Spin and Magnetotransport Properties of Narrow Gap Semiconductors

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Abstract

This thesis describes both experimental and theoretical research into spin dependent phenomena in narrow-gap InSb/In$_{x}$Al$_{1-x}$Sb quantum wells (QWs). InSb QWs are attractive for the study of spin phenomena due to an inherent large spin-orbit coupling that produces a spin splitting of the band structure in zero field. The potential manipulation of the spin splitting with a gate electric field is the basis for a number of device applications and makes this system an exciting candidate for spin-based electrics.

Calculations of the spin-splitting parameters in a range of InSb/In$_{x}$Al$_{1-x}$Sb QWs based on an eight-band $k.p$ model are performed. Important insight concerning the relative significance of the Rashba and Dresselhaus spin splitting and the importance of heterostructure design on the spin dynamics is gained.

Magnetotransport measurements are performed on a series of gated 30 nm wide InSb QWs. The Rashba spin splitting parameter is experimentally determined as a function of carrier density from the analysis of beating patterns observed in the longitudinal resistivity. It is found that InSb QWs have a large and spin-dependent inhomogeneous broadening which significantly impacts on the observed phenomenon.

A fundamental obstacle to the efficient electrical injection of spin into a semiconductor from a ferromagnetic metal is the properties of the interface which must incorporate a tunnel barrier. InAlSb forms a natural Schottky tunnel barrier at the metal-semiconductor interface which can in theory be engineered to optimise the injection and detection of spin. In this thesis the low temperature transport properties of Ti/InAlSb Schottky barriers are characterised using various tunnelling models and it is shown that they can be used as a spin injection contact. Strategies and designs for engineered epitaxial InAlSb barriers are presented.
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Chapter 1

Introduction

1.1 Motivation for narrow gap III-V semiconductors

The development of transistor technology has been rapid and ongoing since the first reported (point contact) transistor by Bardeen and Brattain in 1948 [1]. Since the incorporation of the first field-effect transistors (FET) into integrated computer circuitry in the late 1950s, the number of devices per unit area has risen steadily by a factor of ~2 every 18 months; a trend commonly known as Moore’s Law [2]. Moore’s Law encapsulates the increasing complexity in design of devices and architectures required to maintain the development of computer processing technology. State-of-the-art computer processor chips incorporate complimentary metal oxide semiconductor (CMOS) technology based on Si with the number of devices per chip approaching ≈400 million and sub-50nm gate lengths [3].

As improvements in large scale fabrication techniques allow CMOS technology to be scaled down, fundamental operation issues such as power/heat dissipation, gate leakage and standby power have become evident making the lifetime of such technologies unclear at the present rate and demand of increasing computing power. Moreover, as device dimensions enter the nanoscale, purely quantum mechanical effects manifest which bring with them a degree of
uncertainty to various aspects of the device operation which may not, in the
conventional sense, be beneficial. Research in the CMOS industry is constantly
developing existing and new architecture designs to counter-act the effects of
reduced dimensions, but the need for alternative technologies and routes forward
has long been recognised.

\begin{table}[h]
\centering
\begin{tabular}{lllll}
\hline
 & $E_g$ & $\Delta$ & $m_{cb}^*$ & $\mu$ (300 K) \\
\hline
InSb & 0.235 eV & 0.81 eV & 0.014 $m_0$ & 7.8 \\
InAs & 0.42 eV & 0.38 eV & 0.024 $m_0$ & 3.3 \\
GaAs & 1.519 eV & 0.341 eV & 0.067 $m_0$ & 0.85 \\
Si & 3.2 eV & 0.044 eV & 0.19 $m_0$ & 0.15 \\
\hline
\end{tabular}
\caption{The fundamental band gap $E_g$, spin-orbit energy $\Delta$, effective mass $m_{cb}^*$ and mobility $\mu$ (300 K) for bulk InSb, InAs, GaAs and Si at 10 K [4].}
\end{table}

The intrinsic light effective mass in III-V compound semiconductors result in a
high electron mobility and potentially higher operating speeds than Si based
structures. III-V devices can operate at lower voltages and offer hence lower
power requirements. These properties have attracted considerable research and the
development of III-V based high electron mobility transistors (HEMTs). However, more fundamental draw backs such as the lack of a native oxide, such
as SiO$_2$ which readily forms on Si and eases fabrication have limited their
expansion into consumer electronics to only specific components of products.

Table 1.1 lists some material properties of narrow-gap semiconductors
InSb and InAs and wider gap semiconductors GaAs and Si of interest. InSb has
the lightest effective mass, smallest band gap and largest spin-orbit gap of all III-
V compounds. The electron mobility scales inversely with the effective mass and
for that reason the room temperature mobility in InSb is significantly larger than
other III-Vs and notably almost an order of magnitude greater than that in GaAs.
Nevertheless, research in III-Vs has historically focused on GaAs and its heterostructures. Of note, the discovery of the Gunn effect [5] stimulated a great deal of research toward improving the quality of crystal growth through various growth techniques such as molecular beam epitaxy (MBE).

Due to this past trend in research, it is now desirable both economically and for integration into existing technologies for prospective III-V materials to be grown onto standard production GaAs or Si substrates. This poses a fundamental and challenging problem for the growth of narrow band gap semiconductors due to the large lattice mismatch between the substrate and the target material (≈14.5% for InSb on GaAs). Lattice mismatches can lead to strain induced misfit dislocations at the substrate interface that are detrimental to device performance. Indeed, the difficulties in MBE growth of high quality, low defect density wafers of InSb and InAs on GaAs or Si substrates has significantly impeded their development until more recently [6]. For this reason, immediate research in narrow gap III-V HEMTs has highlighted the ternary In$_{1-x}$Ga$_x$As system [7] as a promising candidate for future high-speed and low power digital logic applications. The small Ga content dramatically reduces the lattice mismatch to the GaAs substrate whilst retaining the properties associated with a narrow band gap.

Advances in the growth of high quality InSb heterostructures have resulted in extrinsic carrier mobilities $\mu$ recently reported in excess of 5 m$^2$V$^{-1}$s$^{-1}$ at room temperature. This attribute makes InSb quantum wells (QWs) particularly attractive for high-speed electronics (HEMTs) [8], ballistic transport devices and magnetic sensor applications such as non-magnetic read heads based on extraordinary magneto-resistance [9]. Recent advances in InSb QW FET technology have demonstrated improvements in performance over Si counterparts based on equivalent device scales [10], maintaining the interest in this material system for future high speed logic applications.
1.2 Semiconductor spintronics

An alternative approach to the traditional charge based electronics is to harness the quantum effects to produce a new type of device functionality, such as utilising and manipulating the electron spin. It is argued that spin-based electronics, so-called spintronics could potentially offer the same performance and functionality as traditional charge-based device but at a fraction of the power [11].

Notable advances in the study of spin transport include, the initial experiments on ferromagnetic-insulator-superconductor tunnel junctions by Tedrow and Meservey that demonstrated the presence of a spin polarized tunnelling current [12] and the subsequent studies of magnetic multi-layers [13] which resulted in the discovery of giant magnetoresistance (GMR) [14] and tunnelling magnetoresistance (TMR). These milestones ultimately lead to the realisation of metallic spin-based devices; some of which are now integrated into consumer-end products such as magnetic read heads based on spin valves in hard disk drives [15].

Spin transport in semiconductor-based devices holds a number of distinct advantages over that in metals, primarily the long spin lifetimes and high electron mobilities. In addition, the prospect of a tunable zero field spin splitting in two dimensional electron gases (2DEGs) formed in semiconductor heterostructures via the Rashba effect (described in chapter 4) provides a new type of device functionality which has seeded a variety of semiconductor spin-based device proposals [16-18]. Perhaps the most cited of these is the electronic analogue of the opto-electric modulator proposed by S. Datta and B. Das in 1990 [16] that operates on the basis that the precession angle of an electron spin traversing the device can be coherently modulated by \( \pi \) radians relative to a magnetised detector electrode by applying a gate electric field via the Rashba effect in a ferromagnet/semiconductor hybrid structure [19]. Coined the ‘spin transistor’, this novel and important proposal provided the impetus for numerous experimental
and theoretical research groups around the world to develop the fundamental physics and understanding of semiconductor spintronics - which is now a rich field of condensed matter physics.

Whilst the development and understanding of the fundamental physics in narrow band gap semiconductors such as InSb and InAs is at a relatively immature stage compared to their more extensively studied wider gap counterparts such as Si and GaAs, the physical properties inherent to narrow gap semiconductors offer unique characteristics which may be beneficial for both existing electronics and future spintronic applications. The Rashba coefficient $\alpha_0$ which parameterises the strength of the interaction with electric field scales inversely with the band gap and hence narrow gap semiconductors offer greater potential for the controlled manipulation of spins via the Rashba effect (see chapter 4). This coupled with the recent advances in the InSb/AlInSb QW FET technologies makes InSb stand out as a promising candidate for developing hybrid spintronic technology.

In general, semiconductor spintronic devices require the satisfaction of three criteria:

(i) The injection of a spin polarised current.

(ii) A means to manipulate the coherent spin ensemble.

(iii) A means to detect the spin polarised current after its transport through the device.

These can be investigated individually using optical and electrical measurements. The second criterion is concerned with the Rashba effect. The first and third criteria are discussed in the following section.
1.3 Introduction to spin injection

Functional spintronic devices such as the GMR based spin valve or the spin transistor require the electrical injection of spins into device to create a non-equilibrium spin population in an otherwise unpolarised medium such as a normal metal or semiconductor. Excitation of spin polarized carriers into the conduction band using pulsed circularly polarised light is an alternative means of optical spin injection. Application of small in-plane magnetic fields result in Larmor precession of the spin ensemble and the subsequent time-resolved detection of the Faraday-rotation of the linearly polarised probe pulse gives a measure of the spin coherence lifetime, $\tau_c$ [20]. This is a well established technique that has been applied to numerous III-V semiconductors, revealing the preservation of spin coherence over practical time scales and in most cases the dominance of the D'yakonov-Perel' mechanism, crucial for device proposals based on or around the Rashba effect (see chapter 4). Room temperature spin lifetimes in $n$-type GaAs, InAs and (undoped) InSb have been reported to be $\tau_c = 100$ ns [20], $\tau_c = 26$ ps [21] and $\tau_c = 2.5$ ps [22] respectively. In addition to this, Kikkawa and Awschalom showed in GaAs that by applying small in plane electric fields (16 Vcm$^{-1}$), lateral transport of the (optically) injected spin ensemble could be achieved over distances exceeding 100 $\mu$m [23].

Despite these achievements, the most fundamental obstacle for realising an all electrical, spin injection/detection device such as a spin valve or spin transistor [16], is the ability to electrically inject and detect a spin polarised current in the semiconductor. Early on it was shown that magnetic semiconductors (ferromagnetic [24] and paramagnetic [25]) could be used as efficient spin injection sources at low temperatures, but the performance rapidly diminishes with increasing temperature limiting their usefulness. Ferromagnetic metals that have Curie temperatures greater than room temperature and are thus attractive for spin injectors. However, initial experiments based on Ohmic contacts failed to inject sizable spin polarisation [26].
1.3. Introduction to spin injection

Summary of Electron Spin Injection Results

Figure 1.1: Spin polarisation results obtained from spin LEDs measurements using electrical injection for various injection schemes including paramagnetic semiconductors (PSC) and ferromagnetic semiconductors (FSC). Data summarises the main results achieved to date. (After [25,27-29]).

An important step towards understanding the physics of ferromagnetic metal-semiconductor interfaces and the mechanisms that govern the injection of spin was made by Schmidt et al., [30] who showed that it is virtually impossible to inject sizable spin-polarized current from a ferromagnetic metal (FM) to a semiconductor (SC) using a simple Ohmic contact technique due to the large conductivity mismatch between the two materials at the interface, typically $\sigma_{FM}/\sigma_{SC} \sim 10^4$. Fert and Jaffres [31] developed these ideas and showed that significant spin polarization of the injected current could be restored by introducing a large spin-preserving interface resistance, such as a tunnel barrier in the form of an ultra thin dielectric or an engineered Schottky barrier.

A large number of experiments have since been performed on devices incorporating interface tunnel barriers that verified these predictions and demonstrated the electrical injection of sizable spin polarised current. These spin
injection experiments typically utilise a spin light emitting diode (spin LED) structure to optically detect spin polarisation from the emission of circularly polarised light (resulting from the radiative recombination of majority spin carriers with unpolarised carriers from the valence band). Engineered Schottky barriers [28] as well as metal-oxide tunnel barriers [29] have both been successfully demonstrated as efficient spin injectors in GaAs QW spin LEDs, with room temperature spin polarisations as high as 32% in the latter. The main (electron) spin injection results obtained from various materials and injection strategies are presented in figure 1.1 according to the maximum spin polarization versus temperature.

Schottky barriers which form naturally at most semiconductor/metal interfaces provide a natural tunnel barrier to electrons without the difficulties of producing discrete pin-hole free oxide film [32]. A like-for-like comparison of spin injection into GaAs via Fe/AlGaAs Schottky and Fe/AlOₓ tunnel barriers was made by van’t Erve et al., (using spin LEDs) [33]. Their results indicated that while the injected spin polarisation was larger in the Fe/AlOₓ/AlGaAs structures (40%) than in the Fe/AlGaAs barrier structures (32%), the operating efficiency of the Fe/AlGaAs Schottky structure was significantly greater (supposedly) due to scattering at the AlOₓ/AlGaAs interface.

The viability of using the InAlSb Schottky for spin injection into InSb QWs is investigated in chapter 6.

1.4 Electrical measurements of zero field spin splitting

The two most common techniques used for experimentally determining the strength of the spin-orbit (SO) coupling are (i) the observation and fitting of quantum interference corrections to the low field magnetoconductance to weak anti-localisation (WAL) theory [34] and (ii) the observation and analysis of beating patterns in the Shubnikov de-Haas (SdH) oscillations in the magnetoresistance ρxx at higher magnetic fields, B.
The effect of zero field spin splitting on the SdH oscillations in a 2DEG was first observed by Lou et al., in the InAs/GaSb QW system [36] as a pronounced beating pattern rather than the simple oscillations periodic in 1/B. A beautiful example of this phenomenon is shown in figure 1.2 taken from [35].

The beating effect observed in $\rho_{xy}$ is analogous to optical beating, produced from the superposition of two frequencies with similar amplitudes, which is frequently been interpreted by various authors as originating from the two spin-split subbands [37-39]. This is often supported by the observation of a distinct double peaked structure in the Fourier transform (FT), corresponding to the frequency and population of each spin-split subband [39]. The interpretation of beating originating from zero field spin splitting can be controversial because several alternative explanations for the occurrence of beating patterns have been proposed, such as magneto inter-subband scattering [40]. Also the influence of
Zeeman splitting on the extracted values of the Rashba parameter is often unaccounted for in analysis [39]. Provided one can justifiably attribute the beating patterns to zero field spin splitting and moreover the Rashba effect, the subsequent analysis yields a quantitative measure of the spin splitting from which the Rashba parameter can be extracted. This type of measurement and analysis is presented in chapter 5.

