of a Gaussian correlation is arbitrary and in practice, the correlation is likely to be random in some cases. Hence estimates of the effect of interface roughness on the mobility are not straightforward to model and difficult to be very precise.
Returning to Fig. 5.6, for the HEMT structure with $n_s$ of about $10^{13}$ cm$^{-2}$, good agreement between the experimental and theoretical results have been obtained with the 300 K mobility of about 1650 cm$^2$ V$^{-1}$ s$^{-1}$, increasing to around 9000 cm$^2$ V$^{-1}$ s$^{-1}$ at 77 K. Similar mobilities have been recently reported by various groups (Wang et al. 1999; Gaska et al. 1999), and Smorchkova et al. (1999) even achieved low temperature mobilities in excess of 50 000 cm$^2$ V$^{-1}$ s$^{-1}$ for high quality Al$_{0.09}$Ga$_{0.91}$N/GaN heterostructures grown by plasma assisted MBE on sapphire. Smorchkova et al. have also investigated the dependence of the 2D electron density and mobility with the changes in the Al composition and the thickness of the AlGaN barrier. They found that increasing the Al composition and the barrier thickness resulted in the increase in 2DEG density and the drop in mobility. Based on these findings, the following conclusions have been drawn:
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(i) The observed increase in $n_s$ is due to the effect of spontaneous and piezoelectric polarisation becoming stronger. Combined with the increasing conduction band offset, a substantial rise in $n_s$ is expected.

(ii) From the theoretical modelling made by Das Sarma and Stern (1985) based on an ideal 2DEG system, the low temperature mobility is calculated to be dominated by the Coulomb interaction of remote charged centres, and the increase in $n_s$ is found to result in improved mobilities due to enhanced screening of carriers. However, in these AlGaN/GaN heterostructures, the increase in $n_s$ corresponds to a decrease in low-temperature mobility, thus ruling out scattering by remote ionised and residual impurities.

(iii) Alloy disorder scattering, which occurs due to the penetration of the electron wavefunction into the AlGaN barrier, increases with thicker barriers since the increase in $n_s$ shifts the charge distribution closer to the heterointerface, resulting in the deeper wavefunction penetration. However, increasing the Al composition pushes up the finite potential barrier height, which reduces the wavefunction penetration. Hence the interplay between these effects needs to be carefully considered for a comprehensive model of alloy disorder scattering.

(iv) Interface roughness scattering, in contrast, becomes stronger by increasing both the Al composition and the barrier thickness. This can be explained by considering the effect of polarisation fields on the 2DEG density (discussed in the previous section). As the Al composition (i.e., lattice mismatch between AlGaN and GaN layers) and the barrier thickness increases, both the spontaneous and piezoelectric polarisation induced charges increase. Hence, a considerable rise in $n_s$ occurs, and a strong band bending can be envisaged. A consequence of this is to push the channel 2D electrons closer to the heterojunction interface and the scattering by interface roughness becomes more effective. This process is likely to be the dominant mobility limiting mechanism at low temperatures.

There are other scattering processes that may be significant in AlGaN/GaN heterostructures and have not been included in the theoretical model, such as by threading dislocations and by grain boundaries. As discussed previously in Chapter 4, the
mobility limited by the dislocations is roughly proportional to temperature (refer to Eq. 4.28), and the polycrystalline nature of wurtzite nitride materials may result in the exponential temperature dependence of the mobility with a small, concentration-dependent activation energy (Fehrer et al. 1998). The earlier results of GaN layers presented in Section 4.2.3 have indicated that these scattering mechanisms play a vital role in limiting the mobility at low temperatures, particularly for low quality materials with a high level of disorder.

The behaviour of the electron mobility and the sheet carrier concentration described so far has shown that there are various factors that govern the transport properties of 2DEGs in AlGaN/GaN heterostructures. Preliminary tests have been carried out in the form of temperature dependent Hall measurements on samples that are grown by MOCVD or MBE with varying Al compositions, of a single heterojunction or of a MODFET structure, and either doped or undoped in the AlGaN barrier. The samples are obtained from various sources (refer to Section 3.2 for a detailed description), and are characterised in this thesis to correlate with the work carried out by other researchers. In particular, comparisons between the experimental data and the theoretical work discussed in this section are made to observe any systematic dependence arising from the range of different sample sources, and will be presented later in Section 5.2.

5.1.2 Magneto-transport in 2DEG systems

Although the exposure of semiconductors to external magnetic fields is of little technological importance with respect to their use in device applications, it is regarded as the most powerful tool in evaluating the physics of semiconductors, particularly for 2DEG systems when combined with an electric field. The resulting physical phenomena can vary qualitatively depending upon the strength of the applied magnetic field and the temperature, and can be divided into two different types of possible effects; the magneto-transport phenomena in weak magnetic fields which can be described by the semi-classical approach (described in this section), and the magneto-transport phenomena in high magnetic fields which require the quantum mechanical approach (discussed in Section 5.1.3). Before these phenomena are discussed, the density of
states for the case of 2DEGs is explained below.

**Density of states in two-dimensions**

The concept of the density of states (DOS) has been introduced in Section 4.1.1 and in a 3D system the DOS scales with the square root of energy, i.e., $E^{1/2}$ (refer to Eq. 4.16). However, the reduction in the dimensionality of a system of electrons profoundly alters the density of available states, and the DOS of a 2D system is given by (Sze 1981)

$$g(E) = \frac{m^*}{\pi \hbar^2},$$

and is therefore independent of energy. This relation is an important feature when discussing the Shubnikov-de Haas effect, and will be duly re-addressed in later Section 5.1.3.

![Density of States](image)

**FIG. 5.7.** Density of ideal electronic states in two and three dimensions.

The difference in the DOS between the ideal 2D and 3D cases is graphically illustrated in Fig. 5.7. In real semiconductor systems however, the presence of disorder gives rise to localised states which result in a band tail rather than the sharp edges described by the ideal DOS variation, and such behaviour is depicted in Fig. 5.8.

Conduction tends to take place in extended states which exist throughout the crystal, while localised states are bound to a finite region in the crystal and do not
contribute to the electron transport (Anderson 1958). Electrons in localised states can only move by being thermally activated to energy states above the mobility edge $E_m$ or by hopping between localised states at low temperatures (e.g., Shin et al. (1999) have investigated such hopping conduction in Silicon-Germanium crystals). The mobility edge is defined as the energy which separates the regions of extended and localised states, and is an important concept regarding the quantum Hall effect (QHE). Note that thermally activated conduction, characterised by an exponential dependence of the conductivity, has not been analysed in this thesis and thus neglected in this chapter. It has been briefly introduced here only for providing general background.

**Classical magneto-transport in two-dimensions**

Standard magneto-transport measurements are performed on isotropic and homogeneous samples in either the van der Pauw or the Hall bar configuration. The principles of the VDP technique has been already described in Section 4.1.1. In this section, the theoretical aspects of magneto-transport in 2D systems will begin by considering the Hall bar geometry shown in Fig. 5.9.

Theoretical aspects of the magneto-transport properties in 2D structures have been reviewed by Harris et al. (1989) and the theory given in this section largely follows their
treatment. Magneto-transport measurements on 2D structures are generally characterised by a corresponding 2D resistivity tensor \( \rho \). It describes the electrical transport in a material through a generalisation of Ohm’s law, which assumes that the current is proportional to the electric field at all points in the sample for small values of the electric field. Thus for a local current density \( \mathbf{J} \), the local electric field \( \mathbf{E} = \rho \mathbf{J} \). The reciprocal of the resistivity tensor gives the conductivity tensor \( \sigma \). Under the influence of a magnetic field \( B \), the components of these tensors are related via

\[
\sigma_{xx} = \frac{\rho_{xx}}{\rho_{xx}^2 + \rho_{xy}^2} \tag{5.5}
\]

and

\[
\sigma_{xy} = \frac{\rho_{xy}}{\rho_{xx}^2 + \rho_{xy}^2} \tag{5.6}
\]

where use has been made of the relationships \( \rho_{xx} = \rho_{yy} \) and \( \rho_{xy} = -\rho_{yx} \), which is appropriate for an isotropic material. Note that the components of \( \rho \), \( \sigma \) and \( J \) are defined with reference to the \( x \)- and \( y \)-axis of the Hall bar.

The form of the conductivity tensor in a magnetic field can be calculated by assuming a constant relaxation time. The semi-classical equation of motion of an electron in an external electric field has already been given by Eq. 4.3. The addition of a magnetic
field perpendicular to the electric field modifies the equation of motion, which can be expressed as

\[ m^* \frac{dv}{dt} + \frac{m^* v}{\tau} = -e(E + v \times B) \]  (5.7)

where \( v \) is defined as the drift velocity and \( \tau \) denotes the average relaxation time. Since the electric field has only components along the plane, i.e., \( E = (E_x, E_y, 0) \), and the magnetic field has only one component normal to the plane, i.e., \( B = (0, 0, B_z) \), the steady state solution of Eq. 5.7 can be separated into the \( x \)- and \( y \)-directions;

\[ v_x = -\mu E_x - \omega_c \tau v_y \]  (5.8)

and

\[ v_y = -\mu E_y + \omega_c \tau v_x \]  (5.9)

where \( \omega_c \) is the cyclotron resonance frequency and \( \mu \) is the electron mobility (described by Eq. 4.9). The cyclotron resonance frequency represents the circular motion of the electron perpendicular to the magnetic field and is given by

\[ \omega_c = \frac{eB}{m^*}. \]  (5.10)

The cycloidal motion is graphically presented in Fig. 5.10. Electrons moving in empty space and starting from rest under the influence of an electric field in the \( x \)-direction and a magnetic field in the \( z \)-direction, execute cycloidal motion with no net velocity in the \( x \)-direction. Without collisions, the electron motion is oscillatory with angular frequency \( \omega_c \).

Extracting the mobility tensor from Eqs. 5.8 and 5.9, and replacing it into Eq. 4.8 leads to a \( 2 \times 2 \) matrices expression for the conductivity tensor

\[ \sigma = \frac{n_s e^2}{m^*} \begin{pmatrix} \frac{\tau}{1 + \omega_c^2 \tau^2} & -\frac{\omega_c \tau^2}{1 + \omega_c^2 \tau^2} \\ \frac{\omega_c \tau^2}{1 + \omega_c^2 \tau^2} & \frac{\tau}{1 + \omega_c^2 \tau^2} \end{pmatrix} \]  (5.11)

where \( n_s \) is the 2D electron density. Incidentally, dividing Eq. 4.9 by Eq. 5.10 yields the relation \( \omega_c \tau = \mu B \). Thus by using this relation, the above equation can be alternatively
expressed as

\[
\sigma = n_s e \mu \left( \begin{array}{cc}
\frac{1}{1 + \mu^2 B^2} & -\frac{\mu B}{1 + \mu^2 B^2} \\
\frac{\mu B}{1 + \mu^2 B^2} & \frac{1}{1 + \mu^2 B^2}
\end{array} \right)
\]  \hspace{1cm} (5.12)

For a standard Hall bar geometry there is no current path in the \( y \)-direction, therefore

\[
\frac{E_y}{J_x B} = -\frac{1}{n_s e} = R_H
\]  \hspace{1cm} (5.13)

and

\[
\frac{J_x}{E_x} = n_s e \mu = \sigma_{xx}
\]  \hspace{1cm} (5.14)

Hence the result represents the classical Hall effect. However, it has been implicitly assumed that all electrons in the sample move with the same velocity. In practice there is a velocity distribution for electrons due to the various scattering processes.
encountered. Consequently, appropriate averages have to be taken for the collision times over the range of carrier energies. As a result of the energy dependence of \( \tau \), Eq. 5.13 is valid only for the condition \( \mu B \gg 1 \). In the low field limit \( (\mu B \ll 1) \), Eq. 5.13 is redefined as \( R_H = -r_H/n_s e \) where the Hall factor \( r_H \) has values determined by the nature of the scattering mechanisms dominating transport (see Section 4.1.1). In 2DEG structures, the carrier distribution is degenerate in which case the energy averages in Eq. 4.4 become the value of the relaxation time at the Fermi energy. Hence the Hall factor described by Eq. 4.23 reduces to unity, resulting in the carrier mobility being equal to the measured mobility (deduced from Eq. 4.25).

For the purposes of evaluating the measured magneto-transport data, the resistivity is related to the measured resistance by the following expressions:

\[
R_{xy} = \rho_{xy} \tag{5.15}
\]

and

\[
R_{xx} = \rho_{xx} \frac{d_{2,4}}{d_{3,7}} \tag{5.16}
\]

with \( d_{i,j} \) being the sample dimensions between the contacts \( i \) and \( j \) of the Hall bar in Fig. 5.9. Finally, the 2DEG density and mobility can be calculated by

\[
n_s = \frac{B}{e\rho_{xy}} \tag{5.17}
\]

and

\[
\mu = \frac{1}{n_s e \rho_{xx}} \tag{5.18}
\]

respectively. Thus it is possible to determine the electron sheet density by simply measuring the transverse voltage and the electron mobility by additionally measuring the longitudinal voltage of the Hall bar.

5.1.3 Transport in a quantising magnetic field

It has been established in the previous section that electrons are forced to move in circular orbits perpendicular to the applied magnetic field with the frequency \( \omega_c \) described by Eq. 5.10, though the motion parallel to the field is unaffected. Under the influence
of strong magnetic fields, the motion of carriers in the plane becomes quantised and
the system can no longer be treated with the semi-classical approach. The kinetic en­
ergy distribution of the carriers is modified into Landau levels due to the quantisation
and the transport properties need to be explained by using the quantum mechanical
approach. This topic has been covered by several textbooks (Singh 1993; Weisbuch
and Vinter 1991; Ridley 1988), and this section presents a summarised extract from
their treatments. To begin with, the effect of strong magnetic fields on 2D systems and
the formation of Landau levels will be discussed, to facilitate the interpretation of the
Shubnikov-de Haas effect as well as the quantum Hall effect which will be explained
subsequently.