1.4.1 Measurements in InSb

Extensive WAL experiments have been performed previously on InSb thin film epilayers grown on GaAs (100) [41] and InSb/CdTe heterojunctions [42], providing unambiguous evidence for the presence of spin-orbit (SO) coupling in 2DEGs formed at the heterointerfaces. In contrast, only a small number of elegant measurements of the SO coupling have been made in InSb QWs; some of these measurements are rather indirect and none use beating effects which have not been observed previously in InSb QWs. A large g-factor means that Zeeman splitting dominates the SdH oscillations at relatively small fields compared to other systems making the observation of beating patterns particularly challenging in narrow gap systems. In addition, the high mobility in InSb QWs suppresses the emergence of the WAL feature; a requirement of which is that the phase coherence time be much greater than the momentum scattering time (WAL is a scattering driven phenomena). Dedigama et al. recently reported the first observations of WAL in a (low mobility) InSb QW supporting the presence of large SO coupling [43]. In an alternative approach, using electron spin resonance measurements Khodaparast et al. [44] extrapolated a spin splitting to zero field in an asymmetric 30 nm InSb/InAlSb QW. Assuming the Rashba interaction to be dominant $\alpha$ was determined to be as high as $1.3 \times 10^{-11}$ eV m. The work presented in chapters 4 and 5 of this thesis contribute both theoretically and experimental to the knowledge of zero field spin splitting and the Rashba
1.4. Electrical measurements of zero-field spin splitting effect in InSb QWs. Notably, magnetotransport data is presented which exhibit beating patterns for the first time from which $\alpha$ is extracted.

1.5 Outline of thesis

Whilst narrow gap semiconductors offer a number of properties advantageous to device applications, their potential for spintronics has yet to be harnessed. The work presented in this thesis was undertaken (i) at QinetiQ Malvern, whilst InSb QW transistor technology was being developed and (ii) during the lifetime of a large EPSRC funded project "spin polarised injection into narrow gap semiconductors", "SPRINGS". The thesis is organised as follows. In chapter 2 an introduction to some of the properties of III-V semiconductors is given such as the basic band structure. Specific emphasis is placed on narrow gap semiconductors and the effect of band non-parabolicity. Useful expressions for the Fermi energy and effective mass are derived which are used later in the thesis.

Chapter 3 describes the growth of InSb heterostructures using MBE and the difficulties associated with mismatched growth. The fabrication techniques used to process the gated Hall bars and three terminal FET geometry devices studied are given along with details of the measurement techniques and the equipment used. Finally, a summary of the all the samples and devices measured are also found here.

Chapter 4 is the first results chapter, presenting the modelling of InSb heterostructures and determination of the Rashba and Dresselhaus spin splitting parameters in realistic devices. The concept of zero field spin splitting originating from the spin-orbit coupling in the presence of inversion asymmetry is introduced and the origins in zincblende crystals. An eight band $k.p$ model is introduced for the spin splitting of conduction bands in narrow gap semiconductors due to inversion asymmetry [45]. Making use of a self consistent Schrödinger-Poisson model, calculations of the zero field spin splitting in InSb/InAlSb heterostructures are performed for a variety of device structures i.e. QW widths and doping and
barrier Al content. A number of new results are presented which are compared to existing results in similar material systems and frequently used approximations. The approach enables the relatively straightforward calculation of the D’yakonov Perel’ spin lifetimes and the chapter is concluded by analysing the anisotropic spin lifetime components in the plane of the 2DEG and the growth direction in the context of the spin lifetime transistor [18].

Other than optical measurement of spin lifetime, few electrical measurements of the spin-orbit coupling in InSb quantum wells exist. Chapter 5 is an experimental results chapter describing the high and low field magnetotransport measurements of gated InSb quantum wells. Low field measurements are used to characterise the momentum scattering processes controlling the electron mobility in the QWs. High field measurements are used to explore the effects of zero field spin splitting which manifest as beating patterns in the Shubnikov de-Haas oscillations. Values for the Rashba spin splitting parameter are extracted as a function of gate bias for the first time in this material system using this technique and the factors that control the appearance of beating patterns are discussed.

Chapter 6 describes the low temperature electrical characterisation of InAlSb Schottky tunnel barriers in a modulation doped InSb/InAlSb heterostructure, and their suitability as spin injectors. Three terminal $I-V$ measurements are analysed between 4.5 K and 100 K using various tunnelling models. It is demonstrated that the InAlSb barrier can support single step tunnelling and has a resistance suitable for a spin injection but not spin detection. A number of anomalous conductance characteristics are observed. Two different approaches to engineering the resistance of the Schottky barrier in InSb heterostructures to be within the desired range for electrical injection and detection of spin are presented.

Chapter 7 summarises the results obtained from the research undertaken and discusses the future research areas. A number of appendices are included at the end of the thesis describing additional details relevant to the modelling performed in the thesis and substantial work that was performed in parallel to that described
in the bulk of the thesis on the fabrication of ferromagnetic-semiconductor hybrid structures in InAs and InSb.

1.6 Key contributions

My project was to aid the development and design of structures for spintronic devices in four ways (i) design epitaxial spin injectors, (ii) develop models to describe the spin properties of InSb QWs, (iii) develop processing strategies to make two-terminal spin valve structures (iv) measure and analyse spintronic devices. Although in the timescale of this project (iv) was not delivered, this thesis represents the work undertaken in (i), (ii) and (iii).

The key contributions to the field are listed here:

(1) It is demonstrated theoretically that the structural inversion asymmetry contribution to zero field spin splitting can not always be assumed dominant and that bulk inversion asymmetry is important in narrow gap InSb. This limits the spin lifetime and the operation of the spin lifetime transistor.

(2) Beating patterns in the magnetoresistance of InSb QWs are observed for the first time and experimental values for the Rashba spin splitting parameter are extracted as a function of carrier density. InSb QWs have an unexpected large level broadening which is spin dependent and can mask the appearance of beating patterns.

(3) It is shown that epitaxial InAlSb Schottky barriers are suitable as spin injection contacts. Designs for optimising the interface resistance for a spin valve device are given.

(4) A proper description of the scattering mechanism in modulation doped InSb QWs is given that describes the experimental temperature dependence of
the mobility well. It is shown that the low temperature mobilities are limited by remote ionised impurities.

(5) It is highlighted that optically injected spins oriented in the [001] direction experience greater relaxation than electrically injected spins in the [1\bar{1}0] direction (in the plane of the QW) and thus standard spin lifetime measurements do not accurately represent the spin dynamics in a lateral device. The extraction of the spin splitting parameters can be made from spin lifetime measurements using the model of Averkiev and Golub for the D'yakonov Perel' spin relaxation rate in the [001] direction.
1.7 List of publications

1.7.1 Key publications


1.7.2 Additional contributed publications


Chapter 2

Properties of narrow gap III-V semiconductors

Compounds III-V semiconductors such as InSb and GaAs have received a great deal of interest due to their intrinsic electrical and optical properties which offer advantages over their binary counterparts Si and Ge, such as high carrier mobility and direct band gap. From the standpoint of spintronics, the crystal lattice structure of III-V semiconductors is of zincblende type which lacks inversion symmetry. This lifts the spin degeneracy in zero magnetic field and will be discussed in detail in chapter 4. Crucially, this property is absent in the diamond crystal structure of Si or Ge and is the basis for a number of spintronic device proposals such as the Datta Das spin transistor [16].

Calculations of the spin-orbit coupling coefficients for the InSb/In_{1-x}Al_xSb quantum well system are performed in chapter 4 based on an eight-band $k.p$ model. An introduction to the band structure and the eight-band model are given here for completeness. Starting from Kane's eight-band model [46], a simplified effective two-band model for the conduction and light hole bands is generated which is valid near the band edges and takes into account band non-parabolicity. This model is used to derive energy corrections to a number of useful transport properties such as the effective mass at the Fermi energy $m^*(E_F)$ and density of
2.1. The zincblende crystal structure

III-V semiconductors typically crystallise into the zincblende crystal structure. It comprises of two interpenetrating face-centred cubic (fcc) sub-lattices, one for each atomic species. Figure 2.1 shows an example of the zincblende structure of the InSb unit cell. The theory of the zincblende crystal has been widely studied and the electronic states and the band structure of materials with this crystal structure are well established [46,47].

The band structure of a crystal, that is the energy-momentum \((E - k)\) space, is linked to the crystal lattice structure via the concept of reciprocal lattice; this is related to the direct crystal lattice through the reciprocal lattice vectors (not shown here), which have dimensions of \(m^{-1}\) i.e. momentum or wave vector \(k\).
2.1. The zincblende crystal structure

In reciprocal \((k)\) space, the Wigner-Seitz cell (which contains all lattice points which are nearer to one particular lattice point than to any other) represents the unit cell and defines the \textit{first Brillouin Zone}. The first Brillouin zone common to both the diamond and zincblende lattice is the truncated octahedron shown in figure 2.2 indicating the important symmetry points and lines. These symmetry points \(L\), \(X\), \(K\), \(U\), etc. are invariant under rotation and reflection about the zone centre \((k = 0)\) denoted by the \(\Gamma\)-point. Hence there are six equivalent \(X\)-points, eight \(L\)-points etc. Due to the periodicity of the lattice in \(k\)-space, it can be shown that all points \(k'\) outside the first zone can be mapped to an equivalent point \(k\) within the first Brillouin zone. Therefore, when considering the band structure of a particular semiconductor, it is sufficient to solve only for energies within the first Brillouin zone for each band. Three directions of \(k\) are generally considered in such calculations which are the \(\Delta\)-line directed along [010], the \(\Lambda\)-line directed along [111] and the \(\Sigma\)-line directed along [100].

\textbf{Figure 2.2:} The first Brillouin zone for the zincblende (and diamond) structure indicating the important symmetry points and lines. \(k_x\), \(k_y\), and \(k_z\) axes are in the \([100]\), \([010]\) and \([001]\) directions respectively.
2.1. The zincblende crystal structure

Examples of the band structure of InSb, InAs and GaAs calculated along these symmetry lines are shown in figure 2.5.

2.2 Band structure of III-V semiconductors

The gross features in the band structure of III-V semiconductors can be described by four bands (eight including spin), likened to one s-type and three p-type atomic orbitals. These are the $\Gamma_{6c}$ conduction band, the $\Gamma_{8v}$ valance band (light and heavy holes) and the $\Gamma_{7v}$ split-off band respectively and are shown schematically figure 2.3.
The fundamental band gap $E_g$ and the spin-orbit splitting of the valance band $\Delta$ are defined. Low temperature values of energy gaps for some bulk III-V compounds of interest are listed in table 1.1 for comparison.

The simplest model for the band structure of a quasi-2D system near the band edge is the effective mass approximation (EMA) which assumes a single, isotropic, parabolic band ignoring any spin-orbit coupling (see also appendix B). More advanced models such as the $k.p$ method provide a more accurate description of the energy bands (i.e. beyond just the conduction band) and allows for the effects of band non-parabolicity and spin-orbit coupling to be included (see also chapter 4). The main idea of the $k.p$ method is to analyse a small region of $k$-space near to the zone centre where the transport takes place. It is important to note however that both the EMA and the $k.p$ method are based on the envelope function approximation (EFA) which modulates the quickly varying lattice-periodic part of the Bloch function illustrated in figure 2.4 [48]. As a result the EFA approach is only an approximation of the true interacting system, valid when
the envelope function $\Psi(r,z)$ varies slowly over the scale of the lattice constant and for energies close to the band edge \[49\]. The solution to the EMA Hamiltonian for the energy dispersion of the conduction band is parabolic and described by \[50\]

$$E_c(k) = E_n + \frac{\hbar^2 k^2}{2m_{cb\perp}}$$

where $m_{cb\perp}$ is the in-plane effective mass at the conduction band edge and $E_n$ is the energy at the bottom of the $n^{th}$ subband ($n = 1, 2, \ldots$). For clarity the subscript $\perp$ will be dropped hereafter. For parabolic bands, $m_{cb\perp}$ is energy independent and can be ascribed to the curvature of the conduction band according to the second derivative of the dispersion with respect to the wave vector $1/m_{cb\perp} = \hbar^2 \left( \frac{\partial^2 E}{\partial k^2} \right)$. The significance of the description “at the conduction band edge” will become clearer when the effects of band non-parabolicity are introduced later in this section.

InSb has the lightest effective mass of all III-V semiconductors, resulting in a high room temperature carrier mobility (see Table 1.1). This is discussed further in chapter 5.

Empirical techniques such as the relativistic tight binding and the non-local pseudo-potential methods \[51,52\] go beyond the EFA based methods and describe the entire band structure within the Brillouin zone of semiconductors, providing useful insight. Examples of the band structures of GaAs, InSb and InAs calculated from the pseudo-potential method are shown in figure 2.5 for the three main directions in $k$-space, $\Lambda \ [111]$, $\Delta \ [010]$ and $\Sigma \ [110]$ (data taken from \[52\]). One can see that the entire band structure near the zone centre consists of sixteen bands (including spin degeneracy).

\[1\] However, in the majority of cases concerning electron transport, conduction takes place within a few tens of meV from the band edge, and a near band edge approach is most appropriate.
2.2. Band structure of III-V semiconductors

Figure 2.5: Band structure of (a) GaAs (top left) (b) InSb (top right) and (c) InAs (bottom) along symmetry lines as calculated from the pseudo-potential method (taken from [52]). Energies are measured in eV relative to the $\Gamma_{8v}$ valence band.

In the case of InSb and InAs [see figure 2.5(b) and (c)] the higher conduction bands $\Gamma_{c7}$ and $\Gamma_{c8}$ and lower valence band $\Gamma_{v6}$ are energetically remote (i.e. $>>E_g$) from the four bands illustrated in figure 2.3 which allows for a simplified treatment of band structure close to the band edge which is discussed...
below. This is not the case in the wider gap GaAs system [figure 2.5(a)], where the separation of the higher conduction bands from the $\Gamma_{ec}$ conduction band is comparable to the band gap $E_g$.

In general, the conduction band of III-V semiconductors becomes increasingly non-parabolic at large values of $k$. Due to its narrow band gap, the conduction band of InSb becomes highly non-parabolic at energies greater than a fraction of the energy gap $E_g$. This results in an energy dependence in the effective mass which is reflected in a number of transport properties. As we will see in following sections these corrections are significant in InSb and are taken into account throughout this thesis. These effects are discussed in the following section for reference in subsequent chapters.

2.3 Band non-parabolicity

The effects of band non-parabolicity can most easily be introduced by Kane's eight-band model [53]. The eight bands considered in this model are those shown in figure 2.3, one for each spin, and all other bands are neglected (for reasons discussed in the previous section). The model successfully describes the conduction bands of narrow gap semiconductors like InSb and InAs as in this case the interactions between the $\Gamma_{6c}$-$\Gamma_{8v}$ and $\Gamma_{6c}$-$\Gamma_{7v}$ (i.e. conduction-valence and conduction-split-off) bands dominate [54]. Although more refined models have since been developed by various authors, the Kane model is commonly used as its parameters are well known [55].

---

2 Often referred to as the three level model as the light and heavy holes bands are degenerate at $k = 0$.

3 For wider gap systems such as the GaAs, it is often necessary to include the more distant bands $\Gamma_{7c}$ and $\Gamma_{8c}$ known as the 14 band or five level model in order to describe experimental data.
The eight-band Kane Hamiltonian matrix (without spin-orbit coupling) is [55,56]

\[
H_s = \begin{pmatrix}
\frac{E_s}{2} & \frac{1}{\sqrt{2}} \hbar c k_z & -\hbar c k_y & \frac{\sqrt{3}}{2} \hbar c k_x & 0 & -\hbar c k_x & -\frac{1}{\sqrt{2}} \hbar c k_x & 0 \\
\frac{1}{\sqrt{2}} \hbar c k_x & \frac{1}{2} E_s - \Delta & 0 & 0 & \hbar c k_y & 0 & 0 & 0 \\
-\hbar c k_y & 0 & -\frac{E_s}{2} & 0 & \frac{1}{\sqrt{2}} \hbar c k_x & 0 & 0 & 0 \\
\frac{3}{2} \hbar c k_x & 0 & 0 & -\frac{E_s}{2} & 0 & 0 & 0 & 0 \\
0 & \hbar c k_x & \frac{1}{\sqrt{2}} \hbar c k_x & 0 & \frac{E_s}{2} & \frac{1}{\sqrt{2}} \hbar c k_y & -\hbar c k_z & \sqrt{3} \hbar c k_x \\
-\hbar c k_z & 0 & 0 & 0 & \frac{1}{\sqrt{2}} \hbar c k_y & -\frac{E_s}{2} - \Delta & 0 & 0 \\
-\frac{1}{\sqrt{2}} \hbar c k_x & 0 & 0 & 0 & -\hbar c k_y & 0 & -\frac{E_s}{2} & 0 \\
0 & 0 & 0 & 0 & \frac{3}{2} \hbar c k_x & 0 & 0 & -\frac{E_s}{2}
\end{pmatrix}
\]

(2.2)

where the energy zero is taken to be at mid-gap, \( k_z = \frac{k_x \pm ik_y}{\sqrt{2}} \) and \( c = \sqrt{\frac{2}{3}} \frac{P}{\hbar} \) (dimensions of speed). \( P \) is Kane’s interband momentum matrix element which couples the bands (\( P \) is nearly constant for all materials [46]).

### 2.3.1 The two-band model

Eight-band calculations of the conduction band can be numerically challenging and in some applications are unnecessary. Under certain approximations a simplified two-band model can be used which captures the main effects of non-parabolicity. The outline of the derivation is given below. The matrix in equation 2.2 can be simplified by choosing the axis of quantisation in the \( z \)-direction. Then \( k_z, k_x = 0 \) and equation 2.2 transforms into the block diagonal form [56]

\[
H_s = \begin{pmatrix}
\bar{H} & 0 \\
0 & \bar{H}
\end{pmatrix}
\]

(2.3)
2.3. Band non-parabolicity

where,

\[
\tilde{H} = \begin{pmatrix}
    \frac{E_g}{2} & \frac{1}{\sqrt{2}} \hbar c k_z & -\hbar c k_z & 0 \\
    \frac{1}{\sqrt{2}} \hbar c k_z & -\frac{E_g}{2} - \Delta & 0 & 0 \\
    -\hbar c k_z & 0 & -\frac{E_g}{2} & 0 \\
    0 & 0 & 0 & -\frac{E_g}{2}
\end{pmatrix}.
\] (2.4)

From inspection of equation 2.4, we see that within this model there exists a dispersionless (i.e. infinite mass) band passing the energy \(-E_g/2\) which is decoupled from the other bands. This is the heavy hole band which can be neglected. For narrow gap semiconductors of interest such as InSb, the split-off energy \(\Delta\) is significantly greater than the band gap \(E_g\) \((\Delta >> E_g)\). Therefore as an approximation, in the eight-band Hamiltonian the coupling to the split-off band, which passes the energy \(-E_g/2 - \Delta\) can also be neglected (i.e. it is sufficiently remote from the conduction and valence bands that its presence can be neglected). Under these approximations and considering that the bands are doubly degenerate (no spin-orbit coupling has been included), equation 2.4 simplifies to an effective two-band Hamiltonian for the conduction and light hole bands. The two-band Hamiltonian matrix is \([55,56]\)

\[
H_2 = \begin{pmatrix}
    \frac{E_g}{2} & \hbar c k \\
    -\hbar c k & -\frac{E_g}{2}
\end{pmatrix}.
\] (2.5)

Diagonalising the eight or two-band Hamiltonians leads to solutions for the energy dispersion. Note that at the zone centre \((k = 0)\) equation 2.2 and 2.5 are
already diagonal. The two-band model is frequently used as it has the advantage that it can be solved analytically. It becomes increasingly less valid as $k$ (and $E$) becomes large. The solutions for the conduction and light hole bands are

$$E_{c\uparrow\downarrow}(k) = \frac{E_g}{2} \sqrt{\frac{4\hbar^2 k^2 c^2}{E_g^2} + 1} \quad (2.6)$$

and

$$E_{\text{lh}\uparrow\downarrow}(k) = -\frac{E_g}{2} \sqrt{\frac{4\hbar^2 k^2 c^2}{E_g^2} + 1}. \quad (2.7)$$

The conduction and light hole band are the mirror image of one another about the centre of the band gap. In exploring the limits of equation 2.6 and 2.7 we find that for small $|k|$ close to the zone centre, the conduction band is parabolic, since to first order $E_{c\uparrow\downarrow} \approx \pm \left(\frac{\hbar^2 k^2 c^2}{E_g} + \frac{E_g}{2}\right)$ where as for large $|k|$ the dispersion becomes linear with $E \approx \hbar kc$. Figure 2.6 shows the conduction band energy dispersion for InSb and GaAs calculated from the two-band model using the parameters listed in table 1.1 (GaAs light hole band is not shown). When comparing the results from the two-band model to the parabolic band approximation (indicated by the black dashed lines) we see that the conduction band of InSb deviates from parabolic behaviour at significantly smaller values of $k$ than in GaAs, demonstrating the relatively large non-parabolicity in the bands of InSb. This result is summarised in table 2.1 which gives the percentage deviation from parabolic behaviour at the Fermi wave vector corresponding to a carrier density of $3 \times 10^{15} \text{m}^{-2}$ in the InSb, InAs and GaAs systems. The main result is that as the band gap is reduced the non-parabolicity of the bands increases.
2.3. Band non-parabolicity

Figure 2.6: Conduction band (green line) and valance band (blue line) of InSb generated from the two-band model compared to the parabolic band approximation (dashed black line). Also shown is the result for the GaAs conduction band using parameters from Table 1.1.

| TABLE 2.1: Percentage deviation of the two-band model from the parabolic band approximation at $n_{2D} = 3 \times 10^{13} \text{m}^{-2}$ |
|---------------------------------|-----------------|-----------------|-----------------|
|                                 | InSb            | InAs            | GaAs            |
| $E_g$                           | 0.235 eV        | 0.42 eV         | 1.512 eV        |
| Deviation from parabola         | 15.5%           | 10%             | 0.7%            |
Substituting $\tilde{E} = (E - E_g / 2)$ into equation 2.7, shifts the energy zero to the conduction band edge. By comparing this result to the parabolic dispersion (c.f. equation 2.2) it is found that the parameter $c$ is related to the effective mass by $c^2 = \frac{1}{2m^*_{cb}}$. The conduction band dispersion can then be expressed in its more familiar form

$$\tilde{E}(1 + \lambda \tilde{E}) = \frac{\hbar^2 k^2}{2m^*_{cb}}$$

where $\lambda = 1/E_g$ is the non-parabolicity factor. The value of the $c$ parameter is approximately $c_0/300$ (where $c_0$ is the speed of light) for all III-V semiconductors \[57\]. The conduction band dispersion in equation 2.8 can be readily implemented to derive the non-parabolic corrections to a number of basic electron transport properties. Some of these will be derived here in. For clarity, the notation $\tilde{E}$ will be dropped and the energy zero will be taken to be at the bottom of the conduction band.

### 2.4 Two-dimensional density of states ($B = 0$)

The density of states (DoS) is the number of states per unit energy per unit area and for parabolic bands is described by

$$N_p(E) = \frac{m^*_{cb}}{\pi \hbar^2} \Theta(E - E_n)$$

Here the subscript $p$ refers to its derivation from a parabolic energy dispersion and $\Theta(E - E_n)$ is the step function centred on the subband edge $E_n$. The derivation of equation 2.9 is given in appendix D. In a quantum well with
multiple occupied subbands, each subband contributes a step in the DoS. Figure 2.7 shows the DoS for the ground state as a function of energy indicated by the solid black line (the energy scale has been normalised to the subband energy $E_n$).

The total carrier density in the 2DEG is the total number of occupied states beneath the Fermi energy $E_F$. This is found by integrating the DoS multiplied by the Fermi-Dirac distribution function according to \[\frac{1}{n_2D} = \int_0^\infty N(E)F(E, T)dE\] (2.10)

where

\[F(E, T) = \left[1 + \exp\left(\frac{E - E_F}{k_B T}\right)\right]^{-1}.\] (2.11)

Here $k_B$ is Boltzmann's constant and $T$ the temperature. At $T = 0$ in the degenerate limit, the carrier density is related to the Fermi energy by $n_{2D} = \frac{m^*_e}{\pi\hbar^2} E_F$. The carrier density can also be expressed in terms of the Fermi wave vector $k_F$ through the simple expression $k_F = \sqrt{2m_{2D} E_F}$. From inspection of equation 2.9, we see that the DoS in narrow gap semiconductors, and particularly for InSb, is small compared to other III-V semiconductors due to the light effective mass. Physically, this means that for the same Fermi energy, the carrier density in InSb is smaller than in a wider gap material like GaAs and higher subbands will become occupied at lower carrier densities.

2.4.1 Implementation of the two-band model

Using the non-parabolic energy dispersion the DoS can be derived revealing additional energy dependences absent in the parabolic band approximation (the derivation is shown in appendix D). The modified DoS for non-parabolic bands is given by,
Two-dimensional density of states (B = 0)

Figure 2.7: Two-dimensional density of States in the parabolic band approximation (black line) and taking into account non-parabolicity through the two-band model (red dashed line).

\[ N_{np}(E) = \frac{m^*_n}{\pi \hbar^2} (1 + 2\lambda E) \Theta(E - E_n) \]  \hspace{1cm} (2.12)

where now the subscript \( np \) refers to its derivation from non-parabolic dispersion.

Figure 2.8 shows the DoS as a function of energy for the two-band model (red dashed line) compared to the parabolic band approximation using parameters listed in table 1.1 for InSb.

We see that for \( E = 0 \), the non-parabolic DoS reduces to result for parabolic bands, whereas for energies of a few tens of meV the DoS increases significantly. Evaluating the carrier density as defined in equation 2.10 using \( N_{np}(E) \) leads to a non-linear energy dependence described by

\[ n_{2D} = \frac{m^*_n}{\pi \hbar^2} E_p (1 + \lambda E_p). \]  \hspace{1cm} (2.13)
It is interesting to note that the expression relating the Fermi wave vector to the carrier density remains unchanged for non-parabolic bands. This can be understood by the following argument; in $k$-space, the Fermi surface for a 2D system is a circle whose radius is the Fermi wave vector $k_F$. The carrier density is the total number of allowed states enclosed by the circle per unit area. By considering the area of the Fermi circle $\pi k_F^2$ and the area per state $\frac{(2\pi)^2}{Area}$ (in $k$-space), we see that neither hold any material parameters. It is then straightforward to show that the carrier density remains related to the Fermi wave vector through $k_F = \sqrt{2\pi m_{2D}}$.

From inspection of equation 2.13, the effect of non-parabolicity can be interpreted as an energy dependent effective mass. In the quasi-free electron approach, the effective mass was related to the second derivative of the energy dispersion with respect to the wave vector. This is only valid for parabolic bands. In general, we define a DoS effective mass which is related to the first derivative of the energy dispersion with respect to the wave vector by [59]

$$\frac{1}{m^*} = \frac{1}{h^2 k} \frac{\partial E(k)}{\partial k}.$$  \hspace{1cm} (2.14)

For parabolic bands the different mass definitions are identical, however, in the case of non-parabolic bands one has to distinguish between them. From equation 2.8 effective mass is then given by

$$m^*(E) = m^*_{cb} \left(1 + \frac{2E}{E_S}\right).$$  \hspace{1cm} (2.15)

Often from an experimental point of view, it is more useful to work with quantities such as the carrier density which is extracted from measurements of the
Hall effect (see chapter 5) rather than energy. The most well known parameters available are the carrier density \( n_{2D} \), the band edge effective mass \( m^{*\text{cb}} \) and the band gap \( E_g \).

Equation 2.13 gives the carrier density in terms of the Fermi energy \( E_F \), \( m^{*\text{cb}} \) and \( E_g \). Equally, the Fermi energy can be expressed in terms of \( n_{2D} \), \( m^{*\text{cb}} \) and \( E_g \) by solving the quadratic for \( E = E_F \) in either equation 2.8 or 2.13 (with the substitution for \( k_F \)) giving

\[
E_F = \left( \frac{E_g^2}{4} + \frac{E_g \pi \hbar^2 n_s}{m^{*\text{cb}}} \right)^{\frac{1}{2}} - \frac{E_g}{2}
\]  

(2.16)

Figure 2.8: The carrier density dependence of the effective mass \( m^{*\text{cb}}(E_g) \) in InSb calculated using equation 2.16 and equation 2.15. Significant deviation from the band edge value \( m^{*\text{cb}} \) is found for moderate carrier densities.
Therefore, for a given carrier density, using equation 2.16 in conjunction with equation 2.15, a more appropriate effective mass at the Fermi energy rather than at the band edge $m_{cb}^*$ can be estimated. The carrier density dependence of the effective mass generated from the two-band model is presented in figure 2.8 using parameters for InSb listed in table 1.1. Figure 2.8 demonstrates that even at relatively low carrier densities of around $3 \times 10^{15}\ m^{-2}$ there is a significant increase in $m^*$ from the band edge value $m_{cb}^*$. This description of the effective mass agrees well with recent experimental data obtained from similar InSb QWs [60] and is used in the analysis of magnetotransport data presented in chapter 5.