Landau levels

The effect of a magnetic field on the motion of an ideal spinless system of non­
interacting electrons is described by the Hamiltonian,

\[ H = \frac{(p - eA)^2}{2m^*} \]  

(5.19)

where \( A \) is the magnetic vector potential. If the \( A \) is chosen where \( A = (0, Bx, 0) \)
giving rise to a uniform magnetic field in the \( z \)-direction, then Eq. 5.19 is given by

\[ H = \frac{p_x^2 + (p_y - eBx)^2 + p_z^2}{2m^*} \]  

(5.20)

The momentum components \( p_y \) and \( p_z \) commute with both \( H \) and \( x \), and are therefore
constants of the motion which may be written as \( p_y = \hbar k_y \) and \( p_z = \hbar k_z \). Thus

\[ H = \frac{p_x^2 + (\hbar k_y - eBx)^2 + \hbar^2 k_z^2}{2m^*} \]  

(5.21)

This Hamiltonian corresponds to that for a simple harmonic oscillator of angular fre­
quency \( \omega_c = eB/m^* \), centered at \( X = \hbar k_y/eB \). The motion of the electron in the plane
perpendicular to the magnetic field is therefore similar to a simple harmonic oscillator.
The term \( \hbar^2 k_z^2/2m^* \) represents the kinetic energy of the electron in the \( z \)-direction and
is independent of \( B \). In a 2D system however, confinement in the growth (\( z \))-direction
causes this energy to be quantised into a number of two-dimensional electric subbands,
\( E_i \). From this approach, the discrete values for the electron energies can be specified.
by the eigenvalues of the Schrödinger equation, and are given by
\[ E_{i,N} = E_i + \left( N + \frac{1}{2} \right) \hbar \omega_c. \] (5.22)

The first term of the above equation represents the orbital motion of the electrons in the \(x-y\) plane and their allowed states. The second term refers to the energy distribution in the plane perpendicular to the magnetic field. Each electric subband is associated with a set of equally spaced energy levels separated by \(\hbar \omega_c\), called the Landau levels. The orbital motion of the electrons in the magnetic field in the \(z\)-direction is characterised by a classical cyclotron radius of the ground state Landau level (termed the magnetic length),
\[ l_B = \left( \frac{\hbar}{eB} \right)^{1/2}, \] (5.23)

which is independent of material parameters. If the electron spin is taken into account in the definition of Landau levels then an additional energy component, the spin magnetic energy, must be included. Hence
\[ E_{i,N,s} = E_i + \left( N + \frac{1}{2} \right) \hbar \omega_c + s g^* \mu_B B, \] (5.24)

where \(g^*\) is the Landé \(g\)-factor, \(\mu_B\) the Bohr magneton and the spin quantum number \(s = \pm 1/2\). The spin magnetic energy term is called the Zeeman energy, and the effect of spin on the electron energy is to split each Landau level into two energy states of opposite spin alignment.

The magnetic quantisation also has an effect on the density of states. As characterised by Eq. 5.4, the energy independent DOS of 2D electrons is changed into a series of delta-functions positioned at the Landau level energies, i.e.,
\[ g(E) = \sum_{i,N,s} n_L \delta(E - E_{i,N,s}), \] (5.25)

where \(n_L\) is the number of states per Landau level, per spin and per unit area, which is given by
\[ n_L = \left( \frac{m^*}{2 \pi \hbar^2} \right) \hbar \omega_c = \frac{eB}{\hbar}. \] (5.26)
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Here a filling factor term $\nu$ may be introduced which defines the ratio between the carrier density and the density of available states;

$$\nu = \frac{n_s}{n_L} = \frac{h n_s}{e B}.$$  \hspace{1cm} (5.27)

Note that in practice, the density of states function given in Eq. 5.25 will be modified because the motion of the electrons in the plane of the 2D gas is not completely free; the electrons will be scattered, and this process is characterised by the mean free path

$$l_e = v_F \tau_t,$$ \hspace{1cm} (5.28)

where $\tau_t$ is the mean time between collisions (transport relaxation time), and $v_F$ is the Fermi velocity given by

$$v_F = \sqrt{2\pi n_s \left( \frac{\hbar}{m^*} \right)}.$$  \hspace{1cm} (5.29)

The Landau quantisation is therefore expected to be effective if $l_e > l_B$. A more detailed account of Landau quantisation is described below.

The ideal and real DOS of 2D electrons under the influence of quantising magnetic field is graphically illustrated in Fig. 5.11. The real situation compared to the ideal one is somewhat different, where the delta-function-like 2D DOS is in practice broadened due to scattering of electrons by structural disorder and scattering processes present in all samples.

All states in the tails of the broadened Landau levels are localised in space and separated in energy from the extended states by the mobility edge (refer to Section 5.1.2). Assuming the thermal energy and the relaxation time are constant, the overlap of Landau levels depends only on the magnitude of the magnetic field. The available states are occupied up to the Fermi energy and a small change in the magnetic field varies the Fermi level smoothly until the Landau level containing the Fermi energy is completely filled. The variation of the Fermi level remains smooth provided that the applied magnetic field is weak which ensures that successive Landau levels overlap.

When the magnetic field is increased, the cyclotron energy becomes large enough that the broadened Landau levels do not overlap, and the Fermi level is forced to jump to the lowest level of the next Landau level. The criterion necessary for this condition
is given by $\omega_c \tau \geq 1$. Theoretical aspects regarding the variation of the Fermi energy with respect to Landau levels are closely related to quantum effects such as the SdH effect and the QHE, presented in the following sections.

**Shubnikov-de Haas effect**

The oscillation of the longitudinal resistivity ($\rho_{xx}$) of a 2D system as a function of the magnetic field at low temperatures is known as the Shubnikov-de Haas effect. This phenomenon is caused by the changing occupation of Landau levels in the vicinity of the Fermi level. With increasing magnetic field, the Landau levels increase linearly in energy due to the cyclotron energy (see Eq. 5.10), and pass through the Fermi level. This effect manifests itself as oscillations in the resistivity (or conductivity), and Fig. 5.12 depicts the variation of the Landau level energy with the magnetic field. It shows that not only the energy of the Landau levels increase but also the energy separation between consecutive Landau levels.

Maximum conductivity occurs whenever the peak of a Landau level passes through the middle of Fermi level since only the DOS close to the Fermi energy is of interest to the conductivity. As the Landau level moves further up in energy, the DOS around the Fermi level becomes smaller and so does the conductivity, until it reaches a minimum when the Fermi level lies exactly between the two adjacent Landau levels.
The reduction of the 2D DOS means that fewer carriers contribute to transport. In addition, these carriers change from being extended to being localised states, and the conductivity drops to zero when the Fermi level lies in the mobility gap. Note that from Fig. 5.12, the increasing energy separation of the Landau levels results in the frequency of the oscillations becoming continuously lower with increasing magnetic field.

The conductivity obtained from SdH oscillations can be divided into oscillatory and non-oscillatory portions, and it is the oscillatory portion of the conductivity which yields the information on carrier concentrations, carrier mobility, effective masses and scattering times. The full expression for the conductivity of the SdH oscillations is given by (Ando et al. 1982)

\[ \sigma_{xx} = \frac{n_s e^2 \tau}{m^*} \left( \frac{1}{1 + \omega_c^2 \tau^2} \right) \times \left[ 1 - \frac{2 \omega_c^2 \tau^2}{1 + \omega_c^2 \tau^2} \frac{\chi}{\sinh \chi} \exp \left( - \frac{\pi}{\omega_c \tau_q} \cos \left( \frac{2\pi^2 \hbar n_s}{eB} \right) \right) \right] \]  

with

\[ \chi = \frac{2\pi^2 m^* k_B T}{\hbar e B} = \frac{2\pi^2 k_B T}{\hbar \omega_c} \]  

FIG. 5.12. Landau fan diagram including the energy of consecutive Landau levels as a function of the magnetic field.
where $\tau_t$ and $\tau_q$ are the transport and quantum relaxation times, respectively. The damping factor for the amplitude of the oscillations is given by the envelope function $(\chi / \sinh \chi) \exp(-\pi/\omega_c \tau_q)$. Whereas the first term in the envelope function is governed by temperature, the second term involves $\tau_q$ which in turn determines the collision broadening of the Landau levels described later by Eq. 5.39.

While Eq. 5.30 provides a theoretical expression for the conductivity, the experimentally measured quantity is always the resistivity. In a magnetic field, both conductivity and resistivity must be expressed as two-dimensional tensors since the Hall effect yields non-zero values for $\rho_{xy}$ and $\sigma_{xy}$. In order to obtain the theoretical expression for $\rho_{xx}$, the resistivity tensor needs to be inverted. This gives

$$\rho_{xx} = \sigma_{xx} \left( \rho_{xx}^2 + \rho_{xy}^2 \right). \quad (5.32)$$

The transverse Hall resistivity can be written as

$$\rho_{xy} = R_H B$$
$$= \frac{\mu_H B}{\sigma_{xx}(B = 0)} \quad (5.33)$$
$$= \rho_{xx}(B = 0) \mu_H B$$

where $\mu_H$ is the Hall mobility. Using Eq. 5.33, we can write

$$\rho_{xx}^2 + \rho_{xy}^2 = \rho_{xx}^2 (B = 0) \times \left[ 1 + \frac{2(\rho_{xx} - \rho_{xx}(B = 0))}{\rho_{xx}(B = 0)} + \frac{(\rho_{xx} - \rho_{xx}(B = 0))^2}{\rho_{xx}^2 (B = 0)} + \mu_H^2 B^2 \right] \quad (5.34)$$

and by assuming that

$$\mu_H B \gg \frac{\rho_{xx} - \rho_{xx}(B = 0)}{\rho_{xx}(B = 0)} \quad (5.35)$$

which is a good approximation in high mobility samples, Eq. 5.34 becomes

$$\rho_{xx}^2 + \rho_{xy}^2 \approx \rho_{xx}^2 (B = 0) \left[ 1 + \mu_H^2 B^2 \right]. \quad (5.36)$$

By combining Eq. 5.30, Eq. 5.32 and Eq. 5.35, and by noting that $\omega_c \tau_t = \mu_H B$, the resistivity can be finally described by

$$\rho_{xx} = \rho_{xx}^2 (B = 0) \frac{n_e e^2 \tau_t}{m^*}$$
$$\times \left[ 1 - \frac{2\omega_c^2 \tau_t^2}{1 + \omega_c^2 \tau_t^2} \frac{\chi}{\sinh \chi} \exp\left(-\frac{\pi}{\omega_c \tau_q}\right) \cos \left(\frac{2\pi^2 h n_e}{eB}\right) \right] \quad (5.37)$$
The most surprising aspect of this transformation is that the resistivity is proportional to the conductivity due to the approximation of Eq. 5.36, and the peaks in the resistivity and conductivity correspond to the point at which the Landau level passes the center of the Fermi level. The whole equation can be viewed as a cosine oscillation, whose frequency is determined by the sheet density and the magnetic field, and whose amplitude is governed by an exponential envelope function which is dependent on the $B$-field and shrinks with increasing temperature. Note that Eq. 5.30 and Eq. 5.37 have been obtained by assuming a single fundamental electric subband in the potential well, since by introducing extra subbands the contribution from higher harmonic terms needs to be incorporated, making the analysis complicated. From Eq. 5.37, all important transport parameters can be extracted and procedures for calculating them will be presented later in Section 5.1.4.

It should be pointed out that experimentally, observing oscillations can be made difficult by two mechanisms; (a) the collision broadening of the Landau levels, and (b) the thermal broadening of the Landau levels.

In order to resolve the oscillations, the collision broadening of the Landau levels, given by $\Gamma$ which is the full width at half maximum (FWHM), should be less than the separation of the levels, i.e.,

$$\Gamma \leq \hbar \omega_c .$$

(5.38)

Alternatively, $\Gamma$ can be determined according to the principle of uncertainty by

$$\Gamma = \frac{\hbar}{\tau_q}$$

(5.39)

which clearly demonstrates that the broadening of the Landau levels is only dependent on the existing scattering processes in the system. Substituting Eq. 5.39 into Eq. 5.38 results in the condition for oscillations to be observed, which is

$$\omega_c \tau_q \geq 1$$

(5.40)

or

$$\mu B \geq 1 .$$

(5.41)
The second condition for quantum effects to take place can be explained by considering the smearing of the Landau levels by temperature. If the thermal energy exceeds the Landau level spacing, the levels will overlap, and from the definition of $\chi$ in Eq. 5.31, the criterion

$$\hbar \omega_c \geq 2\pi^2 k_B T$$

and thus

$$B \geq \frac{2\pi^2 m^* k_B T}{e\hbar^2}$$

must be satisfied. In summary, the oscillations can only be resolved at high magnetic fields and low temperatures, and samples must possess high mobility. Because of the high electron effective mass and a large level of disorder in AlGaN/GaN materials, the electron mobilities in AlGaN/GaN 2DEGs are much lower than those of AlGaAs/GaAs samples (e.g., Harris et al. (1987) achieved mobilities of over $3 \times 10^6$ cm$^2$ V$^{-1}$ s$^{-1}$). The experimental conditions (e.g., $T < 0.1$ K and $B > 10$ T) are certainly achievable in laboratories but well-resolved SdH oscillations in AlGaN/GaN heterostructures could not be observed easily due to difficulties in growing high quality AlGaN/GaN materials. Thus, the improved growth of epitaxial layers using MOCVD and MBE is found to be crucial, since as mentioned earlier in Section 5.1.1, interface roughness scattering plays an important role in limiting the electron mobility at low temperatures.

Recently though, the SdH oscillations in AlGaN/GaN 2D structures have been observed by a number of authors (Elhamri et al. 1998; Smorchkova et al. 1999; Elsass et al. 1999; Shah et al. 2000) with sample mobilities in the range $7000 - 20,000$ cm$^2$ V$^{-1}$ s$^{-1}$ at 1.4 K), and an example of such SdH oscillations for the Al$_{0.18}$Ga$_{0.82}$N/GaN heterostructure with the sheet electron density and mobility of $6.2 \times 10^{12}$ cm$^{-2}$ and $10300$ cm$^2$ V$^{-1}$ s$^{-1}$ respectively, is reproduced in Fig. 5.13 (Wang et al. 2000). As can be seen from the figure, the oscillations indicate the definite presence of a 2DEG and are observed at fields as low as 2 T. At higher fields of above 8 T, even spin-splitting can be observed. As temperature at which the measurement was taken increased, the amplitude of the oscillation decreased as predicted by theory in Eq. 5.37.

The periodic nature of the oscillations and the temperature dependence of the oscillation amplitude can be used to extract material parameters such as $n_s$, $\mu$, $m^*$, $\tau_t$.
and $\tau_i$, and the description of calculation procedure is presented later in Section 5.1.4. In addition, the amplitude of the SdH oscillations can be used as a thermometer for the electron temperature, from which an energy loss mechanism of hot electrons at low temperatures is investigated (discussed in Chapter 6).