It should be clarified that the analytical expressions derived from the Kane model in this chapter are for bulk materials, where $m_{cb}^*$ is the effective mass at the conduction band edge and the energy corrections are for energies measured relative the conduction band edge. In the case of a QW, the Fermi energy is measured relative to the subband edge. In this case, the simplest substitution in the expressions above would be to replace $m_{cb}^*$ with $m_{sb}^*$ to denote the effective mass at the subband edge (the energy dependence is not expected to change). It follows from the results obtained for the bulk that in general $m_{sb}^* > m_{cb}^*$. The subband mass is dependent on the confinement energy, hence it varies with QW width and details of the structure – note that it is increased upon reducing the QW. Accurate calculation of $m_{sb}^*$ for QW heterostructures requires a multi-band Schrödinger-Poisson model, which is beyond the scope of this thesis. Such a calculation has been performed for a similar 30nm InSb QW to those studied in this thesis showing that the disparity is small; $m_{sb}^*$ is $\approx 20\%$ greater than $m_{cb}^*$ [60]. Thus neglect of the confinement energy in the calculation of $m^*$ using equations 2.15 and 2.16 leads to a small overestimation of the experimental Landau level broadening $\Gamma$ and Rashba parameter $\alpha$ presented in chapter 5 of the order $20\%$. 
Chapter 3

Growth, fabrication and experimental techniques

In this chapter, a description is given of the fabrication techniques and experimental methods used in thesis. Section 3.4 summarises the details of the layers and devices studied in chapters 5 and 6.

3.1 Growth of InSb heterostructures

Development in the growth of high quality heterostructures has been significantly accelerated by the techniques of molecular beam epitaxy (MBE) and modulation doping. MBE allows accurate control of layer thickness, elemental composition and the doping profile on the monolayer scale. The ultra high vacuum (UHV) environment in which the growth takes place allows for real time in situ monitoring techniques such as reflection high-energy electron diffraction (RHEED).

The capability of producing sharp atomic boundaries with the MBE technique allows materials of differing lattice constant and band gap to be grown sequentially on top of one another, forming discrete heterointerfaces.
3.1. Growth of InSb heterostructures

By alternating the growth of wider and narrower band gap materials, a ‘square’ quantum well is formed. Because of the potential barriers on both sides, these quantum wells can be grown as narrow as a few nanometres. During the 1980’s significant development were made in the growth of GaAs/AlGaAs heterostructures. It was realised that positioning the doping layer at a distance away from the 2DEG, so called modulation doping, enhances the mobility by several orders of magnitude over that of uniform doped structures. Pfeifer et al. demonstrated low temperature electron mobilities in an AlGaAs/GaAs heterostructure in excess of 100 m²V⁻¹s⁻¹ after illumination [61].

The modulation doped InSb QW samples studied in this thesis were grown by a commercial solid source MBE reactor at QinetiQ Malvern onto semi insulating GaAs (001) substrates. Epitaxial growth onto GaAs substrates is attractive from an economic standpoint because the substrate wafers (typically 3” in diameter) are relatively cheap and readily available. However, in practice the growth of a narrow gap semiconductor onto a wide gap substrate such as GaAs

Figure 3.1: Bandgap energy and lattice constant of various III-V semiconductors at room temperature.
introduces a number of difficulties. Figure 3.1 shows the band gap and lattice constants for various III-V semiconductors. One can see that the lattice mismatch between InSb and GaAs is as high as 14%. The large lattice mismatch introduces strain to the crystal which can result in structural defects such as misfit dislocations [62]. These dislocations propagate away from the heterointerface over large distances (which can be over a micron) and significantly degrade carrier mobility [63]. In addition, structural defects can present 'trap' states for electrons. These can have significant impact in tunnelling experiments if present in the potential barrier (see chapter 6). Lattice strain can be alleviated somewhat by the sequential growth of graded band gap materials i.e. varying Al fraction in the ternary $\text{Al}_x\text{In}_{1-x}\text{Sb}$ compound; this is generally referred to as the buffer layer.

From the above discussion it follows that to grow high quality InSb QWs, it is advantageous to separate the QW region from the heavily defected interface with the GaAs substrate. For this reason, the $\text{Al}_y\text{In}_{1-y}\text{Sb}$ lower barrier is typically
3.1. Growth of InSb heterostructures

grown 3μm thick which acts as a large buffer layer. The heterostructures studied in this thesis have a common structure which is shown schematically in the inset of figure 3.2. A type-I heterostructure is formed providing confinement for both electrons and holes. The Al$_{x}$In$_{1-x}$Sb upper barrier is delta doped with Te ($n$-type donor), separated from the QW by an undoped spacer layer of thickness $S$ which varies from 5 nm to 25 nm in the samples studied. Secondary ion mass spectroscopy (SIMS) of these structures reveal that the Te segregates through the structure in the growth direction. Subsequently, if the Te delta layer is positioned below the QW, ionised Te atoms (impurities) are present in the 2DEG which significantly reduces the mobility. Orr et al. recently reported on carrier mobilities in structures of type shown in figure 3.2 demonstrating a near exponential rise in the mobility with increasing spacer thickness [6]. This clearly underlines the powerful influence of modulation doping as a growth technique.

Growths of wide 30 nm quantum well structures as part of this PhD program showed a significant improvement on the electron mobilities achieved in InSb QWs to-date, the highest of which are presented in chapter 5 which exceed 60,000 cm$^2$V$^{-1}$s$^{-1}$ at room temperature and 400,000 cm$^2$V$^{-1}$s$^{-1}$ at 2 K.

3.2 Device fabrication

Semiconductor devices are fabricated from the as-grown wafer using combinations of photo and electron beam lithography, metal deposition and chemical etching. All the devices studied in this thesis were fabricated using the cleanroom facilities at QinetiQ Malvern. The techniques used to fabricate the devices measured in chapters 5 and 6 are given here. Details on the fabrication of structures used to characterise MgO tunnel barriers grown on InAs and InSb two-terminal spin valve devices are found in appendix C.
3.2.1 Photo lithography

Photo lithography is the technique of transferring a desired pattern from a ‘mask’ (a clear glass plate with an opaque metallic pattern on, usually chrome) onto a polymer photoresist film which covers the semiconductor sample, by exposure to ultraviolet (UV) light. This technique was used to define features larger than 1μm (limited approximately the wavelength of UV light). The photoresist film reacts chemically when exposed to UV light, such that when submersed in a developer solution, the exposed (for positive tone) or unexposed (for negative tone) photoresist is removed. Photoresist (initially in liquid form) is evenly distributed over the sample surface (using a mechanical spin coater) then baked on a hot plate to evaporate the solvents and form a solid film; (positive tone) photoresists used were Shipley S1805, S1813 and PMGI SF6. The thickness of the film depends on the spin speed and time but the recipes used typically result in films between 0.5μm (S1805) to 1.5μm (S1813) thick after baking. Due to the low melt point of InSb (800 K [64] compared to 1513 K for GaAs [65]), samples are baked at relatively low temperatures 85-95°C. A Karl Suss Contact Mask Aligner is used to align the desired pattern on the mask over the sample and expose UV light.

Once developed, the pattern is transferred onto the photoresist film which can then be used as an etch mask or as surface protection for deposition of metal or dielectric. In general, when used as a wet or dry chemical etch mask, a single layer photoresist process is used (S1813), whereas for metallisation, a bi-layer photoresist process is used (SF6/S1805). In the bi-layer process, two types of photoresist are layered upon one another which have different exposure parameters. Consequently, when the bi-layer is exposed to the same intensity of UV radiation, the developed edge profile resembles an ‘undercut’ which improves metal lift-off.
3.2. Device fabrication

3.2.2 Electron beam lithography

E-beam lithography is necessary to define structures with feature sizes <1 μm. The lithographic process is essentially analogous to that of photo lithography, only the resist is sensitive to an electron beam rather than UV light. The resolution is limited by scattering processes in the resist and substrate – using this technique features less than 10 nm can be defined. The desired patterns are designed using computer software, and are written into the resist by a collimated beam of high energy electrons which are accelerated towards the sample (typically 10-30 keV used here) with position controlled by magnetic fields in the SEM column. Once developed, the exposed pattern is transferred onto the resist layer which can be used as a mask for subsequent metal deposition or for etching of small features.

3.2.3 Ohmic contacts

To ensure that conduction is via the 2DEG and not via parallel conduction paths such as the highly defected (and high carrier density) GaAs interface, a shallow etch process is employed. In this process, the desired contact area is exposed to Ar⁺ Ion Beam Milling (IBM) to remove the upper AlₓIn₁₋ₓSb barrier (≈50 nm) and allow for metal deposition directly onto the InSb QW. During the IBM stage, an in situ SIMS facility is used to monitor the etch progress and identify when the QW is reached. The only shortcoming of this approach is that there is no in situ metal deposition capability, and so the sample must be transferred to a metal evaporation chamber which involves a chamber break of vacuum. A 50/350nm Ti/Au bi-layer is deposited using a Balzer Pfeifer PLS500 evaporation system, the Ti layer serving as an adhesion layer. Using this technique, good Ohmic contacts are produced with typical contact resistances of 1 kΩ at room temperature which remain Ohmic to low temperatures (2 K).
3.2.4 Gated Hall bridges

The magnetotransport measurements presented in chapter 5 are performed using the conventional six arm Hall bridge configuration illustrated in figure 3.3. The main features are the following:

(i) \( L \gg W \) i.e. the length of the active region is much greater than the width.
(ii) The current contacts (A and B) are distanced from the voltage probe contacts (C, D and E) and
(iii) The voltage probes are point-like contacts. The Hall probe contacts D and E lie nominally on the same equipotential at \( B = 0 \) thus sampling the Hall voltage only.

Hall bridges were fabricated using photo lithography and wet etching. The conducting mesa is 40 \( \mu \text{m} \) wide and voltage probes were separated by 200 \( \mu \text{m} \). Voltage probes in these devices are located sufficiently away from the current contacts so that geometric contributions to the magneto resistance can be ignored [66]. To investigate the carrier density dependence of various parameters, the device was covered with a sputtered amorphous SiO\(_2\) layer and a Ti/Au gate
3.2. Device fabrication

electrode was evaporated over the length of the 2DEG. This technique of SiO₂ deposition results in a relatively poor quality layer compared to photolytically assisted deposition of Silane (photox) and is susceptible to pin holes.

To mitigate this, sputtered SiO₂ layers were deposited in two stages. In the first stage, half the desired thickness is deposited. The sample is removed from the deposition chamber and subject to agitation in de-ionised water before the remaining thickness of SiO₂ is deposited. Using this method, a high resistance gate oxide layer of 50nm was produced, but with low yield <10 %. To improve the yield, thicker SiO₂ layers were deposited for subsequent samples ≈150 nm thick. Details of the SiO₂ thickness for each individual sample are listed in table 3.2. As will be shown in chapter 5, for devices with a thicker oxide, the majority of applied gate bias is dropped across the oxide resulting in a reduced modulation of the 2DEG carrier density. Figure 3.3 shows a scanning electron micrograph (SEM) of a typical gated Hall bridge.

3.2.5 Three-terminal FET-type devices

The three terminal devices used to study the Schottky barriers in chapter 6 required e-beam lithography to define the small area Schottky contacts (≈200 nm in length). These were patterned using a Raith modified Hitachi S2300 SEM with positive tone PMMA resist (≈150 nm thick film). An SEM of a typical three terminal device is shown in figure 3.4. The e-beam written pattern is highlighted. In the first stage of fabrication, optically defined alignment marks are processed onto the sample. These are used to align the e-beam pattern. Exposed patterns are developed and cleared of resist. The sample is then transferred to a metal evaporation chamber where a thin 5/80 nm bi-layer of Ti/Au deposited (the metal thickness is limited to approximately half the resist thickness to ensure lift-off). Note that the majority of the device is still fabricated using photo lithography. Therefore, the small e-beam written features must be aligned to the optically defined feed metal pattern using the mask aligner.
To alleviate this procedure, large area ‘tabs’ are incorporated into the e-beam design at the ends of the narrow Schottky contacts (see the purple shaded region in figure 3.4). A wet chemical etch is used to define the mesa. It also electrically isolates the contacts and each individual device. Lateral etching during this process completely undercuts regions of the device between central mesa edge and the feed metal forming freely suspended wires known as ‘air bridges’ (see figure 3.4). When used in the standard FET depletion mode, the small area Schottky contacts (implemented as a gate) minimise the leakage currents. In addition, when used for characterising the Schottky barrier, the small contact area minimises the probability of a structural defect residing beneath the contact which may present alternate (high conduction) transport paths (discussed in chapter 6). The device mesa widths varied as 3μm, 6μm or 12μm, with Schottky contacts
3.2 Device fabrication

≈200 nm in length. The Schottky contact areas for each device are listed in Table 3.2.

The three terminal devices were processed onto 12x12 mm samples, partitioned into nine fields of devices. Each field consisted of ten devices. In contrast, the gated Hall bridge devices are much larger in size and a 12x12 mm sample consists of only eight devices. Once fabricated, the samples are cleaved into smaller 4x4 mm sections using a diamond tipped scribe in order to be mounted into 20 pin ceramic chip carriers and wire bonded.

Details on the fabrication of two terminal Co/MgO/InSb lateral structures are given in Appendix C. No results on these structures are reported in this thesis, but an outline is included on the development towards final devices as many aspects of processing problems were resolved during the course of this thesis.

3.3 Experimental techniques

The magnetotransport measurements described in Chapter 5 were performed using the closed cycle magnet system at Imperial College whilst the Schottky barrier measurements presented in Chapter 6 were performed using the He Bath Cryostat system at QinetiQ Malvern.

3.3.1 Magnetotransport measurements

Gated Hall devices were measured in a Cryogenic Ltd 7.5 Tesla vertical field cryogen free superconducting magnet system (CFM) with an integrated variable temperature insert (VTI) at Imperial College. The apparatus allows measurements to be performed over a variable temperature range 2 K < T < 290 K.

The transport probe at the end of the sample stick (provided by Cryogenic Ltd) consists of an anodized Al block on which the sample can be secured either parallel or perpendicular to the field. Eight wires are available for measurements. The eight leads are fed up the length of the sample stick in twisted pairs to a
Fischer connector at the sample stick top plate. The sample temperature is measured using a calibrated Cernox™ sensor in thermal contact with the Al block (in close proximity to the sample). For the transport measurements presented in chapter 5, the chip carrier (in the plane of the 2DEG) is secured in a position perpendicular to the direction of the field. Copper wires are used to connect the contacts on the outside of the chip carrier to the eight pins on the probe. The CFM system has the benefit that no external cryogens are required to reach low temperatures. When the system and He flow rate are optimised, cryogenic temperatures can be maintained for long periods of time. This is particularly important for measurements on gated devices when multiple gate biases may be measured at fixed temperature e.g. for the typical field sweep rate of 2mT/s, measurement of 10 gate biases requires temperature stability for 40 hours (≈4 hours per measurement). However, because the sample probe has only eight wires, only one device can be wired up at any one time.

The longitudinal voltage $V_{xy}$ and the Hall voltage $V_{xx}$ were measured using a four-point low-frequency AC lock-in technique at a measurement current of 500nA. Low drive currents are used to minimise the longitudinal electric field generated across the device and the transfer of heat from the 2DEG to the lattice (Joule heating). This is especially prudent when measuring Shubnikov-de Haas oscillations and the Quantum Hall effect (see chapter 5) since their amplitudes decay with temperature. This effect was encountered at drive currents >1μA.

A schematic of the measurement set-up is shown in figure 3.5. The notation A and B used in the schematic indicates when a differential (A-B) measurement was performed. Delphi computer software written by Dr. Garry Perkins controlled the measurement; generating the AC signal, performing the software lock-in procedure and data collection. The circuit incorporates a variable resistor in series with the sample which is recorded during the measurement and used for determining the current and hence $R_{xx}$ and $R_{xy}$. The computer acquires the voltage signals from the sample and series resistor via a National Instruments Data Acquisition Card (NI-DAQ). Signals $V_{xx}$ and $V_{xy}$ are passed through two
3.3. Experimental techniques

NI-DAQ

Output

\[ V_g \quad V_{ac} \]

Input

Ch2  Ch1  Ch0

A  B

Software Lock-in

Stanford Research Systems SR560 Low Noise Preamplifier (input noise level of 4v nV/√Hz) before feeding the signal to the NI-DAQ card. The computer software also controls the temperature and magnetic field through the magnet power supply and temperature control unit (LakeShore 340). Shielded coaxial cables connect the sample stick with the current source (output from the NI-DAQ card) and pre-amps. Using this measurement configuration, high frequency noise levels of 8nV/√Hz are typically achieved.

The measurement is essentially a constant voltage measurement rather than constant current. As the resistance of the device oscillates due to the
3.3 Experimental techniques

Shubnikov-de Haas effect (see chapter 5) the current responds according. For this reason, the series resistance (1 MΩ) is chosen to be significantly greater than the sample longitudinal resistance so that the current variation is minimised (as long as the current variation is recorded and the response is linear, the true magnetoresistance of the sample is measured).

3.3.2 Schottky barrier measurements

Current-voltage $I-V$ measurements on the three terminal Schottky barrier devices were performed in the transport system at QinetiQ Malvern. An Oxford Instruments Helium (He) Bath cryostat with integrated VTI provided temperature control between 4.2 K to 300 K. Unlike the CFM system used for the magnetotransport measurements, the bath cryostat requires external transfer of liquid Helium into the system. Consequently, cryogenic temperatures are maintained over a relatively short time period compared to the CFM before the He reservoir is depleted e.g. $\approx 10$ hours at 4.2 K. However, since the $I-V$ measurements take a comparably very short length of time to perform, the bath cryostat is more than adequate. The 20 pin chip carrier integrates directly into the sample stick via a 20 pin sprung contact chip socket which has the advantage that all 20 pins, and hence multiple devices are accessible for measurements at one time. This is attached onto the end of a cylindrical copper heat sink, to which a temperature sensor is in thermal contact. Co-axial leads connect the sample stick to the connector box. The sample temperature is maintained using an Oxford Instruments ITC 503 unit which controls both the heater power and the flow of He into the sample space through a fully automated needle valve. Once at 4.2 K, the temperature could be further reduced to 1.6 K by pumping on the sample space with the needle valve closed.

A schematic of the measurement set-up is shown in figure 3.6. Direct current $I-V$ measurements were performed using a Hewlett Packard HP4156B
3.3. Experimental techniques

A semiconductor parameter analyser which provides accurate low resistance measurements suitable for Schottky barrier characterisation.

Figure 3.6: DC measurement set up at QinetiQ Malvern. SMU1 sources the current, SMU2 is set as common ground and VMU1 measures the voltage with respect to the common on the device under test (DUT).

Four source-measurement units (SMUs), two voltage-source units (VSUs) and two voltage-measurement units (VMUs) are available for measurements. The HP4156B was interfaced with a computer which automated the measurement via a Labview program written by Dr James Orr.

A three terminal measurement is used to directly measure the Schottky barrier characteristics independent from the additional series resistance which may arise from the 2DEG channel resistivity and the Ohmic contacts.
Figure 3.7: (a) Schematic diagram of the three point measurement of the Schottky barrier. (b) Equivalent circuit of the DC measurement. The contact resistance, sheet resistance of the 2DEG and the barrier resistance are in series allowing for the isolation of the barrier characteristics when contacts 1, 2 and 3 are in the order shown in (a).

Figure 3.7 shows a schematic and equivalent circuit of the three terminal measurement is shown in (see also figure 3.6). Ohmic contact 1 is biased with respect to contact 2 (Schottky contact) which is common to ground using the SMU. Voltage is measured between contact 2 and an adjacent remote Ohmic contact 3 using the VMU. It can be seen that it is essentially a non-local measurement which, provided no current flows between contacts 2 and 3, measures only the voltage dropped across the Schottky barrier.
3.4 Sample summary

**TABLE 3.1:** Details of pertaining sample parameters and dimensions for the gated Hall bridges investigated in chapters 5.

<table>
<thead>
<tr>
<th>Sample</th>
<th>QW width (nm)</th>
<th>Spacer S (nm)</th>
<th>$\mu$ (m$^2$ V$^{-1}$ s$^{-1}$) 2 K (290 K)</th>
<th>$n_{2D}$ (10$^{15}$ m$^{-2}$) 2 K (290 K)</th>
<th>SiO$_2$ (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2509A</td>
<td>30</td>
<td>20</td>
<td>27.2 (6.78)</td>
<td>2.32 (3.29)</td>
<td>50</td>
</tr>
<tr>
<td>2509B</td>
<td>30</td>
<td>20</td>
<td>26.13 (6.52)</td>
<td>2.51 (3.5)</td>
<td>50</td>
</tr>
<tr>
<td>2504A</td>
<td>30</td>
<td>20</td>
<td>39.5 (6.87)</td>
<td>3.28 (4.56)</td>
<td>150</td>
</tr>
<tr>
<td>2504B</td>
<td>30</td>
<td>20</td>
<td>39.0 (6.93)</td>
<td>3.21 (4.5)</td>
<td>150</td>
</tr>
<tr>
<td>2526</td>
<td>30</td>
<td>20</td>
<td>18.36 (5.07)</td>
<td>1.50 (4.12)</td>
<td>50</td>
</tr>
</tbody>
</table>

**TABLE 3.2:** Details of device parameters and dimensions for the three terminal devices investigated in chapters 6. Wafer number ADJ1125.

<table>
<thead>
<tr>
<th>Devices</th>
<th>QW width (nm)</th>
<th>Spacer S (nm)</th>
<th>$\mu$ (m$^2$ V$^{-1}$ s$^{-1}$) 77 K (290 K)</th>
<th>$n_{2D}$ (10$^{15}$ m$^{-2}$) 77 K (290 K)</th>
<th>Contact Area (μm$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>15</td>
<td>20</td>
<td>6.2 (2.65)</td>
<td>9.3 (10)</td>
<td>0.6</td>
</tr>
<tr>
<td>B</td>
<td>15</td>
<td>20</td>
<td>6.2 (2.65)</td>
<td>9.3 (10)</td>
<td>0.6</td>
</tr>
<tr>
<td>C</td>
<td>15</td>
<td>20</td>
<td>6.2 (2.65)</td>
<td>9.3 (10)</td>
<td>1.2</td>
</tr>
<tr>
<td>D</td>
<td>15</td>
<td>20</td>
<td>6.2 (2.65)</td>
<td>9.3 (10)</td>
<td>2.4</td>
</tr>
<tr>
<td>E</td>
<td>15</td>
<td>20</td>
<td>6.2 (2.65)</td>
<td>9.3 (10)</td>
<td>0.6</td>
</tr>
<tr>
<td>F</td>
<td>15</td>
<td>20</td>
<td>6.2 (2.65)</td>
<td>9.3 (10)</td>
<td>1.2</td>
</tr>
<tr>
<td>G</td>
<td>15</td>
<td>20</td>
<td>6.2 (2.65)</td>
<td>9.3 (10)</td>
<td>2.4</td>
</tr>
<tr>
<td>H</td>
<td>15</td>
<td>20</td>
<td>6.2 (2.65)</td>
<td>9.3 (10)</td>
<td>2.4</td>
</tr>
<tr>
<td>I</td>
<td>15</td>
<td>20</td>
<td>6.2 (2.65)</td>
<td>9.3 (10)</td>
<td>2.4</td>
</tr>
</tbody>
</table>
Chapter 4

Theoretical calculations of the zero-field spin splitting in InSb quantum wells

The operation of many spintronic devices in low dimensional systems is based around manipulating the electron spin during its transport across the device in a controllable manner. Other important aspects of these devices such as spin injection and detection are discussed in chapter 6. This operation is possible because of the spin-orbit splitting of subbands in zero magnetic field, that can be manipulated via the application of an external electric field with a gate. Hence, a proper understanding of how the spin splitting parameters vary with structure and doping and the impact on the spin lifetime is critically important. The work presented in this chapter extends that of [67] by considering a wide range of realistic $n$-InSb/$In_{1-x}Al_x$Sb asymmetric heterostructures with finite barriers. A summary of this chapter is published in [68].

In section 4.1 we first review the origins of zero-field spin splitting in zincblende semiconductors and their heterostructures, and the current understanding of the coupling parameters which determine its magnitude. In section 4.2 the Rashba and Dresselhaus spin-orbit coupling parameters are calculated in a range of InSb/InAlSb quantum well heterostructures using a reduced eight-band $k.p$ model and band profiles generated from a self consistent
4.1. Zero-field spin splitting

Schrödinger-Poisson model (SPM) developed by Dr. Mike Fearn at QinetiQ (see appendix B for details of the SPM). In section 4.3 the spin splitting is calculated and the relative magnitudes of the Rashba and Dresselhaus contributions are discussed. Comparison to theoretical and experimental values of the Rashba parameter in the literature from other relevant material systems is given in section 4.4. In section 4.5 the D'yakonov Perel spin relaxation rates are calculated using the results obtained from earlier calculations. The properties of the spin lifetime transistor are reviewed for the case of InSb and compared to previous studies in different wider gap systems. In particular it is found that the inherent large Dresselhaus splitting in InSb leads to modifications to the conditions for maximum spin lifetime.

4.1 Zero-field spin splitting

In an electron system, the application of a magnetic field $B$ lifts the spin degeneracy of the energy levels and introduces a spin splitting proportional to the magnitude of the magnetic field applied known as the Zeeman effect. The Hamiltonian $\hat{H}_z$ describing the Zeeman effect is

$$\hat{H}_z = \frac{1}{2} g \mu_B \sigma \cdot B$$

where $\sigma$ is the vector of Pauli spin matrices which are given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$\mu_B = e\hbar / m_0$ is the Bohr magnetron and $g$ is the electron Landé $g$-factor. Equation 4.1 leads directly to the Zeeman splitting $\Delta E_z = g \mu_B B$ which is independent of the direction of magnetic field. For a free electron system the $g$-
factor is very close to two. In crystalline solids the g-factor is known to vary from the free electron value depending on the material and is therefore commonly referred to as an effective g-factor denoted by $g^*$. Similar to the effective mass $m^*$, the g-factor exhibits an energy dependence due to the band non-parabolicity [54]. The effective g-factors of some III-V semiconductors of interest are listed in table 4.1 for comparison. One can see that InSb has a very large negative g-factor. This can manifest itself in a variety of ways, one of which is to spin split the Landau level spectrum in magnetic fields which is discussed in chapter 5.

The spin degeneracy of electron (and hole) states in a semiconductor in zero magnetic field is described by $E^{(k)} = E^{(-k)}$. This relationship emerges from the combined requirements of spatial inversion symmetry described by,

$$E_{\uparrow}(k) = E_{\downarrow}(-k)$$  \hspace{1cm} (4.2)

and time-reversal symmetry, known as Kramer's degeneracy described by,

$$E_{\uparrow}(k) = E_{\downarrow}(-k).$$  \hspace{1cm} (4.3)

When the potential through which carriers move is inversion asymmetric, the periodic part of the Bloch functions no longer satisfy equation 4.2 and the spin degeneracy is lifted (Kramer's degeneracy still holds). In this case, a zero-field spin splitting is introduced which is wave vector dependent.

In III-V quantum well (QW) heterostructures, inversion asymmetry originates from two predominant sources, the microscopic potential of the zincblende crystal and the macroscopic electrostatic potential of the heterostructure. These mechanisms are discussed below and are the subject of detailed calculations in realistic InSb QWs in the following sections. It is worth noting that a third contribution to the zero-field spin splitting can arise from the arrangement of atomic bonds at heterointerfaces known as native inversion asymmetry (NIA). NIA can arise in zincblende QWs when the QW and barrier
4.1. Zero-field spin splitting

materials are comprised of differing anions and cations (for example in InAs/GaSb QWs [69]). This is expected to be small in InSb/InAlSb heterostructures and is not discussed further in this chapter.

4.1.1 Bulk inversion asymmetry

As discussed in chapter 2, unlike the diamond lattice structure of elemental semiconductors Si and Ge, the zincblende structure of III-V (and also II-VI) semiconductors such as GaAs, InAs, InSb lack a centre of inversion. This intrinsic inversion asymmetry in the microscopic crystal potential is referred to as *bulk inversion asymmetry* (BIA). In the classic paper by Dresselhaus [47] it was shown that in bulk zincblende semiconductors the spin-orbit coupling in the presence of BIA leads to an anisotropic spin splitting of the conduction band in zero magnetic field proportional to the wave vector cubed, $k^3$ (for small $k$). This is called the *Dresselhaus splitting* and is characterized by the coefficient $\gamma (\text{eV} \cdot \text{m}^3)$.

The anisotropy of the splitting is characterised by a maximum splitting for the [110] direction and zero splitting for the [100] and [111] directions in $k$-space. Estimates of the parameter $\gamma$ can be made from the work of Lommer *et al.* [70] and Winkler [48] who derived analytical expressions from 14-band $k.p$ theory (these involve some band parameters which are not well known e.g. higher conduction band separations). In general, $\gamma$ is expected to increase with increasing spin-orbit gap $\Delta$ and decreasing band gap $E_g$ [48, 70] and is therefore expected to be large in bulk InSb. Table 4.1 lists the estimations of $\gamma$ from [48] for the main III-V bulk semiconductors of interest (using parameters listed therein).

The $\gamma$ related spin splitting is generally small and is difficult to observe experimentally. However, evidence for the presence of Dresselhaus splitting has been demonstrated by Seiler *et al.* in bulk GaSb [71] by analysis of beating effects in the Shubnikov-de Hass oscillations and similarly in bulk InSb under the application of uniaxial strain [72].
4.1. Zero-field spin splitting

**TABLE 4.1:** Spin splitting parameters $\gamma$ (for bulk) and $\alpha_0$ from 14-band $k.p$ theory (taken from [48] unless where stated) along with bulk $g^*$ values for InSb, InAs and GaAs.