Finally, the effect of parallel conduction present in 2DEGs needs to be considered. The interpretation of the magneto-transport properties of 2D structures becomes complicated by it and earlier efforts have developed treatments to correctly model the presence of secondary conducting channel (Chambers 1952; Petritz 1958). Various types of parallel conduction are considered, such as the possibility of more than one subband being occupied and the parallel conduction in the barrier layer. Kane et al. (1987) employed a two-band model, where in the low temperature, degenerate limit, the sheet conductivity, $\sigma_i$, of each channel, index $i$, is given by the tensor relation:

$$
\sigma_i = \frac{n_i e \mu_i}{(1 + \mu_i^2 B^2)} \begin{vmatrix} 1 & -\mu_i B \\ \mu_i B & 1 \end{vmatrix},
$$

(5.44)

where $n_i$ and $\mu_i$ are the 2D carrier density and the mobility, respectively, of individual channels. A characteristic prediction of these calculations is an approximately parabolic increase of $\rho_{xx}$ with $B$ at low fields, and this behaviour has been observed
in a variety of AlGaN/GaN heterostructures (Shah et al. 2000; Saxler et al. 2000). The secondary conducting channel is generally associated with the upper barrier layer in conventional GaAs/AlGaAs compounds. However, as shown earlier in Fig. 5.3, the heavy electric fields generated by polarisation effects in AlGaN/GaN pushes the conduction band of AlGaN above the Fermi level, and the parallel conduction in the barrier region is unlikely (Contreras et al. 2001); instead, a secondary conducting channel is thought to be the GaN layer.

Quantum Hall effect

Another important phenomenon that arises due to the quantisation of the energy spectrum of the electron motion in strong magnetic fields, is the quantum Hall effect, first observed by von Klitzing et al. (1980). They reported that the measured Hall resistance deviates from the predicted classical relation of Eq. 5.17 to form a series of quantised plateaus with Hall resistances given by

\[ R_{xy} = \frac{\hbar}{\nu e^2} \]  

(5.45)

where \( \nu \) is the Landau level filling factor described by Eq. 5.27. Plateaus and zeros of dissipative resistance only occur when the filling factor \( \nu \) is an integer. This is the integer QHE and for its discovery von Klitzing was awarded the Nobel Prize in physics in 1985. A most astonishing aspect of the discovery is the unprecedented accuracy with which Eq. 5.45 is fulfilled (better than 1 part in \( 10^8 \)) irrespective of crystal imperfections and sample geometry.

The QHE is governed by similar principles to the SdH effect, and can be understood by considering the existence of extended and localised states (previously mentioned in Section 5.1.2). Fig. 5.14 shows the relation between the DOS of the Landau levels and the longitudinal and Hall resistivity. As the Fermi level is increased while located in a region of extended states, \( \sigma_{xy} \) is expected to increase due to the increase in total number of occupied extended states. With the Fermi energy located in a localised states region, \( \sigma_{xy} \) is not expected to change its value since the number of occupied extended states does not change. This explanation accounts only for the formation of the plateaus seen in the QHE but not why the Hall resistance has the precise value of
FIG. 5.14. Density of states (top), longitudinal (middle) and transverse (bottom) resistivity for a single Landau level as a function of the filling factor. The shaded areas indicate the localised states.

$h/\nu e^2$.

With the Fermi energy pinned in the localised states region, it might be expected that the Hall resistance value would change significantly (the classical Hall resistance depends on the density of mobile carriers) from the quantised value. Aoki and Ando (1981) have performed calculations of the current flow and obtained the result that the carriers in the extended states make up in current for the localised carriers by increasing their own velocity, and hence suggested a possible explanation for this paradox, which is as follows; the potentials which localise some of the electrons also accelerate the remaining carriers so that the reduction in the number of mobile carriers is exactly
compensated by their increase in velocity, thereby keeping the total current unchanged.

### 5.1.4 Calculation procedures

The previous section demonstrated that investigating the SdH oscillations is a powerful tool in examining transport properties of 2D systems, and samples studied in this chapter have been mainly characterised by utilising the SdH effect. Therefore, this section describes various methods to determine material parameters such as the sheet electron density $n_s$, electron mobility $\mu$, electron effective mass $m^*$, transport relaxation time $\tau_t$ and quantum relaxation time $\tau_q$.

**Electron density and mobility**

The periodicity of longitudinal resistivity oscillations in the reciprocal magnetic field is a signature of the presence of 2DEG, and can be utilised to calculate the 2D sheet carrier density. The DOS of 2D electrons has been given by Eq. 5.4 and found to be independent of energy. Hence in the absence of magnetic field, the Fermi level is defined as

$$E_F = \frac{2h^2 \pi}{m^*} n_s. \quad (5.46)$$

If the resistivity minimum at $B_N$ corresponds to $N$ Landau levels below the Fermi energy, then $E_F$ in the presence of magnetic fields becomes

$$\left(N + \frac{1}{2}\right) \hbar \omega_c = E_F = \frac{2h^2 \pi}{g_sg_v m^*} n_s, \quad (5.47)$$

where $g_s$ and $g_v$ are spin and valley degeneracy, respectively. For successive Landau levels, the following relationship can be obtained,

$$\Delta(1/B) = \frac{1}{B_{N+1}} - \frac{1}{B_N} = \frac{e\hbar}{m^* E_F}, \quad (5.48)$$

which results in

$$\Delta(1/B) = \frac{g_sg_v e}{\hbar n_s}. \quad (5.49)$$

Hence by plotting the reciprocal magnetic field at which the $N$th minimum occurs, against the number of the minimum, a straight line will be exhibited. The gradient of
the line, defined as the fundamental field $B_f$, yields the carrier density by the equation

$$n_s = \frac{g_s g_v e B_f}{h}.$$  \hspace{1cm} (5.50)

This method can only be carried out when only one subband is occupied within the 2DEG. Additional subbands induce the SdH oscillations to be the sum of as many sine waves with different frequencies as there are occupied subbands, and the plot of $N$ vs $B^{-1}_N$ will not be represented by a straight line.

Having determined the sheet density, the electron mobility is found by simply applying Eq. 5.18 for the longitudinal resistivity at low magnetic field. Thus

$$\mu = \frac{1}{n_s e \rho_{xx}(B = 0)},$$  \hspace{1cm} (5.51)

where $\rho_{xx}(B = 0)$ can be obtained from the measured resistance by using Eq. 5.16.

It should be pointed out that the overall gradient of the Hall resistance (from the QHE) can also be used to determine the carrier density from Eq. 5.17, and subsequently the Hall mobility.

Effective mass

The standard treatment of the SdH effect in 2DEG systems is given in the review by Ando et al. (1982) and Coleridge et al. (1989). For the case where the carrier density of the 2DEG is such that only one electric subband is occupied, the oscillating portion of the magnetoresistance can be expressed as

$$\frac{1}{2} \frac{\Delta \rho_{xx}}{\rho_0} = \frac{2}{\sinh \chi} \frac{\chi}{\omega_c \tau_q} \exp \left( \frac{-\pi}{\omega_c \tau_q} \right) \cos \left( \frac{2 \pi \xi}{h \omega_c} - \pi \right),$$  \hspace{1cm} (5.52)

where $\rho_0$ is the zero-field resistivity, $\xi$ is the energy difference between the Fermi level and the minimum of the first electric subband $E_1$ given by $\xi = E_F - E_1 = \pi h^2 n_s / m^*$, and other symbols have been previously introduced.

The effective mass can be determined by examining the variation of amplitudes of the SdH oscillations with temperature. Elhamri et al. (1998) have employed the approximation $\sinh \chi \approx \exp \chi / 2$, and expressed the amplitude $A$ of the SdH oscillation at a given magnetic field as

$$\ln \left( \frac{A}{T} \right) \approx C - \frac{2 \pi^3 k_B m^*}{e h B} T,$$  \hspace{1cm} (5.53)
where $C$ is a temperature independent term. Hence, a plot of $\ln(A/T)$ versus $T$ yields a straight line with a slope of $(-2\pi^2k_Bm^*/e\hbar B)$ from which $m^*$ can be evaluated.

Much work has been devoted to GaN and related materials in determining physical parameters, but only a few reports of the effective mass value has appeared. Early reported values for $m^*$ varied from $0.19m_0$ to $0.27m_0$ (Kosicki et al. 1973; Barker and Ilegems 1973; Rheinländer and Neumann 1974). Recent reports by Drechsler et al. (1995) and Wang et al. (1996) using cyclotron resonance obtained a value of $0.20m_0$ and $0.23m_0$, respectively. The effective mass has also been determined by analysing the temperature dependence of the SdH oscillation amplitude at a fixed magnetic field, where Elhamri et al. (1998), Wang et al. (2000) and Saxler et al. (2000) reported $m^*$ of $0.18m_0$, $0.19m_0$ and $0.21m_0$, respectively. These values are compared with our experimental results later in Section 5.2.2.

**Transport and quantum relaxation time**

The relaxation times (alternatively known as scattering times or lifetimes) can be divided into two classes: the transport relaxation time $\tau_t$ and the quantum relaxation time $\tau_q$. The quantum relaxation time is a measure of the collision broadening of the Landau levels and is related to the half-width of the broadened Landau level through $\Gamma_{1/2} = \hbar/2\tau_q$ (Harrang et al. 1985). The transport relaxation time is governed by the Boltzmann equation (Singh 1993), and is defined as the rate at which the net momentum of all electrons is randomised. It is related to the conductivity of the 2DEG by Eq. 4.7 and thus can be easily calculated by using the relation

$$\tau_t = \frac{m^*\mu}{e}. \quad (5.54)$$

The difference between $\tau_q$ and $\tau_t$ can be better distinguished by formulations which integrate the quantum mechanical transition rates $Q(\theta)$ over all scattering angles $\theta$ (Coleridge 1991), i.e.,

$$\frac{1}{\tau_q} = \int_0^\pi Q(\theta) \, d\theta \quad (5.55)$$

and

$$\frac{1}{\tau_t} = \int_0^\pi Q(\theta) (1 - \cos \theta) \, d\theta, \quad (5.56)$$
In Eq. 5.55, \( Q(\theta) \) is proportional to the probability of scattering through an angle \( \theta \), thus taking into account both small- and large-angle scattering, i.e., all scattering events contribute equally to \( \tau_q \). However, because of the weighting of the transition rates with the momentum loss factor \((1 - \cos \theta)\), \( \tau_t \) is insensitive to small-angle scattering while dominated by large-angle scattering. Note that since the electron distribution at low temperatures in the samples studied is described by degenerate Fermi-Dirac statistics, it is not necessary to perform an energy average in Eqs. 5.55 and 5.56, and the relaxation times are simply evaluated at the Fermi energy.

The significance of these findings is that \( \tau_q \) and \( \tau_t \) are equal for short-range (large-angle) scattering such as by interface charges or ionised background impurities. In contrast, for long-range (small-angle) scattering such as by remote impurities, \( \tau_t \) becomes larger than \( \tau_q \). Hence it is possible to obtain information on the scattering mechanisms by examining the ratio \( \tau_t/\tau_q \) (called the Dingle ratio). Das Sarma and Stern (1985) have pointed out that the Dingle ratio will be close to unity for low mobility materials where short-range scattering is predominant, and much bigger than unity (above 10) for high quality specimens where long-range scattering prevails.

As mentioned previously, \( \tau_t \) can be determined experimentally using Eq. 5.54. The quantum relaxation time can be obtained from the amplitude of the SdH oscillations at a given temperature using a Dingle plot (Coleridge et al. 1989). The resistance amplitude \((\Delta R)\) of the SdH oscillations is given by

\[
\Delta R = 4R_0 \frac{\chi}{\sinh \chi} \exp \left( \frac{-\pi}{\omega_c \tau_q} \right),
\]

where \( R_0 \) is the zero-field resistance. If the logarithm of the amplitude, divided by the thermal damping term \( \chi/\sinh \chi \) to correct for temperature and \( R_0 \), is plotted against \( 1/B \), the quantum relaxation time can be evaluated from the slope of the resulting straight line described by

\[
\ln \left( \frac{\Delta R \sinh \chi}{\chi} \right) = 4 - \left( \frac{\pi m^*}{e \tau_q} \right) \frac{1}{B},
\]

with an intercept (at \( 1/B = 0 \)) of 4. In reality, the Dingle plot deviates from the behaviour predicted by theory (Coleridge 1991); inhomogeneities can produce a plot with two or more beating oscillations, a curvature in the plot indicates field-dependent
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de-phasing from a distribution of densities in 2DEGs, resulting in an intercept greater than 4, and the presence of parallel conduction brings the intercept below 4, though the slope of the line still gives the value of $\tau_q$ to a good approximation.

<table>
<thead>
<tr>
<th>Literature</th>
<th>$\mu$ (cm$^2$ V$^{-1}$ s$^{-1}$)</th>
<th>$\tau_t$ (ps)</th>
<th>$\tau_q$ (ps)</th>
<th>$\tau_t/\tau_q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elhamri et al. (1998)</td>
<td>7480</td>
<td>0.77</td>
<td>0.13</td>
<td>5.9</td>
</tr>
<tr>
<td>Saxler et al. (2000)</td>
<td>19000</td>
<td>2.34</td>
<td>0.50</td>
<td>4.7</td>
</tr>
<tr>
<td>Shah et al. (2000)</td>
<td>8000</td>
<td>1.04</td>
<td>0.15</td>
<td>6.9</td>
</tr>
<tr>
<td>Braña et al. (2000)</td>
<td>2078</td>
<td>0.26</td>
<td>0.05</td>
<td>5.2</td>
</tr>
</tbody>
</table>

Table 5.2 lists a collection of relaxation times data recently reported by various groups. As can be seen from the table, the Dingle ratio values are found to be comparable irrespective of different electron mobilities represented by $\tau_t$. The values are relatively low compared to high mobility materials such as AlGaAs/GaAs heterostructures implying more large-angle scattering; however, the difference between $\tau_t$ and $\tau_q$ can be attributed to the presence of additional small-angle scattering, likely to be due to charged defects at the epilayer/substrate interface. Wang et al. (2000) compared the $\tau_t/\tau_q$ ratio of AlGaN/GaN systems between structures with an undoped AlGaN and a deliberately Si-doped AlGaN layer, and reported much lower $\mu$ and $\tau_t/\tau_q$ for the doped sample. They attributed this decrease to a rise in the number of scatterers due to Si doping, where, as discussed earlier in Section 4.2.2, intentional Si doping for n-GaN may produce both donor and acceptor levels, which when ionised, can act as scattering centres. The relaxation times of the samples studied in this chapter have been evaluated, and by comparing them to the results of Table 5.2, the significance of evaluated values will be discussed later in Section 5.2.2.

5.2 Results and discussion

This section presents the results of transport properties of AlGaN/GaN heterostructures grown on sapphire by MBE and MOCVD, based on interpretations of the Hall and low temperature SdH measurements data. Descriptions of the Hall mobility variation with temperature are given in Section 5.2.1, from which the general quality of
the samples can be assessed regarding the scattering processes present in 2D structures. Low temperature magneto-transport experiments, utilising the QHE and the SdH effect, have been commonly used to investigate the properties of 2DEGs in AlGaAs/GaAs heterojunctions, but it is only recently that reports of similar studies on a limited number of AlGaN/GaN layers have appeared. From low temperature measurements, the presence of a 2DEG can be confirmed. In addition, material parameters such as $m^*$, $\tau_q$ and $\tau_t$ can be determined. In this chapter, a variety of samples has been characterised to look for systematic variations, and in particular, the Dingle ratio ($\tau_t/\tau_q$) values have been investigated which provide information on the type of dominant scattering mechanism present in the samples at low temperatures. Such analysis of magneto-transport data below 10 K will be presented in Section 5.2.2.