<table>
<thead>
<tr>
<th></th>
<th>$\gamma$ (eVÅ$^3$)</th>
<th>$\alpha_0$ (Å$^2$)</th>
<th>$g^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>InSb</td>
<td>760.1</td>
<td>523.0</td>
<td>-48.7</td>
</tr>
<tr>
<td>InAs</td>
<td>130 [73]</td>
<td>117.1</td>
<td>-15.4</td>
</tr>
<tr>
<td>GaAs</td>
<td>27.58</td>
<td>5.206</td>
<td>-0.44</td>
</tr>
</tbody>
</table>

Eppenga and Schuurmans studied spin splitting due to BIA in GaAs/AlGaAs quantum wells (QWs) and showed that in a spatially inhomogeneous structure (not necessarily a QW) where the $z$-axis is in the growth direction, the Dresselhaus term is separated into two contributions,$^4$ a $k$-cubic term and a $k$-linear term characterized by the coefficient $\beta$ (eVm) defined as [74]

$$\beta = \langle \hat{k}_z \hat{k}_z \rangle. \quad (4.4)$$

The brackets represent the average over the probability density of the confined state and $\hat{k}_z$ is the operator form of the confinement wave number (see footnote). Thus, for barriers of finite height, $\beta$ has contributions from the well and barrier. It was highlighted that for wide QWs, $\beta$ can be approximated by the formula

$$\beta \approx \gamma_{\text{bulk}} \left( \frac{\pi}{W} \right)^2 \quad (4.5)$$

$^4$ This is because when $z$ is in the growth direction $k_z$ is replaced by its operator form $-i \partial / \partial z$ within the envelope function approximation.
4.1. Zero-field spin splitting

where $W$ is the well width and $\gamma_{\text{bulk}}$ is the $k^3$ splitting parameter for the bulk QW material. This is strictly the high barrier limit where $\frac{\pi}{W} = k_z^W$ is the quantised wave number in the well. This approximation suggests that $\beta$ is also a material parameter independent of the details of the heterostructure and is frequently used in qualitative discussions due to its simplicity [18,75]. In the following sections it will be demonstrated that this is a poor approximation in the InSb QW system.

4.1.2 Structural inversion asymmetry

The second source of inversion asymmetry is related to a change in the macroscopic potential and bandstructure through a heterojunction interface, known as structural inversion asymmetry (SIA), described by Bychkov and Rashba [19]. This produces an additional spin splitting linear in $k$ and is characterized by the coefficient $\alpha$ (eVm), and is commonly referred to as the Rashba effect. An important feature of the Rashba effect is that the asymmetry of the heterostructure potential and hence the magnitude of $\alpha$ can in principle be tuned by means of an external gate electric field. For this reason the Rashba effect has attracted considerable interest for spintronic device applications in recent years and is the basis for the operation of the fabled spin transistor proposed by Datta and Das in 1990 [16]. The phenomenological Rashba Hamiltonian is given by [19]

$$\hat{H}_{SO} = \alpha (\sigma \times k) \vec{k}$$  \hspace{1cm} (4.6)

where $\vec{k}$ is the unit vector in the growth direction. When applied to a QW system with growth parallel to the $z$-direction, equation 4.6 reduces to the well known form

$$H_{SO} = \alpha (k_y \sigma_y - k_z \sigma_z)$$  \hspace{1cm} (4.7)
4.1. Zero-field spin splitting

The solution for the subband dispersion yields two branches (one for each spin) described by

$$E_s(k) = \frac{\hbar^2 k^2}{2m^*_b} \pm \alpha k$$  \hspace{1cm} (4.8)

which leads directly to a spin splitting $\Delta E = 2\alpha |k|$. The dispersion curve is illustrated in figure 4.1. Although the single band Rashba model neglects any energy dependences of band parameters (arising from band non-parabolicity), the simplicity of the model and the ease of its implementation makes it attractive for use in simulations and deriving analytical spin dependent corrections to various transport properties e.g. see equation 5.19 in chapter 5 [39,75].
4.1. Zero-field spin splitting

Following early theoretical works and subsequent interpretations of the Rashba model, the Rashba coefficient $\alpha$ was taken to be proportional to the electric field in the conduction band [76,77]. This lead to the frequently quoted formula for $\alpha$ [78-80]

$$\alpha = \alpha_0 \langle E_z \rangle$$  \hspace{1cm} (4.9)

where again the brackets represent the expectation value of the electric field $E_z$ in the QW. In this form, the parameter $\alpha_0$ is a material specific parameter (dependent on $E_g$ and $\Delta$) describing the strength of the Rashba interaction. Recently however, it was shown by Pfeffer and Zawadzki [81] that $\alpha$ can not be directly related to the electric field in the conduction band. Nevertheless, the analytical models that have been derived for $\alpha_0$ provide useful insight to the influence of the band parameters on the strength of the Rashba interaction [48,79]. Predicted values of $\alpha_0$ for InSb, InAs and GaAs taken from [48] are listed in table 4.1 for comparison. We see that InSb has the largest Rashba coupling $\alpha_0$ indicating that a large change in the spin splitting will result from a relatively small change in electric field (e.g. from a gate electrode). This re-emphasises why InSb is considered a promising candidate for spintronic applications.

The combined spin-orbit (SO) Hamiltonian for SIA and BIA induced couplings for a two dimensional electron gas (2DEG) confined in the $x-y$ plane is of the form [45,74]

$$H_{SO}(k_{||}) = \alpha(k_x \sigma_y - k_y \sigma_x) + \beta(k_x \sigma_x - k_y \sigma_y) + \gamma(k_x^2 k_y \sigma_y - k_x k_y^2 \sigma_x)$$  \hspace{1cm} (4.10)

This Hamiltonian can equally be rewritten in the form $H_{SO}(k_{||}) = \hbar \sigma \cdot \Omega(k_{||})$ which is analogous to the Zeeman term in equation 4.1. Here $\Omega(k_{||})$ is given by
4.1. Zero-field spin splitting

\[ \Omega(k) = \frac{1}{\hbar} \left[ \left( \beta \gamma - \alpha \gamma \right) k_x k_y, \left( \alpha \gamma - \beta \gamma \right), 0 \right]. \]  \hspace{1cm} (4.11)

Therefore, the spin splitting induced by the SO coupling in equation 4.11 can be described by a \( k \)-dependent effective magnetic field \( B_{\text{eff}}(k) \) about which spins precess with an effective Larmor frequency \( \Omega(k) = g^* \mu_B B_{\text{eff}}(k) / \hbar \). The rate of spin precession is thus determined by the magnitude of the spin splitting through \( k \) and the coupling parameters \( \alpha, \beta \) and \( \gamma \).

This is essentially the basis for the D'yakonov and Perel' (DP) spin relaxation mechanism [82] i.e. the decoherence of an initially aligned (polarized) population of spins is driven by their individual precession about the vector \( \Omega(k) \).

For a spin polarized current in a diffusive system, the presence of momentum scattering randomly changes the wave vector \( k \) in the time \( \tau_p \) which in turn changes the orientation of the effective magnetic field, and precession vector. For frequent momentum scattering events the average precession frequency and hence spin relaxation rate is slowed (known as motional narrowing) leading to a characteristic spin relaxation rate \( \tau_s^{-1} \propto \tau_p \). The DP spin relaxation mechanism has been shown to be present in most III-V semiconductor systems over a broad range of temperatures [83,84]. It is essential for spintronic devices as the dominance of this mechanism is necessary for the gate modulation of spin populations through the tunability of \( \alpha \) [85]. Recent experimental results from \( n \)-type InSb/InAlSb QWs which appear to be consistent with the DP mechanism, indicate that it is dominant over a broad range of temperatures [86].

4.2 SIA and BIA coefficients in InSb quantum wells

Rashba splitting in symmetric InSb QWs was previously studied in the high barrier limit by Stanley et al. using Kane’s eight-band \( k.p \) theory [67]. It was
found that the spin splitting in InSb was up to a factor of two times greater than that in equivalent InAs QWs due to the larger split-off and smaller band gap energies. The work presented in this chapter extends that of [67] by considering a wide range of realistic $n$-InSb/In$_{1-x}$Al$_x$Sb asymmetric heterostructures with finite barriers. Critically, by considering finite barriers, the penetration of the wave function into the barriers is taken into account, adding a dominant contribution to the Rashba coefficient $\alpha$ [81]. It is also demonstrated that the same effect influences the calculations of $\beta$.

Counter to the assertion that the Rashba effect is dominant in narrow gap semiconductors [45,77,87], the theoretical results presented here indicate that for certain structures the BIA terms can give a significant contributions (>50 %) toward the total spin splitting and should not be neglected.

4.2.1 The $k.p$ model

To calculate the conduction band SO coupling parameters, we employ the eight-band $k.p$ model described by Pfeffer and Zawadzki [45]. The model has successfully reproduced experimental results from the InGaAs/InAlAs system and more recently achieved agreement with spin resonance results obtained from InSb/In$_{0.91}$Al$_{0.09}$Sb asymmetric QWs by Khodaparast et al. [44,87], which is of particular relevance to the structures studied here.

As discussed in chapter 2, the three-level $k.p$ model for the conduction, valence (light and heavy hole) and split-off bands respectively, results in an 8x8 matrix Hamiltonian (see for example equation 2.2). For the case of a heterostructure with $z$ in the growth direction i.e. parallel to [001], $k_z \rightarrow \hat{k}_z$ and the potential $V(z)$ is included along the diagonal. The band parameters are now position dependent. (Note that the Rashba term naturally appears from evaluating the Hamiltonian with the $\hat{k}_z$ operator). The 8x8 matrix is reduced by substitution to a 2x2 matrix for the conduction band. The resulting 2x2 Hamiltonian for the conduction band is [87]
4.2. SIA and BIA coefficients in InSb quantum wells

\[
\begin{pmatrix}
\hat{A} - \lambda & \hat{K} \\
\hat{K}^* & \hat{A} - \lambda
\end{pmatrix}
\begin{pmatrix}
\Psi_1(z) \\
\Psi_2(z)
\end{pmatrix} = 0
\] (4.12)

where \( \lambda \) is the energy eigenvalue and

\[
\hat{A} = -\frac{\hbar^2}{2} \frac{\partial}{\partial z} - \frac{1}{m^*(z, \lambda)} + \frac{\hbar^2 k_z^2}{2m^*(z, \lambda)} + V(z).
\] (4.13)

The off-diagonal term \( \hat{K} = \hat{K}_{\text{SIA}} + \hat{K}_{\text{BIA}} \) consists of two parts for the SIA and BIA interactions given by

\[
\hat{K}_{\text{SIA}} = -i\sqrt{2}k_y \hat{\alpha}(z, \lambda)
\] (4.14)

\[
\hat{K}_{\text{BIA}} = -i\sqrt{2}k_k k_y \hat{\gamma}(z, \lambda) + \sqrt{2}k_y \hat{\beta}(z, \lambda)
\] (4.15)

where here we define,

\[
\hat{\alpha}(z, \lambda) = \frac{P^2}{3} \frac{\partial}{\partial z} \left( \frac{1}{\tilde{\varepsilon}_i(z, \lambda)} - \frac{1}{\tilde{f}_i(z, \lambda)} \right),
\] (4.16)

\[
\hat{\beta}(z, \lambda) = \frac{\partial}{\partial z} \tilde{\gamma}(z, \lambda) \frac{\partial}{\partial z},
\] (4.17)

and

\[
\tilde{\gamma}(z, \lambda) = \frac{2BP}{3} \left( \frac{1}{\tilde{\varepsilon}_i(z, \lambda)} - \frac{1}{\tilde{f}_i(z, \lambda)} \right),
\] (4.18)

where \( k_z = (k_x \pm ik_y) / \sqrt{2} \). The energies \( \tilde{\varepsilon}_i(z, \lambda) = -E_{gi} + V(z) - \lambda \) and \( \tilde{f}_i(z, \lambda) = -E_{gi} - \Delta_i + V(z) - \lambda \) describe the valence and split-off band edge.
energy profiles measured relative to \( \lambda \). The subscript \( i \) on the energy gaps \( E_g \) and \( \Delta \) refers to the different regions of the heterostructure e.g. upper barrier (UB), QW and lower barrier (LB). \( V(z) = -e\phi(z) + dV_{UB}\Theta(-z) + dV_{LB}\Theta(z+W) \) is the conduction band edge energy profile throughout the heterostructure where \( e \) is the electron charge, \( \phi(z) \) is the smoothly varying electrostatic potential and \( dV_{UB}\Theta(-z) \) and \( dV_{LB}\Theta(z+W) \) are step functions characterising the conduction band offsets \( dV_{UB} \) and \( dV_{LB} \) at the two interfaces located at \( z = 0 \) and \( z = W \) respectively. \( B \) is the Kane parameter [46] and \( P \) is the interband momentum matrix element related to the \( k.p \) interaction term \( E_p \) by \( P^2 = \hbar^2 E_p / 2m_e \). \( B \) and \( E_p \) are taken to be -31.4 eVÅ\(^2\) [88] and 23.1 eV [4] (\( P = 9.37 \) eVÅ), respectively for InSb (the value of \( B \) is discussed later). Due to the lack of data on the ternary alloys, these are assumed to be the same for In\(_{1-x}\)Al\(_x\)Sb. This is a reasonable approximation for \( E_p \) since it is approximately constant for most III-V compounds [46], however, \( B \) may be expected to be smaller in the alloy due to the large band gap. To be consistent with the model of Pfeffer and Zawadzki [45], potential energies are measured relative to the conduction band edge at \( z = 0 \) in the QW such that \( V_{QW}(0) = 0 \) (see figure 4.2).

The spin-orbit coupling parameters \( \alpha, \beta \) and \( \gamma \) are calculated explicitly by evaluating the expectation values of equations 4.16 to 4.18 with respect to the wave function \( \Psi(z) \) i.e. \( \alpha = \langle \Psi(z) | \hat{\alpha}(z, \lambda) | \Psi(z) \rangle \) etc.

### 4.2.2 Heterostructure details

Electrostatic potentials \( \phi(z) \) and the normalised electron wave functions \( \Psi(z) \) for each structure are obtained self consistently at 10 K without spin splitting from solutions of \( \hat{A}\Psi(z) = \lambda\Psi(z) \) [45], using a one-band Schrödinger-Poisson model (SPM) tailored to narrow band gap materials (details are given in Appendix B) [6,89,90]. A typical solution for a 20nm wide QW is shown in figure 4.2.
4.2. SIA and BIA coefficients in InSb quantum wells

Figure 4.2: Typical conduction band profile $V(z)$ (left axis) and normalised probability density function $|\Psi(z)|^2$ of the 1st subband (right axis) of a δ-doped $In_{0.8}Al_{0.2}Sb/InSb/In_{0.85}Al_{0.15}Sb$ 20 nm QW heterostructure. The doping density $N_{2D}$, spacer thickness $S$ and resulting carrier density $n_{2D}$ for this solution are given. $E_i$ is the energy of the ground state and $\lambda$ is the energy eigenvalue. The left-hand axis is normalized to $V_{QW}(0) = 0$.