5.2.1 Temperature dependent Hall measurements

Temperature dependent Hall measurements have been conducted on AlGaN/GaN 2DEG samples (VDP squares) using the CCC system (described in Section 3.1.1) at temperatures in the range 10 – 300 K, and the corresponding results are presented in this section. A list of 2DEG samples and their details has been given earlier in Table 3.2 in Section 3.2.2. Only samples D952 and G99 have been investigated by the Hall measurements. G91 exhibited prolonged drift with time during the measurement readings, making it difficult to measure voltages correctly and reliably, and hence the G91 data were neglected. C251199 and J401 were not included in the Hall measurements due to lack of time available before a visit to Grenoble for low temperature magneto-transport experiments, and because of the difference between the CCC and the VTI in the socket arrangement that houses the samples.

As mentioned previously in Section 5.1.1, Yu and Brennan (2001) have calculated the electron mobility of individual scattering mechanism present in 2DEGs, and for a Al$_{0.2}$Ga$_{0.8}$N/GaN HEMT structure with $t_{\text{AlGaN}}$ of 50 nm, they obtained the resultant mobility of about 9000 and 1600 cm$^2$V$^{-1}$s$^{-1}$ at temperatures of 77 and 300 K, respectively (refer to Fig. 5.6). The measured Hall mobility data are plotted in Fig 5.15 and their result is also included in the figure for comparison.

The mobility variation of G99 and D952 exhibits similar dependence to the theor-
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FIG. 5.15. A plot of electron Hall mobility as a function of temperature for samples G99 and D952. The solid line is the theoretical variation calculated by Yu and Brennan (2001) for a Al$_{0.2}$Ga$_{0.8}$N/GaN HEMT structure.

Experimentally, the Hall values are found to be much lower. At 300 K, the mobility values of G99 and D952 are approximately 1000 and 900 cm$^2$V$^{-1}$s$^{-1}$ respectively, while at 77 K, the mobilities correspond to 4370 and 1790 cm$^2$V$^{-1}$s$^{-1}$ respectively. The difference between the experimental and theoretical values is smaller at higher temperatures, and above 200 K, the dominant mobility limiting mechanism is expected to be polar optical scattering. Although the overall trend of the mobility variation is characteristic of 2DEGs in general, the large discrepancy at low temperatures needs to be accounted for. Yu and Brennan (2001) attributed the low temperature mobility to scattering by interface roughness, where interface roughness parameters $L = 1.5$ nm and $\Delta = 0.1$ nm are assumed. As mentioned previously in Section 5.1.1, the mobility limited by interface roughness scattering is inversely proportional to $L^2 \Delta^2$, and small changes in these parameters can induce a large decrease in the mobility. Neglecting relatively small differences in the Al composition and the barrier thickness between the samples, it is therefore possible that G99 and D952 may be governed by a larger degree of interface roughness.
Note that since G99 is of a HEMT structure with an intentionally doped region 10 nm from the interface, whereas the structure of D952 consists of an undoped AlGaN layer, comparing G99 results to the theoretical values (based on modulation-doped structures) is expected to yield a more accurate investigation. Apart from interface roughness scattering, scattering by ionised centres could also play an important role. The Si doping level of G99 was about $1.2 \times 10^{19}$ cm$^{-3}$, while for the calculated results, the doping level was assumed to be $3 \times 10^{18}$ cm$^{-3}$. In theory, all of the dopants are assumed to be ionised and transfer free electrons to the 2DEG. For the case of G99, the Si doping can produce ionised donors, neutral donors which lie below the Fermi level, and acceptors which may or may not be ionised. A consequence of this is that some ionised acceptors may act as extra scattering centres and contribute further to the reduction in mobility. The mobility values of G99, albeit about 50% lower than theory, are much higher than those of D952 which is undoped, and this may be due to a greater level of compensation in D952. This is reasonable since the high degree of compensation in GaN layers has already been demonstrated from the results presented in Section 4.2.3. In summary, a combination of increased scattering by rougher interfaces and a higher density of ionised scatterers could be partly responsible for the low mobility observed in the measured samples. In addition, it is possible that structural quality related processes such as scattering by threading dislocations and grain boundaries may have a profound effect on limiting the low temperature mobility. This is consistent with the results discussed previously in Section 4.2.3, where these scattering mechanisms were also found to play an important role in degrading mobility in bulk GaN samples.

Unfortunately, an accurate interpretation of the scattering processes involved in AlGaN/GaN 2DEGs cannot be obtained based on the Hall results alone. It should be pointed out that a detailed understanding of nitride-based materials and their physical properties has proven to be difficult over the years due to the high density of structural defects arising from non-optimised growth techniques, thereby resulting in material characterisation being very much sample dependent. In addition, a wider range of samples needs to be investigated in order to determine systematic behaviour in transport properties. The low temperature magneto-transport results presented in
Section 5.2.2 aim to provide more reliable findings by studying the $\tau_I/\tau_q$ ratio over a wider variety of samples, and further discussions on scattering in AlGaN/GaN 2DEG systems will be given later.

![Graph of electron Hall concentration as a function of temperature for samples G99 and D952.](image)

**FIG. 5.16.** A plot of electron Hall concentration as a function of temperature for samples G99 and D952.

Fig 5.16 plots the temperature dependence of electron Hall concentration for the samples G99 and D952. The samples exhibit a confined 2D electron gas characterised by a nearly constant, temperature independent carrier concentration, though some 15% increase is observed from 77 to 300 K for G99. The slight activation is an indication of parasitic conduction in the bulk GaN buffer layer, and a GaN base with insulating properties would be required to eliminate parallel conduction effects (Zhang et al. 1998). Below 77 K, both samples display almost constant variation with a change of less than 5%, and the 10 K electron sheet density of about $4.4 \times 10^{12}$ and $8.4 \times 10^{12} \text{ cm}^{-2}$ is observed for G99 and D952, respectively. Modulation doping was employed for G99, and with an intentional Si doping density of $1.2 \times 10^{19} \text{ cm}^{-3}$ in the structure, a large 2D sheet electron density $n_s$ may be due to the charge transfer from the AlGaN layer. However, D952 was grown with an undoped AlGaN barrier, and yet the obtained $n_s$ is found to be nearly twice the measured value in G99. Clearly, it can be seen that
the charge transfer from the AlGaN barrier alone cannot provide an explanation for the above finding, and the large 2D electron densities in the samples are likely to be induced by additional sources.

As mentioned theoretically in Section 5.1.1, the high \( n_s \) values are expected to be induced by spontaneous and piezoelectric polarisation effects in AlGaN/GaN heterostructures. The lattice mismatch between the GaN and AlGaN layers and internal strain in the barrier increases with increasing \( x \), resulting in increased contributions from both spontaneous and piezoelectric polarisation. Hence, the polarisation induced 2D electron density is expected to be larger in D952 than in G99, where, although the samples have been grown by MOCVD with similar AlGaN barrier thicknesses, the Al content of 0.23 was used during D952 growth, which is more than twice the value of G99. In the next section, further comparisons will be made with the transport results obtained from the low temperature magneto-transport measurements, from which the role of polarisation fields on the formation of 2DEG in each measured sample is discussed.

5.2.2 Low temperature magneto-transport measurements

The magneto-transport measurements have been carried out at low temperatures and under high magnetic fields, and a description of experimental procedures for such measurements is given earlier in Chapter 3. All 2DEG samples were measured at 4.2 and 1.3 K using the VTI system (described in Section 3.1.2), with the magnetic field sweeping up to 15 T. Standard a.c. lock-in measurement techniques have been employed for data acquisition of the samples which are mostly of a Hall bar configuration and contacted with Ti/Al (refer to Section 3.1.4 for a detailed account). The driving current of 100 nA (at 10.96 Hz) was typically applied to minimise electron heating effects, and from preliminary studies, these effects were found to be negligible below about 1 \( \mu \)A. Oscillations in longitudinal magneto-resistivity have been observed in all samples, and by analysing the obtained data, transport parameters including \( n_s \), \( \mu \), \( \tau_2 \) and \( \tau_q \), are determined and presented in this section. Samples J401 and G99 have been further characterised at higher temperatures (up to 10 K) using the VTI, and at lower temperatures (down to 50 mK) using the DLF system (described in Section 3.1.3). The
obtained variation of oscillation resistivity with temperature has been investigated to extract $m^*$, and is also included here.

**Resistivity variation with magnetic field**

The longitudinal magneto-resistivity data of J401 is plotted in Fig. 5.17 for temperatures of 4.1 and 1.3 K. As can be seen from the figure, strong Shubnikov-de Haas oscillations are clearly observed, indicating the presence of a 2DEG at the AlGaN/GaN interface. As has been discussed theoretically in Section 5.1.3, the SdH oscillations are described by Eq. 5.37 where the frequency is determined by $n_s$ and $B$, and where the amplitude is governed by an exponential envelope function which is dependent on $B$, $\tau_q$ and $T$. As can be seen from the figure, the effect of the thermal damping factor $\chi/\sinh \chi$ in Eq. 5.37 is to reduce the oscillation magnitude with increasing temperature.

![Fig. 5.17](image)

**FIG. 5.17.** A plot of magneto-resistivity $\rho_{xx}$ as a function of magnetic field $B$ for J401 ($\text{Al}_{0.18}\text{Ga}_{0.82}\text{N/GaN}$), measured at 4.1 (solid line) and 1.3 K (dotted line).

The 1.4 K carrier concentration of the sample obtained from the periodicity of the SdH oscillations in reciprocal magnetic field, was found to be $5.8 \times 10^{12} \text{ cm}^{-2}$ with a
corresponding $\mu$ of about 9950 cm$^2$V$^{-1}$s$^{-1}$. Compared to high quality GaAs/AlGaAs 2DEGs, these values are a relatively high concentration and low mobility for SdH measurements, but the oscillations are clearly resolved, and spin-splitting is even observed above $B = 8$ T. The onset of the oscillation occurs at around 2 T which indicates good material quality, and is lower than previously reported AlGaN/GaN heterostructures with mobilities in excess of $10^4$ cm$^2$V$^{-1}$s$^{-1}$ (Gaska et al. 1999; Saxler et al. 2000; Elsass et al. 1999). It should be pointed out that depending on which pair of contacts is used, the recorded mobility calculated from the low-field resistivity spans the range 8120 – 28250 cm$^2$V$^{-1}$s$^{-1}$, suggesting that the quality of material varies within the sample. This variation in mobility (or resistivity) was evident in the rest of the samples, though the difference in mobility in these cases were markedly lower than J401 ($\leq 20\%$). As for the carrier density, no variation was observed throughout the samples. The non-uniformity aspect will be further discussed regarding the nature and distribution of scatterers, by studying the relationship between $\tau_l$ and $\tau_q$ later in this section.

![Graph of Hall resistance vs. magnetic field](image)

**FIG. 5.18.** A plot of Hall resistance $R_{xy}$ as a function of magnetic field $B$ for the samples.

Fig. 5.18 shows the Hall resistance $R_{xy}$ variation with $B$ for the measured samples.
Considering J401, the Hall resistance also exhibited plateaus at the minima in $\rho_{xx}$ (quantum Hall effect), which supports the experimental finding that a 2DEG is formed at the AlGaN/GaN interface. The plateaus are not as well defined as those seen in good quality AlGaAs/GaAs samples, and this could suggest the presence of a parallel conduction path. However, the carrier density calculated from the Hall gradient ($5.6 \times 10^{12}$ cm$^{-2}$) is close to the SdH carrier density, which implies the absence of significant parallel conduction. This is confirmed by the behaviour of the $\rho_{xx}$ minima, which continue to decrease with increasing $B$, almost reaching zero at 15 T (Reed et al. 1986).

The definition of Hall plateaus are much weaker in other samples than in J401, and parallel conduction effects are likely to be stronger, particularly in samples G91 and D952 which do not exhibit any plateaus. The Hall resistance results can be further compared with the magneto-resistivity variations which are plotted in Fig. 5.19, 5.20, 5.21 and 5.22 for samples C251199, G99, G91 and D952, respectively.

![Graph](image)

**FIG. 5.19.** A plot of magneto-resistivity $\rho_{xx}$ as a function of magnetic field $B$ for C251199, measured at 4.1 K.

From the oscillation curves, comparisons can be made in terms of the field at which the oscillations start to appear ($B_{\text{onset}}$), and the amplitude and the shape of the
oscillations. $B_{\text{onset}}$ occurs at around 2, 6.5, 4, 7.5 and 8 T for J401, C251199, G99, G91 and D952, respectively. As mentioned earlier in Section 5.1.3, the oscillations appear in the quantum regime where the conditions $\omega_c\tau_q \gg 1$ (Eq. 5.40) and $\mu B \gg 1$ (Eq. 5.41) are satisfied. Hence, oscillations can be observed earlier in higher mobility samples with smaller scattering rates. The oscillation amplitude is also controlled by the quantum lifetime which is a measure of collision broadening of the Landau levels. Thus from Eq. 5.37, it can be seen that greater amplitudes are represented by larger $\tau_q$, suggesting qualitatively that J401 and G99 are likely to be associated with bigger $\tau_q$. This prediction, along with systematic behaviour of $B_{\text{onset}}$, is considered and given more fully later.

As mentioned earlier in Section 5.1.3, the effect of a parallel conducting channel on 2DEG transport is manifested by an approximately parabolic variation of $\rho_{xx}$ with $B$, and this trend is clearly observed in C251199. This parabolic increase has been reported by (Shah et al. 2000; Contreras et al. 2001) and is thought to be due to the parallel conduction in the GaN layer. Referring to Table 3.2, C251199 contains a thick C-doped GaN buffer layer (1.4 μm), on top of which a thin (0.18 μm) GaN
channel layer is grown. Carbon was chosen as the compensating dopant for achieving resistivities greater than $10^6 \, \Omega \, \text{cm}$ (Webb et al. 1999). The insulating property of the thick GaN layer is expected to prevent parallel conduction through the GaN buffer layer, and thus in C251199's case, the secondary conducting channel is expected to be the undoped $n$-type GaN channel region.