This SPM is a good approximation when the spin splitting is small giving $\Psi_1(z) = \Psi_2(z) = \Psi(z)$ [45]. In real device structures it is beneficial for carrier confinement, mobility and surface gate leakage to have an increased alloy content in the upper barrier with respect to the lower barrier [91]. For this reason, the various well widths considered here are modelled with barriers of varying $In_{1-x}Al_xSb$ compositions to best meet this criterion. Accordingly, Al content in the barrier increases as the well width is narrowed. This has a profound effect on the dependence of $\alpha$ on well width that, namely that for a given carrier density, $\alpha$ is unexpectedly largest in wide well structures. This is discussed in detail below.
4.2. SIA and BIA coefficients in InSb quantum wells

For each well width, the doping density \( N_d \) and spacer thickness \( S \) are varied, providing sixteen different SPM solutions for a given well width \( W \). A 5% difference in Al composition between the upper and lower barrier is maintained in each structure for comparison. \( \Delta q_W \) is taken as the bulk value for InSb (\( \Delta = 0.810 \text{eV} \) [4]) for all QW widths whereas split-off energies for the barriers are estimated from a linear interpolation between the known values for bulk InSb and bulk AlSb (0.750eV [4]) due to the lack of data on the ternary alloys. For the calculations performed here, we restrict ourselves to solutions for zero bias and vary the doping parameters \( N_d \) and \( S \) such that only the lowest subband is occupied.

4.2.3 The Rashba Coefficient \( \alpha \)

The doping parameters \( N_d \) and \( S \) in the SPM calculations acutely influence the conduction band edge potential profile and the wave function asymmetry, defined here as the difference between the probability density at the interfaces \( \Delta \Psi_i^2 = \Psi_i^2(0) - \Psi_i^2(W) \). The carrier density in the well \( n_{2D} \) is determined by the amount of carriers transferred into the well from the \( \delta \)-layer which increases with \( N_d \) and decreasing \( S \). Therefore the effects of \( N_d \) and \( S \) on \( \alpha \) can be interpreted as just the variation of \( \alpha \) with \( n_{2D} \) as presented in figure 4.3 for the various well widths. Each data point thus represents a separate SPM solution from varying \( N_d, S \) and \( W \). At small carrier densities the magnitude of \( \alpha \) increases approximately linearly with \( n_{2D} \). This is due to an increased conduction band bending in the top barrier which increases the electric field in the QW and weights the wave function towards the top interface (thus increasing \( \Delta \Psi_t^2 \)). The most striking result of figure 4.3 is that contrary to previous studies [55,79], for a given carrier density, \( \alpha \) is greatest in the wide QW structures, albeit with the drawback of a greatly reduced capacity of the ground state subband before the occupation of the second subband compared to the narrow wells. This ultimately limits the range of allowed \( n_{2D} \) for single subband occupancy in this model.
Beyond this limit for wider wells, we see that larger Rashba coefficients are achieved in narrower wells at higher carrier densities (see figure 4.3).

The electric field in the conduction band is equal to

\[ E_e = \frac{1}{e} \frac{d\phi(z)}{dz} + dV_{UB} \delta(z) - dV_{LB} \delta(z-W) \]

i.e. the electrostatic potential gradient plus the interface contributions. Pfeffer and Zawadzki [45] showed that the Rashba coupling parameter can be separated into a term proportional to the electric field \( \frac{d\phi(z)}{dz} \) and interface terms resulting from the differentiation over the discontinuities in \( V(z) \) at the heterointerfaces, \( dV_{UB} \Theta(-z) \) and \( dV_{LB} \Theta(z+W) \).
The three terms are given by [45]

\[
\alpha = \frac{P^2}{3} \left[ \left( \frac{\partial \phi}{\partial z} D_1 \right) \right] + \frac{P^2}{3} \left[ dV_{UB} D_0 \Psi^2(0) - dV_{LB} D_w \Psi^2(W) \right] + \frac{P^2}{3} \left[ \Psi^2(0)(C_0 - dV_{UB} D_0) - \Psi^2(W)(C_a - dV_{LB} D_w) \right]
\]

(4.19)

where \( D_1 = \frac{1}{\varepsilon_i^2} - \frac{1}{\tilde{f}_i^2} \), \( C_0 = \Delta_{QW} / \varepsilon_{QW}(0) \tilde{f}_{QW}(0) - \Delta_{UB} / \varepsilon_{UB}(0) \tilde{f}_{UB}(0) \), and \( C_a = \Delta_{QW} / \varepsilon_{QW}(W) \tilde{f}_{QW}(W) - \Delta_{LB} / \varepsilon_{LB}(W) \tilde{f}_{LB}(W) \). The first term in equation 4.19 is assigned the label \( F_1 \) and the second \( F_2 \) such that the total ‘field’ term is \( F = F_1 + F_2 \) (see figure 4.4 inset). The third term in equation 4.19 is the ‘interface’ term \( I \). These are shown individually in figure 4.4 for a 20nm QW.

**Figure 4.4:** Results for \( \alpha \) from a 20 nm QW showing the contributions from the ‘field’ and ‘interface’ terms. The inset shows the two components of the field term \( F \) which result in the observed dependence on \( n_{2D} \).
It is clear that the interface dominates the contribution $\alpha$. The coefficients within the interface term, $C_0 - dV_{ub} D_0$ and $C_w - dV_{lb} D_w$, are negative and vary weakly with $n_{2D}$ compared to $\Psi(0)$ and $\Psi(W)$. As such, one finds that the total contribution to $\alpha$ is proportional to the asymmetry of the electron probability density at the interfaces ($\Delta\Psi_i^2$). The role of the electric field can then be interpreted as facilitating the asymmetry of the QW profile necessary to weight the wave function toward or away from an interface, thus varying $\Delta\Psi_i^2$. The total field term is positive because the electric field at the interfaces in $<\Psi(z)|E|\Psi(z)>$ results in the addition of a large positive step (the same step is subtracted from the interface term). The observed small variation of the field term $F$ with carrier density results from the competition between the two component field terms $F_1$ and $F_2$ which have opposite dependences on $n_{2D}$ as shown in the inset of figure 4.4 by the red dashed and red dotted lines respectively. Since $F_2 > F_1$ we find that the electric field contribution to $\alpha$ is largely determined by the band offsets rather than the average electric field.

The observed trend of $\alpha$ increasing with QW width can be explained using the following argument. The increased confinement energy in narrow wells compared to that in wider wells had been assumed to increase the wave function penetration into the barriers and hence $\alpha$ (if the underlying asymmetry is the same in each case) [55]. Whilst this is certainly true for wells of fixed barrier height, in the structures considered here which are a better reflection of real devices, the Al content in the barriers and hence barrier heights (with respect to the subband energy $E_i$) are generally increased in the narrower well structures. This reduces the penetration of the wave function into the barriers ($\Delta\Psi_i^2$), and therefore $\alpha$, compared to the wider wells. The results in figure 4.3 also indicate that the wider well structures should exhibit an increased sensitivity of $\alpha$ (i.e. $\frac{\partial\alpha}{\partial n_{2D}}$) to $n_{2D}$.

These results for $\alpha$ can be summarised by the general assertion that for a single-sided $\delta$-doping structure of given QW width and barrier composition, $\alpha$ is proportional to $n_{2D}$ (where $n_{2D}$ varies as a result of doping). This statement is true
also for δ-doping located in the bottom barrier. However, a distinction between
the two becomes evident when using an external electric field to vary \(n_{2D}\) and \(\alpha\).

For structures doped below the QW, the direction of the electric field across the
QW is reversed and although \(n_{2D}\) increases with positive bias, the QW asymmetry, and hence \(\alpha\), decreases. This description is consistent with the
experimental results of Schapers et al. [92] and Nitta et al. [93] for InGaAs QWs.

Structures doped above the QW (such as those studied here and also chapter 5)
are expected to exhibit the opposite behaviour of \(\alpha\) increasing with positive gate
bias. Data obtained from magnetotransport measurements is presented in chapter
5 that is consistent with this expected trend.

4.2.4 Dresselhaus coefficients \(\beta\) and \(\gamma\)

The BIA parameters \(\beta\) and \(\gamma\) exhibit a relatively weak dependence on \(n_{2D}\) and
energy \(\lambda\) compared to \(\alpha\) (this is demonstrated for \(\beta\) in figure 4.3).

To compare the Dresselhaus coefficients for different QW widths, \(\gamma\) and \(\beta\)
are plotted for a fixed Fermi energy in figure 4.5(a) and (b) as indicated by the
solid and dotted lines, respectively. The increase in \(\gamma\) with well width is due to the
reduced confinement which lowers the energy \(\lambda\). An estimate for the value of \(\gamma\) in
bulk InSb at the zone centre, \(\gamma_{\text{bulk}}\), can be made from the eight-band model used
here by evaluating equation 4.18 directly with an unstrained energy gap
\(E_g = 235.2\) meV [4] and assuming \(\lambda = V(z) = 0\) in the bulk. This approach yields
\(\gamma_{\text{bulk}} \approx 646.5\) eVÅ\(^3\). By comparison to the results in figure 4.5(a) we see that the
value of \(\gamma\) for the widest well shows a ≈30% reduction from the bulk value due to
the presence of subband confinement (i.e. \(E_1\)) in the QW. Hence
when \(W \rightarrow \infty, E_1 \rightarrow 0\), the value of \(\gamma\) will approach that of the bulk.

The estimation of \(\gamma_{\text{bulk}}\) from equation 4.18 can be compared with results in
the literature. It is somewhat greater than that estimated from the sixteen-band \(k.p\)
4.2. SIA and BIA coefficients in InSb quantum wells

Figure 4.5: Calculated results for the BIA SO coupling parameters $\gamma$ (top panel) and $\beta$ (bottom panel) as a function of $W$ width $W$ for fixed Fermi energy $E_F = 40$ meV. Also shown in (b) are the results for the calculation of $\beta$ from $\gamma < k_z^2 >$ (red line) and $\gamma_{\text{bulk}}(\pi/W)^2$ (green line) for comparison.

model of Cardona et al. [49] given as $\gamma^\text{bulk}_{\text{bulk}} = 563.9 \text{ eVÅ}^3$ and is somewhat lower than that given in [48] of $\gamma^\ast\text{bulk} = 760 \text{ eVÅ}^3$. Discrepancies in the literature arise from the different number of bands accounted for in the models and more so to the uncertainty in the values of the parameters which enter them (which are generally determined theoretically). For example values of Kane's $B$ reported in the literature vary significantly [4,48,72]. $B$ has been calculated from k.p theory to be $-32.2 \text{ eVÅ}^2$ [48] and $-31.4 \text{ eVÅ}^2$ [88] and determined experimentally from magnetoresistance measurements (by analysis of strain induced beating patterns) on bulk InSb by Seiler et al. [72] to be $-12.6 \text{ eVÅ}^2$. These values differ by over a factor of two which would feed directly through to the results here for $\gamma$ and $\gamma_{\text{bulk}}$. The experimental technique of Seiler et al. is somewhat unreliable, predominantly
due to the inherent large effective g-factor in bulk InSb which contributes to the splitting in magnetic field from which the value of $B$ is extracted (see chapter 5 for further discussion in QW systems). For the modelling presented in this chapter, the value of $B = -31.4$ eVÅ$^2$ is taken from reference [88] as the results listed therein follow the trends of III-V semiconductors e.g. $B = -16.8$ and $-4.86$ eVÅ$^2$ for InAs and GaAs, respectively. The close agreement with the results of Cardona et al. [49] provides additional confidence in the value used, although a direct comparison between the values of the parameters used here and by Cardona et al. [49] can not be made. (In the sixteen (or fourteen) band model $\gamma$ is no longer proportional to $B$, but rather the momentum matrix element $Q$ which couples the valance bands to the higher order conduction bands, not included in the eight band model [49,77,81]).

The calculation of $\beta$ as a function of well width $W$ is indicated by the solid line in figure 4.5(b). A weak quadratic behaviour is exhibited, decreasing with increasing well width that can be compared to the $1/W^2$ dependence appearing in the high barrier limit of $\beta$ given in equation 4.5 (indicated by the dot dashed line in figure 4.5(b)). Although instructive as a qualitative comparison, the high barrier approximation overestimates the magnitude of $\beta$ by a factor of two compared with the evaluation of equation 4.17, even for the widest well. This is a direct result of the finite barriers used in the modelling presented here and the larger value of $\gamma_{\text{bulk}}$ used in the approximation. A second expression for $\beta$ that also appears in the literature and has been used by various authors is given by [17,18,80]

$$\beta = \gamma <k_z^2>.$$  \hspace{1cm} (4.20)

where $\gamma$ is calculated for the heterostructure and $<k_z^2>$ is the squared $k_z$ operator averaged over the ground state. The result of this approach is presented in figure 4.5(b) by the dashed line. By comparison, one finds that values of $\beta$ obtained using this approach are smaller by a factor of $\approx 1.2$ compared to the evaluation of
4.2. SIA and BIA coefficients in InSb quantum wells

Equation 4.17 in the widest well. The disparity is due to an oversight of an additional two terms that arise in $\beta$ from the differentiation of $\tilde{\gamma}(z, \lambda)$ over the interfaces. These terms are comparable to the field and interface terms appearing in $\alpha$ (see equation 4.19). The complete expression for $\beta$ consists of three terms given by [68]

$$
\beta = \frac{-2PB}{3} \left[ \frac{\partial \psi(z)}{\partial z} D_i \left( \frac{\partial \psi(z)}{\partial z} \right) + V_{UB} D_0 \psi(0) \left( \frac{\partial \psi(0)}{\partial z} \right) - V_{LB} D_H \psi(W) \left( \frac{\partial \psi(W)}{\partial z} \right) \right] 
$$

$$
- \frac{2PB}{3} \left[ \psi(0) \left( \frac{\partial \psi(0)}{\partial z} \right) (C_0 - V_{UB} D_0) - \psi(W) \left( \frac{\partial \psi(W)}{\partial z} \right) (C_w - V_{LB} D_H) \right]
$$

$$
+ \frac{2PB}{3} \left[ \psi(z) \left( \frac{\partial^2 \psi(z)}{\partial z^2} \right) \psi(z) \right],
$$

(4.21)

where $\psi(0)$, $\psi(W)$, $\partial \psi(0)/\partial z$ and $\partial \psi(W)/\partial z$ are the values of the wave function and its derivative at the interfaces $z = 0$ and $z = W$. Note that the third term in equation 4.21 is formally equivalent to the expression in equation 4.20. From inspection of the results, it is found that the $2^{nd}$ term (interface term) dominates over the $1^{st}$ term (field term), as is the case for $\alpha$. However, the third term $\gamma < k_z^2 >$ contributes to $\approx 75\%$ of the total, justifying the use of this approximation by previous authors [17,18,80]. These results demonstrate the interface contribution to $\beta$ and thus confirms that the $k$-linear Dresselhaus term can be linked to both BIA and SIA mechanisms [55,74,94].