The shape of $\rho_{xx}$ is rather different in the remaining samples (G91, G99 and D952), where the general behaviour is described by a decreasing $\rho_{xx}$ with $B$, which presents superimposed SdH oscillations at high magnetic fields and a fast decrease with $B$ at very low magnetic field. The continuous decreasing component of $\rho_{xx}$, with a parabolic negative magneto-resistivity in the low $B$-field range, has been observed in high mobility GaAs/AlGaAs (Choi et al. 1986). This phenomenon has also been reported by Braña et al. (2000) in AlGaN/GaN heterostructures, who have attributed it to diffusive electron-electron interactions. The fast decrease of $\rho_{xx}$ at very low magnetic field may arise due to weak localisation which is the quantum interference of the conducting electrons with the defects of the system (Weisbuch and Vinter 1991). In an ideal 2D system, the electrons behave like particles with a trajectory determined
by elastic scattering off the potential walls as they travel through a region having an applied electric field. However, in real systems, some electrons may be scattered by impurities and defects so much that they become trapped in a small region and are unable to contribute to conduction, resulting in a weakly localised state and low conductivity. Along with the samples G91, G99 and D952, this behaviour has also been observed by Shah et al. (2000) in AlGaN/GaN heterostructures due to a large amount of disorder thought to be present in these systems.

The resistivity description given above has been concentrated on the deviations from the ideal SdH oscillation behaviour. The effects of significant parallel conduction and electron-electron interactions are the degradation of the quantum Hall effect and Shubnikov-de Haas oscillations, and analysis of the carrier densities and mobilities may need to be modified to accurately model the transport properties of the carriers. However, as will be seen later, the 2DEG density calculated from $\rho_{xx}$ and $R_{xy}$ plots are found to be comparable in all samples (refer to the results listed in Table 5.3), suggesting the absence of significant parallel conduction and electron-electron interactions. Consequently, the influence of these effects is regarded to be minimal, and
neglected in the analysis.

**Carrier density and mobility comparisons**

Table 5.3 lists the low temperature 2DEG electron sheet density and mobility extracted from magneto-transport results using the calculation procedure given in Section 5.1.4. The values represent averages of the data at different temperatures, though they varied little within the measurement temperature range and were almost temperature independent. Comparing the carrier densities evaluated using the SdH and the Hall resistance data (\(n_s[\text{SdH}]\) and \(n_s[\text{Hall}]\) respectively), it can be reiterated that parallel conduction effects are small, judging from the slight difference between the two densities (< 15%). Incidentally, the SdH carrier density has been calculated using the gradient of the plot of reciprocal magnetic field at which the \(B_{xx}^{-1}\) minimum occurs against the number of the minimum \((N)\). Most samples, except G91, exhibited well-resolved SdH oscillations, and the carrier density was easily determined. As shown in Fig. 5.21, the SdH minima of G91 were difficult to identify, and thus the \(\rho_{xx}\) curve was normalised and then the decreasing background component subtracted to pinpoint the oscillation minimum. The \(B_{N}^{-1}\) vs \(N\) plot yielded a straight line for all samples, justifying the assumption made in theory (see Section 5.1.3) that only one subband contributes to conduction.

An interesting feature is observed when looking at the carrier density and mobility values of G91 and D952, and comparing them to the measured quantities obtained from the VDP experiments in Section 5.2.1. The mobilities evaluated from the magneto-transport measurements are approximately half the values obtained from the VDP experiments, though the carrier densities show a closer agreement. This remarkable discrepancy may be due to various reasons:

(i) Inhomogeneities in the layer, as the Hall bar and VDP samples are processed at different regions of the wafer. Note that in J401’s case, the mobility change within a Hall bar was found to be up to 3-fold, depending on which pair of contacts are used for the measurements.

(ii) Different current distributions between the Hall bar and VDP configuration. The
current lines in the Hall bar flow through a confined area, much smaller than that of the VDP arrangement. Greater freedom is provided in a VDP sample where current flow between the contacts becomes less tortuous, thereby resulting in reduced $\rho$ and a rise in $\mu$.

(iii) Problems due to sample processing. Mixing of the $\rho_{xx}$ and $\rho_{xy}$ components could occur due to errors during the lithography etch of a Hall bar.

It should be pointed out that the above factors are only speculative; systematic studies have yet to be carried out to verify these possibilities. Further work is required to investigate this mobility discrepancy, and precisely determine the source of anomaly.

**TABLE 5.3.** Summary of the electron density and mobility determined from the low temperature magneto-transport data. Approximate 2DEG densities induced by polarisation effects (Ambacher et al. 1999) corresponding to a similar Al content and AlGaN thickness to the measured samples, are also included for a comparative study.

<table>
<thead>
<tr>
<th></th>
<th>D952</th>
<th>G91</th>
<th>G99</th>
<th>C251199</th>
<th>J401</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x$ (%)</td>
<td>23</td>
<td>20</td>
<td>10</td>
<td>~ 5</td>
<td>18</td>
</tr>
<tr>
<td>$t_{\text{AlGaN}}$ (nm)</td>
<td>35</td>
<td>12</td>
<td>32</td>
<td>200</td>
<td>120</td>
</tr>
<tr>
<td>$n_s[\text{SdH}]$ ($\times10^{12}$ cm$^{-2}$)</td>
<td>10.8</td>
<td>2.6</td>
<td>4.2</td>
<td>3.9</td>
<td>5.8</td>
</tr>
<tr>
<td>$n_s[\text{Hall}]$ ($\times10^{12}$ cm$^{-2}$)</td>
<td>9.8</td>
<td>3.1</td>
<td>4.1</td>
<td>4.3</td>
<td>5.6</td>
</tr>
<tr>
<td>$n_s[\text{SP+PZ}]^f$ ($\times10^{12}$ cm$^{-2}$)</td>
<td>~ 11.0$^a$</td>
<td>~ 5.3$^b$</td>
<td>~ 3.0$^c$</td>
<td>~ 10.0$^*$</td>
<td></td>
</tr>
<tr>
<td>$\mu$ (cm$^2$ V$^{-1}$ s$^{-1}$)</td>
<td>960</td>
<td>1650</td>
<td>2380</td>
<td>5070</td>
<td>8120 – 28250</td>
</tr>
</tbody>
</table>

$^f$ From the results shown in Fig. 5.5(b) calculated by Ambacher et al. (1999) with similar $x$ and $t_{\text{AlGaN}}$.

$^a$ For $x = 0.23$ and $t_{\text{AlGaN}} = 30$ nm.

$^b$ For $x = 0.20$ and $t_{\text{AlGaN}} = 10$ nm.

$^c$ For $x = 0.10$ and $t_{\text{AlGaN}} = 32$ nm.

$^d$ Difficult to compare since C251199 is of a superlattice structure.

$^e$ Theoretical results only extend $t_{\text{AlGaN}}$ to 30 nm, and since J401 consists of a much thicker (120 nm) AlGaN layer, the maximum sheet charge $\sigma/e$ based on a structure with $x = 0.18$ is given instead (refer to Fig. 5.5(a)).

Also included in Table 5.3 is the maximum carrier density induced by spontaneous and piezoelectric polarisation $n_s[\text{SP+PZ}]$ previously shown in Fig. 5.5, which has been theoretically calculated by Ambacher et al. (1999). The presence of high carrier densities in G99 and D952 obtained by the Hall measurements has been explained qualitatively with regards to the polarisation effects in Section 5.2.1. A closer inspection of the SdH results on a wider range of samples is presented below (Note
that C251199 is omitted in the discussion, because of difficulties in comparing with theory as C251199 is of a superlattice structure).

- **D952**: Close agreement between experiment ($1.1 \times 10^{13}$ cm$^{-2}$) and theory ($1.08 \times 10^{13}$ cm$^{-2}$) is achieved, indicating that in this sample, which is undoped, the 2DEG density relies both on spontaneous and polarisation induced effects.

- **G91**: $n_s[SdH]$ is found to be around half of $n_s[SP+PZ]$, and the lower carrier density of G91 is attributed due to strain relaxation of the barrier. As stated earlier in Section 5.1.1, Ambacher et al. (1999) have found, based on their theoretical calculations, that a complete relaxation of strain results in zero piezoelectric component, and that the piezoelectric and the spontaneous contribution each induces an approximately equal amount of charges. This implies that the AlGaN layer of G91 is heavily affected by the propagation of dislocations due to non-optimised growth conditions, and consequently the barrier is thought to be unstrained (non-pseudomorphic).

- **G99**: Unlike the case of G91, the extracted carrier density of G99 is about 30% higher than $n_s[SP+PZ]$. The theoretical calculations have been performed assuming an undoped AlGaN barrier, whereas G99 was modulation-doped with the Si doping level of $1.2 \times 10^{19}$ cm$^{-3}$ (refer to Section 5.1.2 for G99 growth details). Hence the difference in $n_s$ can be explained by an addition of carriers by charge transfer from the doped region in the AlGaN layer.

- **J401**: As given in table 3.2, the AlGaN layer of J401 is undoped with $t_{AlGaN} = 120$ nm, which is much thicker than the critical layer thickness, estimated by Fischer et al. (1994), at which pseudomorphic growth can no longer occur. Hence, similar to the case of G91, the 2DEG density is expected to be induced by spontaneous polarisation only. From the calculated sheet charge density results shown in Fig. 5.5(a), $\sigma/e$ induced by spontaneous polarisation is estimated to be just below $6 \times 10^{12}$ cm$^{-2}$, which matches closely with $n_s[SdH]$ of J401.

From Table 5.3, the overall trend of mobility with increasing carrier density is not clear, inconsistent with the finding given in theory (Section 5.1.1) that by increasing
the Al composition, greater carrier densities are induced by polarisation effects, thereby increasing interface roughness scattering and reducing low temperature mobility. In addition, as mentioned earlier in Section 5.2.1 regarding the Hall measurements, the measured mobilities lie well below the mobility limited by interface roughness, and other processes such as scattering by remote ionised donors, threading dislocations and grain boundaries, can be proposed as the dominant scattering mechanism at low temperatures. The extremely high mobility of J401 in particular indicates a decreased dislocation and grain boundary scattering, arising from a much improved material quality compared to the rest of the studied samples. Better understanding of mobility limiting processes at low temperatures can be achieved from the interpretation of $\tau_t/\tau_q$ results, which is given below.

**Determination of relaxation times**

Transport and quantum relaxation times are evaluated using the calculation procedure described in Section 5.1.4, where $\tau_t$ was extracted from the low field resistivity, and the determination of $\tau_g$ was derived from Dingle plots of the SdH oscillation amplitudes. Typical Dingle plots are shown in Fig. 5.23 for samples D952 and J401B, all displaying good linear variation. There are differences in the $y$-intercept of the plots though, where for C251199 and J401 the intercept was close to the theoretical value of 4; in other samples, it was slightly lower (see Table 5.4 for details). As discussed in the work carried out by Coleridge (1991), the presence of parallel conduction brings the intercept below 4, though he added that the slope of the plot still gives the value of $\tau_g$ to a good approximation (refer to Section 5.1.4). In addition, as mentioned earlier in the previous results (see Table 5.3), the close agreement between $n_s[SdH]$ and $n_s[Hall]$ demonstrates that there is no strong evidence of parallel conduction effects.

The extracted relaxation times are listed in Table 5.4. It was mentioned earlier that J401 exhibited marked non-uniformity, where, although the carrier density did not vary, the low field resistivity changed by almost a factor of 3 between different sets of contacts to the Hall bar. Hence, the results of J401 are given as J401A, B, and C, and are considered more fully later. An initial look at the results shown in Table 5.4 indicates that the comparison of the Dingle ratios for a range of samples with different
structures which, despite having fairly similar carrier densities, display a wide range of transport mobilities. However, before discussing likely scattering processes present in relation to relaxation time ratios, the \( B_{\text{onset}} \) dependence on \( \mu \) and \( \tau_q \) is investigated below.

As mentioned earlier in Section 5.1.3, the magnetic field at which the SdH oscillations start to occur is controlled by the relations, \( \omega_c \tau_q \gg 1 \) and \( \mu B \gg 1 \). From the \( B_{\text{onset}} \) values listed in Table 5.4, it can be seen that, except for G99, \( B_{\text{onset}} \) decreases with increasing \( \mu \). The low \( B_{\text{onset}} \) of G99 can be explained by considering the variation in \( \tau_q \), where G99 exhibits \( \tau_q \) which is about twice the values of D952, G91 and C251199. Hence the condition \( \omega_c \tau_q \gg 1 \) can be achieved at a lower magnetic field for G99 than C251199 which has a higher mobility. Similar argument can be applied to the relatively large oscillation amplitudes of G99 compared to D952, G91 and C251199. The amplitude of oscillations is also governed by \( \tau_q \) in Eq. 5.37, where an increase in \( \tau_q \) resulting in greater amplitudes. The largest mobility and quantum relaxation time are obtained in J401, and thus, its \( \rho_{xx} \) shown in Fig. 5.17 is characterised by the lowest \( B_{\text{onset}} \) and well-resolved oscillations with the biggest amplitudes.

**FIG. 5.23.** Dingle plots for samples D952 and J401B, showing good linear dependences, but differences in intercept.
**TABLE 5.4.** Summary of magneto-transport properties of the samples investigated, including parameters such as $\tau_\ell$ and $\tau_\eta$. J401 is divided into 3 regions corresponding to different sets of contacts to the Hall bar.

<table>
<thead>
<tr>
<th>Sample</th>
<th>$n_s \times 10^{12}$ cm$^{-2}$</th>
<th>$\mu$ cm$^2$ V$^{-1}$ s$^{-1}$</th>
<th>$B_{\text{onset}}$ (T)</th>
<th>$\tau_\ell$ (ps)</th>
<th>$\tau_\eta$ (ps)</th>
<th>Dingle ratio $\tau_\ell/\tau_\eta$</th>
<th>$y$-intercept</th>
</tr>
</thead>
<tbody>
<tr>
<td>D952</td>
<td>10.8</td>
<td>960</td>
<td>8</td>
<td>0.12</td>
<td>0.08</td>
<td>1.5</td>
<td>1.1</td>
</tr>
<tr>
<td>G91</td>
<td>2.6</td>
<td>1650</td>
<td>7.5</td>
<td>0.16</td>
<td>0.09</td>
<td>1.7</td>
<td>0.93</td>
</tr>
<tr>
<td>G99</td>
<td>4.2</td>
<td>2380</td>
<td>4</td>
<td>0.29</td>
<td>0.18</td>
<td>1.6</td>
<td>2.2</td>
</tr>
<tr>
<td>C251199</td>
<td>3.9</td>
<td>5070</td>
<td>6.5</td>
<td>0.63</td>
<td>0.10</td>
<td>6.3</td>
<td>4.2</td>
</tr>
<tr>
<td>A</td>
<td>5.8</td>
<td>8120</td>
<td>2</td>
<td>1.02</td>
<td>0.35</td>
<td>2.9</td>
<td>4.1</td>
</tr>
<tr>
<td>B</td>
<td>5.8</td>
<td>9340</td>
<td>2</td>
<td>1.17</td>
<td>0.36</td>
<td>3.3</td>
<td>4.3</td>
</tr>
<tr>
<td>C</td>
<td>5.8</td>
<td>28250</td>
<td>2</td>
<td>3.53</td>
<td>0.30</td>
<td>11.8</td>
<td>4.3</td>
</tr>
</tbody>
</table>

Table 5.4 shows a roughly monotonic increase in the ratio of $\tau_\ell$ to $\tau_\eta$ with increasing mobility, but with a fairly large spread; this is plotted in Fig. 5.24. Since the electrons are in most of these samples are generated solely as a result of polarisation effects, and modulation doping was only used in G91 and G99, it is difficult to make a direct comparison with theoretical models based on GaAs/AlGaAs systems (Das Sarma and Stern 1985; Harrang et al. 1985), where modulation doping is generally employed. Nevertheless, to obtain a semi-quantitative indication, a power law fit to the experimental data reported by Coleridge (1991) is included in Fig. 5.24 (solid line), but scaled to lower values along the mobility axis by the ratio of GaAs to GaN effective masses, to give equivalent transport relaxation times (the spread of data is approximately ±50% about this line). The GaN data lie well below this line, indicating that for a given scattering rate, there is much more large-angle scattering in this material. Also included in Fig. 5.24 are the result from Elhamri et al. (1998), Saxler et al. (2000), Shah et al. (2000), Braña et al. (2000), and Wang et al. (2000), and these appear to be consistent with the data presented in the figure.

Overall neutrality of the material demands that a density of positive charges equal to the 2DEG concentration exists in each of these structures, and this may be fixed or mobile, or a combination of both, but the distribution of these charges is currently unresolved (Harris et al. 2000). The general upward trend in the Dingle ratio for the undoped samples (D952, C251199 and J401) indicates that higher mobilities are
FIG. 5.24. Dependence of lifetime ratio, $\tau_l/\tau_q$, on transport mobility for all samples studied, together with previously reported literature values, where a) Elhamri et al. (1998), b) Shah et al. (2000), c) Braña et al. (2000) and d) Wang et al. (2000). The solid curve represents scaled results for GaAs/AlGaAs 2DEGs.

generally associated with a reduction in large-angle scattering. In addition, samples C251199 and J401, with the thickest AlGaN layers, have the highest mobilities and relatively large $\tau_l/\tau_q$ ratios is consistent with a model in which the compensating positive charges are remote from the 2DEG, and possibly located at the surface. The role of deliberate Si doping in samples G91 and G99 is found to be a relative increase in large-angle scattering compared to other layers, as demonstrated by their deviations (lower $\tau_l/\tau_q$) from the upward trend in the Dingle ratio of undoped samples. As mentioned earlier in Section 5.1.4, Wang et al. (2000) have noted a reduction in transport mobility when intentional modulation doping with Si is used, and this is clearly borne out here.

Two other scattering processes which may be significant in these samples, and are suggested in the theory (see Section 5.1.1) and in the previous results (refer to Section 5.2.1), are by threading dislocations and by grain boundaries. Since dislocations extend from substrate to surface across the 2DEG, they will presumably act as large-
angle scatterers, producing reductions in both \( \tau_t \) and \( \tau_q \). Differences in the dislocation density and distribution may thus account for some of the variations between samples seen in Fig. 5.24.

\[ \]

**FIG. 5.25.** Schematic diagram of grain boundaries with different sizes, where (a) the cyclotron motion of an electron is unaffected due to a large grain size (J401C), and (b) the motion is hampered by a small grain size (J401A and B), resulting in strong grain boundary scattering.

The unusual results obtained from J401 can be also explained by grain boundary scattering. The high mobility obtained in region C suggests this is material in which the density of scatterers near the 2DEG, and the dislocation density, are both relatively low; this is confirmed by the large \( \tau_t/\tau_q \) ratio. As Table 5.4 shows, it is only the transport mobility which is reduced in regions A and B, and this could be the result of a locally smaller grain size in these areas, so that grain boundary scattering becomes the limiting mechanism. The effect of grain boundaries with different thicknesses on the cycloidal motion of carriers is illustrated in Fig. 5.25. Using the transport mean free path, given by Eq. 5.28, as a measure of the average grain size suggests they are \(~ 1 \mu m\) across, respectively, and since this is larger than the maximum cyclotron radius, described by Eq. 5.23, which has been used in the determination of \( \tau_q \), \(~ 14 \text{ nm at 3.5 T} \), it seems likely that \( \tau_q \) will not be significantly degraded in these regions (indeed, experimentally, there is a small increase of about 20\%). Speculating further along these lines, the broken trend line in Fig. 5.24 is a suggested limit for dominant grain boundary scattering, assuming that \( \tau_q \) is approximately constant, so that the
ratio is proportional to $\tau_t$. Interestingly, J401C lies close to this line (although to a lesser degree than in J401A and J401B), indicating that, even in this region, grain boundary scattering may be an important effect.

**Determination of effective mass**

As described by the calculation procedure given in Section 5.1.4, the effective mass is evaluated by measuring the amplitude of the SdH oscillations at a fixed magnetic field for each temperature. Samples exhibiting the largest amplitudes (J401 and G99) are selected for the analysis using a the VTI system at temperatures in the range 1.3 - 15 K. The results of J401 and G99 are plotted in Fig. 5.26 and Fig. 5.27, respectively.

![Linear fits](image)

**FIG. 5.26.** $\ln(A/T)$ as a function of $T$ at various $B$ for J401. The solid lines represent the best fit to the data. The effective mass, calculated from the average of the slopes, is $(0.22 \pm 0.04)m_0$.

The effective mass was extracted at several values of the magnetic field, yielding an average value of $m^*$ to be $(0.22 \pm 0.04)m_0$ for J401, and $(0.25 \pm 0.08)m_0$ for G99. Both quantities are slightly higher compared to the reported values calculated using the variation of SdH oscillation amplitudes with $T$ (refer to Section 5.1.4 for more details). This small difference could be due to either the experimental procedures or
the material itself. While there is an assumption involved in the derivation of Eq. 5.53 to determine $m^*$ ($\sinh \chi \approx \exp \chi/2$), the possible errors are small provided the temperature is not too low. In addition, the $\rho_{xx}$ variation with $B$ in these samples show well-resolved SdH oscillations which do not display visible deviations from sinusoidal behaviour with temperature. The effective mass can vary depending on the substrate used during growth, where Elhamri et al. (1998) reported $m^*$ of $0.18m_0$ for an AlGaN/GaN heterostructure grown on SiC substrate. The lower lattice mismatch using SiC can profoundly influence the residual strain in GaN layers, and Yang et al. (1993) reported of the change in $m^*$ arising from strain variations. Nevertheless, a reasonable agreement between experiment and theory is achieved, where the obtained $m^*$ of J401 and G99 are within the previously reported range of $0.19m_0 - 0.27m_0$. In particular, the GaN electron effective mass value of J401 matches closely with that employed in the analysis throughout this thesis given by Perlin et al. (1996), and this is somewhat demonstrated by the superior material quality of J401 compared to G99.
Chapter 6

Phonon Processes in AlGaN/GaN Structures

In this chapter, an investigation of phonon emission processes in AlGaN/GaN heterostructures at low temperatures is presented. The process of hot carrier energy relaxation is central to the behaviour of semiconductor devices. In addition to its relevance to modelling device performance, information concerning the electron-phonon interaction which is of fundamental importance in the semiconductor physics can also be obtained. As demonstrated in the previous chapter, the Shubnikov-de Haas effect has been utilised to obtain a wide variety of transport parameters, where the measurements employed sufficiently low currents to avoid electron heating. The amplitude of the SdH oscillations can also be used as a thermometer for the electron temperature by deliberately increasing applied current, and studies as a function of current can yield the temperature dependence of power input per electron. As far as the author is aware, this is the first time that, for a AlGaN/GaN 2DEG system, the phonon scattering behaviour and its effect on the electron temperature at very low temperatures are examined. It should be pointed out here that this work was carried out in collaboration with Dr. A. J. Kent from the Physics Department at Nottingham University, who was responsible for the numerical modelling. The theoretical background related to these studies is provided in Section 6.1, followed by discussions on the experimental findings and their comparisons with theoretical analysis in Section 6.2.
6.1 Theoretical considerations

Under equilibrium at low temperatures, electrons are characterised by a temperature which equals that of the lattice. As applied current is increased, the electrons acquire more energy, and when the electron temperature exceeds the lattice temperature, they can be regarded as \textit{hot}. This results in a net loss of energy and momentum to the lattice by the electron system, and in Section 6.1.1, energy relaxation by hot electrons in semiconductors is theoretically described, concentrating mainly on acoustic phonon emission processes. Previous studies of these processes are reviewed in Section 6.1.2, where the concept of the \textit{dirty limit} in disordered systems is introduced. Finally, Section 6.1.3 presents procedures for data analysis.

6.1.1 Phonon emission by hot electrons

The interaction between electrons and the thermally vibrating lattice is represented by a scattering process in which phonons are either absorbed or emitted by the carriers. Phonons can be seen as quantised lattice vibrations with energy

\[ E(\omega_q) = \left( n(\omega_q) + \frac{1}{2} \right) \hbar \omega_q , \]  

where \( n(\omega_q) \) is the statistical average occupation number of phonons in the phonon frequency mode \( \omega_q \), which at thermodynamic equilibrium is given by the Bose-Einstein function

\[ n(\omega_q) = \frac{1}{\exp(\hbar \omega_q / k_B T) - 1} . \]  

Now consider an electron, which is initially in a state described by its wavevector, \( \mathbf{k} \). Upon emission of a phonon of wavevector \( \mathbf{q} \) the electron is scattered into a new state \( \mathbf{k}' \), where \( \mathbf{k} = \mathbf{k}' + \mathbf{q} \). In this process, which is depicted in Fig. 6.1, the electron loses momentum \( \hbar q \) and energy \( \hbar \omega_q \). The conservation of momentum during an electron-phonon interaction requires

\[ k'^2 = k^2 + q^2 - 2kq \cos \phi . \]  

Note that when considering an absorption of a phonon, the negative sign is replaced by the plus sign. Remembering that energy is also conserved in the phonon scattering,
the energy of the final state in a spherical parabolic band is given by

\[ \frac{\hbar^2 k'^2}{2m^*} = \frac{\hbar^2 k^2}{2m^*} - \hbar \omega_q. \]  

(6.4)

For the case of acoustic phonons,

\[ \omega_q = v_s q, \]  

(6.5)

where \( v_s \) is the velocity of sound. Combining Eqs. 6.3 and 6.4 yields

\[ \cos \phi = \frac{q}{2k} + \frac{m^* \omega_q}{\hbar k q}. \]  

(6.6)

Representing the right-hand side of Eq. 6.6 by \( f(q) \), energy and momentum conservation can be imposed by the constraint \(-1 \leq f(q) \leq 1\). In degenerate 2DEG systems, the only electrons able to be scattered lie near the Fermi level energy, and the electron wavevector \( k \) is effectively described by the Fermi wavevector \( k_F \) which can be directly obtained by the expression

\[ k_F = \sqrt{\frac{2\pi n_s}{\hbar^2}}. \]  

(6.7)

Thus by using Eq. 6.5 and the relation \( \hbar k_F = m^* v_F \),

\[ f(q) = \frac{q}{2k_F} + \frac{v_s}{v_F}. \]  

(6.8)

\[ \text{(a)} \quad \text{(b)} \]

\[ \text{FIG. 6.1. Geometry of the phonon scattering: (a) an electron is scattered from state } k \text{ to } k' \text{ (both close to the 2D Fermi surface) and (b) a phonon, wavevector } q \text{ is emitted at angle } \theta \text{ to the 2DEG normal.} \]
It follows from the conservation limit that no solution exists for $v_F < v_s$, and an electron must travel with a group velocity in excess of the sound velocity in order to emit a phonon. Therefore, provided $v_F \gg v_s$, the electron-phonon interaction is effectively cut off for $q > 2k_F$. This corresponds to a maximum phonon energy $2\hbar v_g k_F$, which, at a sufficiently high temperature, is less than the average thermal energy of the electrons $k_B T_e$. Hence the acoustic phonon emission by hot electrons can be divided into two temperature ranges; (i) for $T_e > 2\hbar v_g k_F / k_B$ in the so-called equipartition (EP) regime, and (ii) for $T_e \leq 2\hbar v_g k_F / k_B$ in the Bloch-Grüneisen (BG) regime. It should be noted that at very high temperatures (above the EP regime), the dominant mechanism of energy relaxation by hot electrons in semiconductors is by optic phonon emission, which is considered to be an inelastic process due to the high optic phonon energy $\Phi_{op}$. In GaAs, $\Phi_{op} \approx 36$ meV, and the changeover at which optic phonon emission becomes dominant is found to occur at around 30 K (Hawker et al. 1992). The optic phonon energy of GaN is much larger ($\approx 92$ meV), and the changeover is expected to occur at a high temperature (Stanton et al. 2001 recently reported the changeover temperature of about 70 K).

Below the optic phonon limited regime, energy loss from hot electrons is dominated by acoustic phonons, whereas momentum loss can also take place by interacting with ionised impurities. As mentioned earlier, the interacting acoustic phonon energies are restricted by momentum conservation to be smaller than $k_B T_e$ in the equipartition range (for the case of samples studied in this chapter, $T_e > 20$ K), and the scattering is regarded to be quasielastic. The equilibrium phonon (Bose-Einstein) occupation factor given earlier in Eq. 6.2 can be approximated to $k_B T / \hbar \omega_q$, resulting in a linear temperature dependence of energy loss rate. When the energy exchange becomes comparable to $k_B T_e$, i.e., as the temperature becomes lower in the Bloch-Grüneisen range ($T_e \ll 20$ K), collisions occurring in acoustic phonon scattering can be approximated as elastic for momentum loss, but not for energy. The effect of screening increases and scattering involves smaller wavevectors. This gives rise to a stronger temperature dependence of the scattering rate (Kawamura and Das Sarma 1992), which can be investigated by studying the relationship between the input power per electron $P_e$ and the electron temperature $T_e$ (discussed more fully below). As will be evident later in
Section 6.2, the BG regime is mainly of interest with regard to these results since the experiments are carried out in the temperature range 0.05 – 10 K.

In equilibrium, $P_e$ is balanced by the energy loss to phonons. To obtain an expression for $P_e$ in terms of the measurable parameters, the basic dynamical equations that describe the momentum and energy conservation of an electron system are considered, which are given by:

$$\frac{d(m^*v_e)}{d\tau} = eF - \frac{m^*v_e}{\tau_m}$$

(6.9)

and

$$\frac{dE}{d\tau} = eFv_e - \frac{(E - E_0)}{\tau_E},$$

(6.10)

where $v_e$ is the electron velocity, $F$ is the electric field, $E$ is the energy, $E_0$ is the energy at zero field, $\tau_m$ is the momentum relaxation time, and $\tau_E$ is the energy relaxation time.

In the steady state,

$$v_e = \frac{e\tau_m}{m^*} F = \mu F$$

(6.11)

and

$$E = E_0 + \frac{\tau_m \tau_E (eF)^2}{m^*},$$

(6.12)

where the mobility $\mu$ is field-dependent through the energy dependences of the momentum relaxation time and the effective mass. Combining Eqs. 6.11 and 6.12, the total emitted power $P_T$, i.e., $(E - E_0)/\tau_E$, is therefore expressed as

$$P_T = e\mu F^2.$$  

(6.13)

Note that since $P_T$ represents the net energy loss rate by hot electrons, it needs to be divided by the carrier density $n_s$ in order to obtain the input power per electron, $P_e$. The procedures for obtaining $P_e$ and $T_e$ from the experimental data will be described later in Section 6.1.3.

In the analytic formulation for acoustic phonons described by Ridley (1988), $P_e$ is proportional to $T_e^\varphi - T_L^\varphi$, where $T_L$ is the lattice temperature. The exponent $\varphi$ can vary, depending on conditions such as the mode of coupling and the degree of screening. As
briefly introduced earlier in Section 4.1.2, electrons interact with acoustic phonons by deformation-potential (DP) and piezoelectric (PZ) scattering. For the case of energy relaxation by piezoelectric coupling with and without screening in the BG regime, the power emitted follows a $T^5$ and $T^3$ dependence, respectively, i.e.,

$$P_e = \frac{30e^2K_{av}^2m^*\epsilon_0}{\pi\rho c^2\hbar^2\nu_k^2\nu_F^2} \left[ (k_BT_e) - (k_BT_L) \right]$$

(6.14)

and

$$P_e = \frac{4e^2K_{av}^2m^*\epsilon_0}{7\pi\rho c^2\hbar^2\nu_k^2\nu_F^2} \left[ (k_BT_e) - (k_BT_L) \right]^3$$

(6.15)

where $K_{av}$ is an average piezoelectric coupling coefficient, $\epsilon_0$ is the reciprocal Debye screening length, and other symbols have their usual meanings (refer to Table 4.1 in Section 4.1.5). The effect of screening is taken into account using the quasi-static approximation (Stern and Howard 1967):

$$\epsilon_u = \left(1 + \frac{\epsilon_0}{\epsilon} \right)$$

(6.16)

where

$$\epsilon_0 = \frac{m^*\epsilon}{2\pi\rho c^2\hbar^2}$$

(6.17)

For the case of energy relaxation by DP coupling in the BG range, $\varphi = 7$ and 5 in the screened and unscreened limits, respectively. The dominant phonon emission mechanism in GaN at low temperatures will be discussed further at the end of this section.

Similar approach to the formalism given above has been successfully applied to AlGaAs/GaAs 2DEG systems at low temperature (Challis et al. 1987; Fletcher et al. 1992), although it has been shown that a more accurate modelling is achieved when calculating the energy loss rates numerically at intermediate temperatures (Kent 1998). As mentioned previously at the beginning of this chapter, phonon emission processes in AlGaN/GaN heterostructures are investigated in conjunction with Nottingham University, where the results obtained from the SdH experiments are compared with the theoretical analysis based on the numerical approach of Kent (1998). The model used the variational method to describe the ground state electron wave function of the
confining potential which is given by (Stern and Howard 1967):

\[ \Psi_0(z) = \sqrt{\frac{1}{2}} \gamma^3 z^2 \exp \left( -\frac{1}{2} \gamma z \right), \]  

(6.18)

where \( \gamma \) is a variational parameter, representing the average separation of the electrons from the heterointerface in terms of the 2D sheet density \( n_s \) and the depletion charge per unit area in the channel \( n_{depl} \), and is described by

\[ \gamma = \left[ \frac{48 \pi m^* e^2}{\varepsilon_s \hbar^2} \right]^{1/3} \left( n_{depl} + \frac{11}{32} n_s \right)^{1/3}. \]  

(6.19)

The static approximation used in Eq. 6.16 is also employed to incorporate screening, and the values of the material parameters required for the numerical calculations are listed later in Table 6.1 (see Section 6.1.3). It should be pointed out here that a complete account of the numerical analysis is beyond the scope of the thesis, and thus for further details, refer to the treatment elucidated by Kent (1998).

Experimentally, there are various methods to measure energy relaxation rates including photoluminescence (PL) and transport experiments, which have been extensively applied to GaAs and related materials. PL has proved effective for measuring energy loss by hot electrons in GaAs (Shah 1992), although these measurements are susceptible to inhomogeneous line broadening effects which are particularly severe in GaN material of current quality. Sakaki et al. (1984) have adopted a similar approach to that employed in this chapter, where the temperature dependence of SdH oscillation amplitudes is used to determine the energy loss rate in GaAs. This method requires high mobility samples, and thus cannot be utilised on bulk GaN whose mobility is not sufficiently high. The previous results presented in Section 5.2.2 already demonstrated high mobilities and well-resolved SdH oscillations in 2DEG samples characterised in this thesis, and the experimental findings discussed in Section 6.2 correspond to the first investigation of phonon emission processes in AlGaN/GaN heterostructures at low temperatures using the SdH approach.

Stanton et al. (2001) recently reported studies of hot electron relaxation in MBE grown bulk GaN using a combination of pulsed electrical transport and heat pulse phonon measurements, which have been successfully used for GaAs devices (Kent et al. 1997). The pulsed transport measurements were employed to determine carrier
temperatures, and in the heat pulse experiments, information about the mode and wavevector of the emitted phonons was obtained. Based on comparisons between theoretical calculations and the results of GaN samples with 300 K electron concentration in the range $10^{24} - 10^{25} \text{ m}^{-3}$, the following conclusions have been drawn:

- Below 20 K (in the BG range), emission of PZ coupled phonons in the unscreened limit, i.e., $\varphi \approx 3$, is found to be much stronger than the DP coupling. The dominant interaction between electrons and PZ coupled phonons over DP coupled phonons is explained by the high PZ constant of GaN (about 5 times greater than GaAs); in contrast, the DP coupling constants of GaN and GaAs are similar in value.

- Power emitted follows a linear temperature dependence between 20 – 70 K, in agreement with theory for the equipartition regime. Above about 70 K, optic phonon emission takes over as the dominant mechanism.

Heat pulse studies of the energy relaxation rate of hot electrons are also carried out by Hawker et al. (1999) on n-type GaN samples where, similar to the layers investigated in Section 4.2.3, carrier transport is heavily affected by an impurity band. They identified coupling to PZ acoustic phonons with screening as the dominant energy relaxation mechanism at $T < 10$ K, though the dependence was $P_e \propto T_e^4$ which is an order of magnitude lower than predicted by theory for the screened PZ coupling. The reduced temperature dependence is attributed to the dirty limit, which becomes more effective in defect-ridden materials such as group III nitrides; this is discussed more fully in the following section.

6.1.2 Dirty limit effect

Various authors have discussed a hydrodynamic theory of phonon emission for disordered materials, where frequent collisions of the electrons with the disorder potential enhance the phonon emission efficiency (Chow et al. 1996; Chow et al. 1997; Fletcher et al. 2000). Their findings establish the concept of dirty limit for

$$ql_e \ll 1 ,$$  \hspace{1cm} (6.20)
where the emitted phonon wavevector is given by

\[ q \approx \frac{k_B T_e}{\hbar \omega_s} . \]

(6.21)

Here, \( l_e \) the elastic mean free path for impurity and defect scattering given earlier by Eq. 5.28. The temperature below which the dirty limit arises is deduced from Eq. 6.20, and is defined by

\[ T_d = \frac{\hbar \omega_s}{k_B l_e} . \]

(6.22)

In the case of piezoelectric coupling with screening, the temperature dependence of \( P_e \) was found to be reduced from \( T_e^5 \) to \( T_e^4 \) in the dirty limit. The nitride-based systems are known to contain many dislocations, defects and traps, etc., and the evidence of dirty limit behaviour for a GaN epilayer with \( \mu \approx 10 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1} \) at low temperatures, corresponding to \( T_d \) of about 20 K, has been reported by Hawker et al. (1999). However, in relatively high mobility 2DEG samples studied in this chapter, \( l_e \) is much higher so that the onset of the dirty limit is expected to occur at a much lower temperature. The presence of the dirty limit effect in AlGaN/GaN heterostructures will be discussed further in Section 6.2.2.

### 6.1.3 Data analysis

As mentioned previously in Section 6.1.1, for higher currents at a fixed cryostat temperature, electron heating occurs (i.e., \( T_e > T_L \)) and this results in weaker SdH oscillations. The change in the SdH oscillation amplitude with temperature can be utilised as a thermometer for the electron temperature, and calculation procedures for obtaining the variation of the power emitted by hot electrons as a function of \( T_e \) from the experimental data are presented below:

(i) The SdH oscillation amplitudes at different temperatures were measured for several fields in the range \( 3 < B < 5 \text{ T} \), where the driving current was kept low (about 100 nA) to avoid electron heating effects. From the plot of the SdH amplitude as a function of \( T \), a polynomial fit to the data is made, representing the calibration of \( T_e \).
(ii) With the sample at the base temperature, the SdH amplitude was then measured for a series of different currents, again using several oscillations in the range $3 < B < 5 \text{T}$. By comparing these amplitudes with those from the calibration run, the value of $T_e$ corresponding to each level of current can be obtained.

(iii) The input power per electron can be calculated from the current, the sample resistance and geometry, and the carrier density; at equilibrium, this equals the electron energy loss rate by phonon emission, which is a function of $T_e$ and $T_L$.

Eq. 6.13 is used to calculate $P_e$, where the electric field $F$ is extracted by dividing the voltage drop along the Hall bar by its length which, in this case, is $375 \mu\text{m}$.

(iv) Finally, the experimental relation between phonon emission rate and electron temperature can be examined by plotting $P_e$ logarithmically against $T_e$.

The obtained results are compared with theoretical analysis based on numerical calculations conducted by Dr. A. J. Kent at Nottingham University (refer to Section 6.1.1), and the parameter values used in the modelling are listed in Table 6.1.

### Table 6.1. GaN parameter values used in the theoretical model. All quantities were obtained from Madelung (1991) and Edgar et al. (1999), except for the PZ constants, which are from Bernardini et al. (1997) and O'Clock and Duffy (1973).

<table>
<thead>
<tr>
<th>GaN parameters</th>
<th>Symbols</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Effective mass (kg)</td>
<td>$m^*$</td>
<td>0.21$m_0$</td>
</tr>
<tr>
<td>Permittivity (F cm$^{-1}$)</td>
<td>$\epsilon_s$</td>
<td>9.5$\epsilon_0$</td>
</tr>
<tr>
<td>Density of mass ($\times$10$^3$ kg m$^{-3}$)</td>
<td>$\varrho$</td>
<td>6.15</td>
</tr>
<tr>
<td>Speed of sound ($\times$10$^5$ m s$^{-1}$)</td>
<td>$v_a$(LA)</td>
<td>6.56</td>
</tr>
<tr>
<td></td>
<td>$v_a$(TA)</td>
<td>2.68</td>
</tr>
<tr>
<td>Piezoelectric constant (C$^2$ m$^{-4}$)</td>
<td>$K_{av}(LA)$</td>
<td>0.22</td>
</tr>
<tr>
<td></td>
<td>$K_{av}(TA)$</td>
<td>0.23</td>
</tr>
</tbody>
</table>

$K_{av}$ is a directional average of the three independent piezoelectric tensor elements for wurtzite GaN, $c_{31}$, $c_{12}$ and $c_{33}$. For longitudinal acoustic (LA) phonons: $K_{av} = \frac{1}{8}[\frac{3}{2}(c_{31} + \frac{3}{2}c_{33} + 2c_{12})^2 + \frac{7}{4}c_{33}^2]$.

For transverse acoustic (TA) phonons: $K_{av} = \frac{1}{8}[(c_{31} - c_{33} - \frac{1}{3}c_{12})^2 + \frac{5}{6}c_{33}^2]$. 

---

1 For transverse acoustic (TA) phonons: $K_{av} = \frac{1}{8}[(c_{31} - c_{33} - \frac{1}{3}c_{12})^2 + \frac{5}{6}c_{33}^2]$. 

6. Phonon Processes in AlGaN/GaN Structures

6.2 Results and discussion

J401B and G99 have been selected to investigate the energy loss mechanism by hot electrons at low temperatures. They were chosen because of their relatively large $\rho_{xx}$ amplitudes, and by comparing the results of the layers with considerably different material quality (J401B being superior to G99), information regarding the effects of structural defects on the phonon emission process can be deduced. The dominant energy loss mechanism of J401B and G99 at low temperatures is identified in Section 6.2.1, followed by discussion of results in Section 6.2.2 concerning the possible existence of dirty limit phenomenon. Note that a combination of DLF and VTI equipment is employed to measure SdH oscillations at various temperatures (50 mK – 10 K) and currents (100 nA – 140 $\mu$A). For more details on the experimental procedures, refer to Section 3.1.

6.2.1 Dominant energy loss mechanism

Figs. 6.2(a) and (b) plot $\rho_{xx}$ vs $B$ for J401B at different temperatures and currents, respectively, and show that the amplitude of the SdH oscillations falls with both increasing lattice temperature, and increasing current. At currents of 100 nA or less, the amplitude was found to be independent of current for a given magnetic field, showing that in this range electron heating was negligible, i.e., $T_e = T_L$. Thus measurement of the $\rho_{xx}$ oscillations at different cryostat (and hence lattice) temperatures using a constant $I = 100$ nA enables a calibration of the relationship between amplitude and $T_L$, and hence $T_e$, to be determined. The data analysis has been carried out using the procedure described in Section 6.1.3, where the oscillations between $3 < B < 5$ were examined (well away from the region with spin-splitting).

The extracted values of $P_e$ are plotted as a function of $T_e$ in Fig. 6.3 for J401B. The slope of the graph gives the value of $\varphi$ in the power law: $P \sim T_e^\varphi$, which was found to be $4.4 \pm 0.3$ (in these energy loss experiments, $T_L$ was 50 mK so the $T_L^{\varphi}$ term in Eqs. 6.14 and 6.15 is negligible). This result is only slightly less than $\varphi = 5$ expected for the screened piezoelectric interaction in the Bloch-Grüneisen regime as described earlier in theory (see Eq. 6.14 in Section 6.1.1). However, some of the data falls in the
intermediate range of temperature and so a slightly weaker temperature dependence is expected. Also included in Fig. 6.3 are the results of a numerical calculation of $P_z$ for piezoelectric coupling.

At elevated temperatures (the equipartition regime), the theoretical energy relaxation tends to a linear dependence on $T_e$, whereas at electron temperatures between 1 and 10 K, $P_z$ follows $T_e^{4.4}$ and $T_e^{3.0}$ dependences for the screened and unscreened situations. The comparison between the theoretical and experimental results, particularly the temperature dependences, suggests PZ coupling with screening as the likely phonon emission process. As mentioned earlier in Section 6.1.1, this is reasonable because of the high values of the piezoelectric coupling constant and the carrier density, and agrees well with the finding reported by Hawker et al. (1999). Although remark-
FIG. 6.3. A double-logarithmic plot of $P_e$ vs $T_e$ for J401, obtained from the SdH oscillation amplitudes at various currents. The squares and circles represent experimental data of J401B and J401C, respectively, and the solid line is a power law fit to the data, with the slope of $4.4 \pm 0.3$. The dashed and dotted lines are theoretical results for unscreened and screened piezoelectric coupling, respectively, using $n_s = 5.8 \times 10^{12}$ cm$^{-2}$ in the calculations.

able agreement in the temperature dependence is achieved, there are discrepancies in the magnitude between experiment and theory. For a given $P_e$, the $T_e$ values obtained from experiment are about 40% smaller than the calculated values for screened PZ coupling. Part of the difference may come from uncertainties in the parameters used in the calculations, such as $m^*$, $K_{av}$ and $\varepsilon_s$, where the exact values for nitrides are still under debate (Monemar 1999). It could also be explained by considering the model used to describe the screening. The numerical results describe PE coupling in the strongly screened limit, arising from the static screening approximation (refer to Eq. 6.16), which represents the maximum level of carrier screening. Using a dynamical screening model in the simulation would reduce $T_e$ for a given $P_e$, giving an improved agreement between experiment and theory.

However, an interesting point can be made when considering the energy loss rate dependence of J401C. Remembering previously in Section 5.2.2, the low field resistivity and mobility values of J401C were found to be approximately three times smaller and
greater, respectively, than those of J401B, the $P_e$ values of J401B are scaled so that they are equivalent to $P_e$ of J401C (also plotted in Fig. 6.3). The scaled values match closely with the theoretical behaviour of screened PZ coupling. The significance of this result will be more fully discussed later in Section 6.2.2.

For the case of G99, similar steps to J401B have been taken to analyse the SdH oscillations and arrive at the temperature dependence of the energy loss rate, which is shown in Fig. 6.4. A much closer agreement between experiment and theory than J401B is achieved in terms of the magnitude, though the temperature dependence is slightly lower ($\varphi = 4.0 \pm 0.5$). Again, phonon emission by piezoelectric acoustic phonons in the screened limit can be proposed as the dominant energy relaxation mechanism at low temperatures. The small discrepancy in $\varphi$ could be due to experimental error, though the influence of the dirty limit may also play an important role. This aspect is investigated further in the next section.
6.2.2 Discussion of results

In the previous section, the magnitude difference between the experimental data of J401B and theory was partly attributed to the overestimation of the screening. In fact, the closer match achieved in J401C can be explained by considering the varying degree of screening between grain boundaries. It has been established throughout this thesis regarding the importance of grain boundary effects on transport properties of GaN and related materials. As shown earlier in Fig. 4.18, the interface between two grains is effectively described by a double Schottky barrier, where the region beneath it is depleted. The depletion implies less carriers and consequently, screening is less effective under the barrier region. In contrast, within a grain, electrons are free to move and particularly at the center of the grain, carriers are not affected by the depletion effects and thus exert efficient screening. Hence, the electron-phonon interaction is weaker in the grain than within the grain boundary. Taking the mean free path as a measure of average grain size, it can be seen that J401B and C have a diameter of about 0.3 and 1.1 μm, respectively. Thus a greater fraction of carriers in J401B are depleted by the grain boundaries than in J401C; the power loss by acoustic phonons in J401B is more enhanced relative to the situation in J401C due to less effective screening. This explanation agrees well with the experimental finding of J401B, where the lower $T_e$ than predicted by theory for a given $P_e$ is accounted for by the overestimation of screening.

Although the slight discrepancy in $\varphi$ of G99 between experiment and theory is within experimental error, it may also be caused by the dirty limit effect. The onset of the dirty limit can be estimated by using Eq. 6.22 in Section 6.1.2, and for G99, $T_d \approx 0.7$ K. This is just below the measurement electron temperature range of $0.8 \leq T_e \leq 5$ K (refer to Fig. 6.4), indicating the absence of the dirty limit. However, the close proximity between $T_d$ and the minimum experimental $T_e$ suggests that the dirty limit behaviour below 0.7 K may have an effect, albeit weak, above 0.8 K. This is reasonable since:

(i) As mentioned earlier in Section 6.1.1, the numerical calculations have been carried out at intermediate temperatures, i.e., $P_e \sim T_e^5$ is obtained as $T_e \to 0$ K,
and above the absolute zero temperature, a weaker temperature dependence is predicted. Hence the presence of the dirty limit is likely to exert influence above 0.7 K.

(ii) Theoretically an order of magnitude reduction in the temperature dependence is expected for the dirty samples, but as a result of the weak influence of the dirty limit effect, the reduction in $\varphi(G99)$ compared to theory is only about 0.3.

Incidentally, it should be pointed out that the temperature at which the dirty limit arises is estimated to be 0.1 and 0.04 K for J401B and C, respectively. As shown in Fig. 6.3, these values are clearly below the measurement electron temperature range of $0.6 \leq T_e \leq 5$ K. This is consistent with our finding that in this temperature range, the dominant process of energy relaxation by hot electrons in J401 is by acoustic phonon emission via piezoelectric coupling with screening in the clean limit.

Combined with the results presented in Chapter 5, the energy loss rate studies discussed here further demonstrate the versatility of using the SdH effect as a characterising tool. However, one drawback of using this method for the energy loss investigation of hot electrons is that, owing to rapid disappearance of the SdH oscillations with increasing temperature, the measurements can only be performed to less than around 10 K. Further collaborative work with Nottingham University is currently under way to extend the experimental temperature to 300 K by using the zero-field measurements on J401, and initial indications from the correlated work show encouraging signs (private communication).
Chapter 7

Conclusions

A combination of Hall and low temperature magneto-transport measurements has been successfully implemented in this thesis to investigate electrical properties of n-type GaN layers and AlGaN/GaN 2DEG systems. Group III nitrides contain a high level of disorder arising mainly from non-optimised growth conditions, and from transport studies of the samples, information on the role of structural defects and their effects regarding device application is obtained. In this chapter, an overall summary of the main results discussed in this thesis is presented, followed by a list of suggestions for future work.

7.1 Overall summary

The temperature-dependent Hall effect in n-GaN samples grown on sapphire by MBE and MOCVD has been analysed using a model with and without an impurity band. Transport properties of non-degenerate GaN layers unaffected by an impurity band conduction have been investigated by simultaneously fitting the Hall mobility and concentration data, and found that (a) at high temperatures (> 200 K), polar optical scattering dominates the mobility, whereas at lower temperatures, ionised impurity scattering is the dominant mobility limiting mechanism, (b) the $N_A$ values extracted from the low temperature mobility fit indicate compensation in the range 20 – 40%, where a higher mobility is associated with the less compensated sample, (c) the obtained donor activation energy ($\approx 10$ meV) agreed closely with the theoretical quanti-
ties predicted for the hydrogenic donors with a screening effect.

For the samples with doping densities in excess of $1 \times 10^{18} \text{ cm}^{-3}$ (Mott criterion), the presence of a parallel conduction channel (impurity band) and its effect on electron transport are studied by de-convoluting the temperature-dependent Hall data. The de-convoluted results indicated that (a) the electrical properties are not systematically dependent on growth technique, (b) Si and unintentional donors show similar behaviour, (c) the impurity band is approximately $(30 \pm 9) \text{ meV}$ below the conduction band edge at low impurity densities, but this energy reduces with increasing impurity content, (d) the mobility degradation mechanisms have the same relative effect on electron transport in the conduction and impurity bands, and (e) structural defects such as grain boundaries are associated with potential fluctuations which could be partially responsible for reducing mobility.

Transport properties of AlGaN/GaN heterostructures grown on sapphire by MBE and MOCVD have also been studied, based on interpretations of the Hall and low temperature magneto-transport measurements (mainly utilising the SdH effect). The presence of a 2DEG is confirmed by the clear SdH oscillations which have been seen in the wide range of samples characterised, covering the mobility from about 1000 to 28 000 cm$^2$ V$^{-1}$ s$^{-1}$. The high 2D sheet electron densities in the range $(2.6 - 10.6) \times 10^{12} \text{ cm}^{-2}$ have been mainly attributed to the charges induced by spontaneous and piezoelectric polarisation effects, which become stronger with the increasing Al composition and barrier thickness. Deviations from the ideal $\rho_{xx}$ variation with $B$ have been observed in some of the samples, arising from the parallel conduction effects and electron-electron interactions. However, the close agreement between the carrier density values obtained from the SdH magnetoresistance and Hall resistance suggested that these effects are minimal. The effective mass values calculated from the SdH oscillation amplitudes are found to be $0.22m_0$ and $0.25m_0$ for the samples with high and low material quality, respectively, and within the previously reported range.

A fairly consistent underlying trend in the scattering behaviour, independent of growth technique, is observed by studying the relationship between $\tau_q$ and $\tau_l$. For a given scattering rate, the results show that there is a greater proportion of large-angle scattering in nitride samples ($1 \leq \tau_l/\tau_q \leq 12$) than in GaAs/AlGaAs heterojunctions.
(\tau_l/\tau_q \gg 10). The smaller Dingle ratio values probably occur from the presence of dislocations, higher background impurity densities and more severe interface roughness. The large variation of mobility exhibited within one sample (up to 3-fold) corresponds to inhomogeneities in the layer, and this evidence seems to point to grain boundary scattering as the dominant mobility limiting process. The properties of two samples containing deliberate modulation doping display greater short-range scattering, partly due to the increase in the density of scatterers arising from the Si incorporation. The observation that the two samples with the thickest undoped AlGaN layers have the highest mobilities and \tau_l/\tau_q ratios suggests that the positive charges which compensate the 2DEG are remote from it, and possibly reside mostly at the surface.

The versatile nature of using the SdH effect as a characterising tool has been further demonstrated by using the amplitude of the \rho_{xx} oscillations to calibrate the electron temperature. From the measured temperature dependence of the energy loss rate in AlGaN/GaN heterostructures, the phonon emission processes below 10 K were investigated. For the high-quality sample, the power emitted followed \( T_e^{4.4} \) dependence, and the comparison with calculated theoretical results indicated that the dominant mechanism of energy relaxation by hot electrons is acoustic phonon emission via piezoelectric coupling with screening. However, around 40% discrepancy in the magnitude between experiment and theory is observed. This is probably caused by the over-estimation of the screening effect, where, considering the depletion of carriers in the Schottky barrier region formed at the grain boundary interface, it can be seen that for a given sample, the screening effects are expected to be lower in a region with a smaller grain size. This explanation is supported by the close agreement with the numerical modelling achieved in another region of the studied sample containing larger grains.

The presence of the dirty limit is suggested for the low-quality sample, where the energy loss rate followed \( T_e^{4.0} \) dependence, slightly lower than predicted by theory for the screened piezoelectric coupling in the clean limit. Although the temperature below which the dirty limit occurs (\( T_d \)) is estimated to be just below the measurement electron temperature, the dirty limit effect is thought to be still weakly present above \( T_d \).
7. Conclusions

7.2 Future work

One of the main emphasis of the future work would be on the improvement of the material quality of the grown samples. In addition, a wider range of samples needs to be studied in order to obtain a more accurate picture of the transport behaviour in nitride materials. Collaborative work with the grower, where feedback provided by electrical characterisation enables a full systematic dependence on growth conditions to be determined, is essential to co-ordinate the optimisation process. Setting aside the growth issue, the future work regarding experimental techniques is also significant, and this can be classified into two categories; further analysis of the SdH data, and correlated work with other characterisation techniques.

From the temperature- and field-dependent longitudinal conductivity in the Landau level tails of 2DEG structures at low temperatures, the charge transport by hopping conduction can be investigated. In SdH experiments, the temperature dependence of the conductivity minima is generally proportional to $(1/T) \exp[-(T_0/T)^{1/2}]$, where $T_0$ is the characteristic temperature. Information on the localisation of states by the magnetic field and variable-range hopping between those states can then be obtained by analysing the magnetic field dependence of $T_0$. Breakdown of the integer quantum Hall effect can also be determined from the SdH measurements in the extreme quantum limit. As shown previously in Fig. 5.17, sample J401 which is of a high material quality, exhibited oscillation minima approaching zero near the maximum magnetic field of 15 T. It is thus expected that by increasing $B$ further, clear dissipationless minima is observed in the SdH curves. Indeed, the measurements on J401 under magnetic fields of up to 28 T have been carried out, showing such behaviour. The temperature dependence of the widths of these minima have enabled a phase diagram for breakdown of the QHE to be partially mapped out, and this work has been reported by Harris et al. (2001).

One common feature of the results presented in this thesis is the detrimental effect of structure-related defects, and in particular, the grain boundaries is found to play a crucial role in transport behaviour of both GaN and AlGaN/GaN layers. Therefore, linking the current work with other characterising methods that reveal information on
the structural properties is imperative. The proposed programme can be briefly listed as follows:

(i) Correlating with characterisation techniques such as atomic force, transmission electron and scanning tunnelling microscopy (AFM, TEM and STM, respectively). As an example, the dislocation density in GaN samples, determined from TEM, can be used in the scattering calculations carried out in Chapter 4, thus resulting in a more complete analysis. Also, the formation of grain boundaries and its effect as a function of the grain size can be verified from AFM and STM investigations.

(ii) From Capacitance-Voltage measurements, information on the concentration of doping atoms and their depth profile is obtained. Comparing these quantities with the values determined from the Hall data would be beneficial in assessing the accuracy of the analysis. In addition, the behaviour of contacts (e.g., leakage currents and Schottky barrier heights), knowledge which is useful in device fabrication, can be investigated by combining with Current-Voltage experiments.

(iii) Evidence of heavy compensation by deep acceptors in bulk GaN and dominant scattering by impurities introduced by intentional Si doping in AlGaN/GaN HEMT structures, has been discussed in this thesis. Hence, deep level transient spectroscopy (DLTS), where studies of the capacitance and current transients by thermally excited emptying of electrons or holes from traps are performed, allows quantitative information on the presence of deep carrier defects to be obtained.

(iv) Using transmission line methods (TLM), maximum carrier mobility and saturation velocity as a function of applied electric field can be established in 2DEG structures over a range of carrier densities. Group III nitrides show promising potential for high power, high temperature microwave devices, and comparing Monte-Carlo simulations of velocity-field characteristics with the TLM results would provide valuable information towards the device development research.
Bibliography


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