It is worth commenting on the underlying barrier asymmetry in these structures i.e. $dV_{UB} - dV_{LB} > 0$. This counteracts the direction of the field in the QW, reducing the asymmetry of the probability densities at the interfaces $\Delta \Psi_i^2$. Intuitively, one would therefore expect the Rashba coefficient to be greater in symmetric barrier structures. In varying the upper barrier alloy composition $x$, we find that although $\Delta \Psi_i^2$ does indeed increase as the barrier asymmetry is reduced, the coefficients within the dominant interface term associated with the top
interface which depend on band parameters, decrease in such a way as to counteract this expected behaviour. Consequently, for a fixed carrier density, $|\alpha|$ increases with barrier asymmetry. This is demonstrated in figure 4.6 for a 20 nm QW. The upper barrier composition has been reduced from In$_{0.8}$Al$_{0.2}$Sb to In$_{0.85}$Al$_{0.15}$Sb using interpolated band parameters from [4]. The same behaviour is seen in wells of different widths (not shown). $\beta$ also increases with barrier asymmetry as indicated by the open symbols in figure 4.6. In contrast, $\gamma$ shows negligible variation with barrier asymmetry because the contribution from the QW dominates over that from the barriers.

The results for these calculations highlight the influence of heterostucture design on $\alpha$ and $\beta$. For a large Rashba coefficient $\alpha$, the carrier density $n_{2D}$ should be maximised for a given well width $W$ (maintaining single subband occupation) with consideration given also to the barriers i.e. upper and lower barrier composition and asymmetry.

![Figure 4.6](image)

**Figure 4.6:** Calculated parameters $\alpha$ and $-\beta$ as a function of barrier asymmetry for a 20 nm QW with fixed carrier density $n_{2D} = 2.6 \times 10^{11}$ cm$^{-2}$. The solid lines are a guide to the eye.
4.3 Spin splitting

The total spin splitting at the Fermi energy $\Delta E_{\text{Tot}} [k_F (\theta)]$ depends on the direction of in plane momentum $\theta(k_{||})$ and is calculated within the eight-band model used here by

$$\Delta E_{\text{Tot}} [k_F (\theta)] = 2 \left| \Psi(z) \right| \hat{K}_{SLA} + \hat{K}_{BLA} \left| \Psi(z) \right|$$

(4.22)

where $\hat{K}_{SLA}$ and $\hat{K}_{BLA}$ are the off-diagonal elements of the Hamiltonian as defined before. The Fermi wave vector is a function of $\theta$ given by $k_F (\theta) = k_F (\cos \theta, \sin \theta, 0)$ and $k_F$ is calculated from carrier densities obtained from the SPM solutions through the relationship $k_F = \sqrt{2m_2 D \omega}$. This is equivalent to the spin splitting from the effective field $\Delta E_{\text{Tot}} [k_F (\theta)] = 2\hbar \left| \Omega [k_F (\theta)] \right|$. Evaluating equation 4.22 yields the spin splitting at the Fermi energy, as a function of $\theta$

$$\Delta E [k_F, \theta] = 2k_F \left\{ \alpha^2 + \beta^2 + \alpha \sin 2\theta (\gamma k_F^2 - 2\beta) - \beta \gamma k_F^2 \sin^2 2\theta \left( \frac{\nu^2 k_F^2}{4} - \beta \right) \right\}^{\frac{1}{2}}$$

(4.23)

Figure 4.7 shows the spin splitting as a function of in plane wave vector for three 15 nm QW structures with different Fermi wave vector using parameters $\alpha$, $\beta$ and $\gamma$ obtained in the previous two sections.
4.3. Spin splitting

The spin splitting $\Delta E[k_F(\theta)]$ originating from SIA and BIA separately exhibit an isotropic and a symmetric four-lobed [74] behaviour respectively. Thus the oscillatory behaviour in $\Delta E_{tot}[k_F(\theta)]$ gives a clear indication that the cubic terms in $k$ from BIA contribute significantly to the total spin splitting.

The strong anisotropy about the [110] and [\(\bar{1}10\)] directions is due to the presence of both BIA and SIA simultaneously which are non-additive within equation 4.22. The minimum spin-splitting is observed for $k_F(\theta)$ parallel to the
4.3. Spin splitting

$4V = 15 \text{nm}$
$W = 20 \text{nm}$
$W = 25 \text{nm}$
$f - F = 30 \text{nm}$

\[0 \quad 0.6 \quad 0.5 \quad 0.4\]
\[^3 = 0.4\]

Figure 4.8: Fraction of the total averaged spin-splitting contributed from BIA as a function of carrier density for the different well widths. The dashed line indicates the point when both SIA and BIA contribute equally to \(< \Delta E_{\text{Tot}} > (k_F)\).

[1 1 0] direction which also shows a strong non-linear dependence on $k_F$ (this is also the direction of the minimum for $\Omega[k_F(\theta)]$ since $\Delta E_{\text{Tot}}[k_F(\theta)] = 2\hbar |\Omega[k_F(\theta)]|$).

The average spin splitting is found by integrating equation 4.23 over the Fermi circle $k_F(\theta)$ i.e. all angles $\theta$. Odd terms (e.g. $\sin \theta$ and $\sin^3 \theta$) integrate to zero, resulting in a simplified expression given by
4.3. Spin splitting

\[ < \Delta E_{\text{Tot}} > (k_F) = 2k_F \left( \alpha^2 + \beta^2 + \frac{k_F^4}{8} - \frac{k_F^2}{2} \beta \gamma \right)^{1/2}. \] (4.24)

In this case the SIA and BIA terms are decoupled and the separate contributions may be extracted. (Note that when SIA dominates, the usual spin splitting associated with the Rashba effect is recovered, i.e. \( < \Delta E_{\text{SIA}} > = k_F |\alpha| \)).

The significance of the BIA contribution to spin splitting in the structures studied here is quantified in figure 4.8 which shows the fraction of the total spin splitting originating from BIA as a function of carrier density for the four well widths. The carrier density dependence stems primarily from the Rashba parameter, showing that for small carrier densities where the Rashba effect is small, the BIA contribution is relatively large, whereas with increasing carrier density its significance decreases as the Rashba effect is enhanced. Furthermore, the total (average) spin splitting for a given carrier density is greater in the narrow well structures: For \( k_F = 1.26 \times 10^8 \text{ m}^{-1} \), \( < \Delta E_{\text{Tot}} > (k_F) = 1.80 \text{ meV} \) and \( 1.42 \text{ meV} \) for the 15 nm and 30 nm QW, respectively.

It is therefore found, contrary to the results of Pfeffer and Zawadzki for the InAlAs/InGaAs system [45], that in these InSb heterostructures the SIA cannot always be considered as the dominant mechanism as the BIA contribution is significant and in some cases dominant [68].

From the calculations performed here, it is noted that the characteristic anisotropy of the BIA spin splitting \( \Delta E_{\text{BIA}}(k_F(\theta)) \) exhibits a marked dependence on the ratio of \( \beta / \gamma \) and \( k_F \). For particular values of \( \beta / \gamma \) and \( k_F \) the anisotropy, defined here as \( \Delta E_{[100]} / \Delta E_{[110]} \), undergoes a \( \pi/4 \) phase shift compared to that reported by Eppenga et al. [74], such that the maximum spin splitting is found along the [110] direction and not the [100] directions. This macroscopic change in anisotropy occurs smoothly and it can be shown from equation 4.23 (with \( \alpha = 0 \)) that the transition occurs when the condition \( 4 \beta / \gamma k_F^2 = 1 \) is satisfied (at which point \( \Delta E_{\text{BIA}}(k_F(\theta)) \) is completely isotropic). When both SIA and BIA are
present the total spin-splitting will not become isotropic due to the crossed terms involving $\alpha\beta$, $\alpha\gamma$ and $\beta\gamma$ which appear in equation 4.23. The behaviour of $\Delta E_{\text{tot}}(k_F(\theta))$ becomes completely symmetric about the [100] direction when $2\beta/\gamma k_F^2 = 1$, whereas we find for $2\beta/\gamma k_F^2 < 1$ the minimum spin splitting is found along the [110] direction i.e. a $\pi/2$ phase shift compared to the data presented in figure 4.6 where $2\beta/\gamma k_F^2 > 1$.

An optical experiment whereby the spin splitting is determined as a function of the in plane wave vector could in principle detect such a change in symmetry when the carrier density is varied such that the condition of $\beta/\gamma = k_F^2 / 2$ is traversed. For example, this information could be gained from the side emission of a gated LED structure in the [110] and [1$ar{1}$0] directions, a Raman scattering experiment such as that performed by Jusserand et al. [95] or even from the spin galvanic effect [96]. With knowledge of the carrier density, such an experiment would yield direct measurement of the ratio $\beta/\gamma$, which could be compared to calculations and also to a spin galvanic type experiment [94].

4.4 Comparison to previous experiment and theory

The values of $\alpha$ calculated here can be compared to previous experimental and theoretical studies of narrow gap InSb and InAs QWs available in the literature. Consistent with previous studies of InSb [87], $\alpha$ is found to be negative. This result can be deduced from inspection of equation 4.19 and the direction of the electric field across the well, whereby, provided that the coefficients $C_0 - dV_{UB}D_0$ and $C_W - dV_{LB}D_W$ are negative, $\alpha$ is negative so long as $\Delta\Psi_i^2 = \Psi^2(0) - \Psi^2(W)$ is positive. It follows from this argument that $\alpha > 0$ in structures that are doped below the QW as was demonstrated by Nitta et al. in the InGaAs system [93].
4.4. Comparison to previous experiment and theory

Khodaparest et al. [44,97] studied the spin splitting in finite magnetic fields in symmetric InSb/In_{0.91}Al_{0.09}Sb QWs by spin resonance. Assuming that the spin splitting at zero field originated solely from SIA a value of $\alpha \approx 1.3 \times 10^{-11}$ eVm was estimated for a well width of 30 nm. Their results have been described by Pfeffer and Zawadzki [87] using an eight-band $k\cdot p$ model applicable to $B \neq 0$ and neglecting BIA. Their extracted value is somewhat greater than calculations performed here. However, recent measurements performed on InSb QWs by the same group [98] claim to find better agreement with theory using smaller values of $\alpha$, more consistent with those calculated here.

Grundler [99] investigated the gate dependence of $\alpha$ in symmetric 4nm InAs/InGaAs QWs via the beating of Shubnikov-de Haas oscillations extracting values in the range $\alpha = 2-4 \times 10^{-11}$ eVm. These values were estimated using an expression derived by Engels et al. [39] relating $\alpha$ to the difference in the populations of the spin-split subbands $\Delta n = n^+ - n^-$ determined from Fourier analysis of the beating patterns at low $B$ fields (this is discussed in further in chapter 5). In fact, the Rashba coefficient is rarely measured in narrow gap semiconductors by this method due to the presence of large Zeeman splitting, which dominates the transport at relatively low fields compared to wider gap systems (see Chapter 5 for further detailed discussion) [44,100,101].

All of the above methods are based on the assumption that the zero-field spin splitting is dominated by the SIA mechanism. The results of the calculations presented in this thesis indicate that this assumption should not always be considered true and can be the source of erroneous estimations of $\alpha$. More recently, a novel experimental approach for direct measurement of the Rashba and $k$-linear Dresselhaus coefficients was proposed by Ganichev et al. [94] from analysis of the angular dependence of the spin-galvanic photocurrent [96]. Values for the ratio of Rashba and Dresselhaus coefficients in 15nm InAs/InGaAs QWs are estimated at $\alpha / \beta \sim 2.15$ using this method, agreeing with ratios from $k\cdot p$ calculations in the InGaAs QW system of $\sim 1.85$ using the method described in this chapter [45]. In comparison, the ratios calculated here for equivalent InSb
4.4. Comparison to previous experiment and theory

QW structures are typically smaller than those quoted above because of the significantly larger Dresselhaus coefficient $\gamma$ in InSb which enhances $\beta$.

4.5 D'yakonov Perel' spin relaxation

Averkiev and Golub [102] calculated the spin relaxation in [001] oriented QWs based on the DP mechanism and predicted a large anisotropy with respect to the in-plane momentum and a large enhancement of the spin lifetime under certain conditions from the interference between SIA and BIA induced (SO) interactions. Following their work, two device proposals emerged (apparently simultaneously) by Cartoxia et al. [18] and Schleimann et al. [17] for a spin lifetime field effect transistor (SL-FET). The functionality of these devices is based on achieving the conditions of $\alpha = \beta$ and $\alpha \neq \beta$ which are shown to significantly change the spin lifetime and provide current modulation. Formally, this is the diffusive regime equivalent to the Datta-Das spin transistor. This change in spin lifetime occurs since for $\alpha = \pm \beta$ the direction of the precession vector $\Omega(k_{||})$ (when disregarding $\gamma$) no longer depends on $k$, i.e. from equation 4.15 we see that

$$\Omega(k_{||}) \propto \alpha(\pm k_x - k_y)[1,\pm1,0]$$

(4.25)

so that scattering events change only its magnitude and not direction, allowing long spin lifetimes for spins oriented in the [110] and [1\bar{1}0] directions respectively, i.e. when parallel to $\Omega(k_{||})$ [102]. Experimental verification of the spin relaxation anisotropy has now been demonstrated by Averkiev and Golub [103] by means of Hanle effect measurements in the GaAs/AlGaAs system, where a variation in the spin lifetime of a factor of four was observed between spins oriented along the [1\bar{1}0] and [001] directions. Although the concept of the SL-FET has received some criticism as being a counter productive incarnation of the original Datta-Das spin transistor [104] (based primarily on arguments of
realistic and achievable spin injection efficiencies) it is interesting to investigate the viability of balancing the SIA and BIA interactions for the purpose of enhancing the spin lifetime in the InSb/In$_{1-x}$Al$_x$Sb QW system.$^5$

The original proposals for the SL-FET neglected the $k^3$ contribution ($\gamma$) to the Dresselhaus splitting [102]. Kainz et al. [105] later calculated the spin lifetime in the AlGaAs/GaAs and GaAlSb/InAs systems including the $k^3$ contribution. The main result was that by taking into account $\gamma$ in the calculation, a carrier density and well width dependence of the spin lifetime was observed, which was previously overlooked. It is expected that the influence of the $\gamma$ terms in the InSb system will be even more significant and is taken into account in the following calculations.

For the In$_{1-x}$Al$_x$Sb/InSb structures considered, the parameters $\alpha$ and $\beta$ are of opposite sign. Following the results of Averkiev et al. [80], for this case a maximum enhancement in the spin lifetime should occur for spins injected parallel to [1 1 0]. For this reason, the calculations presented here focus on this direction. For a degenerate 2DEG the spin relaxation rate for spins oriented parallel to the [1 1 0] direction is given by [80]

$$\frac{1}{\tau_{d[110]}} = \frac{2\tau_1}{\hbar^2} \left[ \frac{(\alpha + \beta)^2 k_F^2}{2} - \frac{1}{2} \gamma (\alpha + \beta) k_F^4 + \frac{1 + \tau_3 / \tau_1}{16} \gamma^2 k_F^6 \right]$$

(4.26)

$\tau_1$ and $\tau_3$ are the lifetimes associated with the harmonics of the scattering cross-section of the form

$$\tau_n^{-1} = \frac{1}{\hbar^2} \int |U_{kk'}|^2 (1 - \cos n\theta) d\theta$$

(4.27)

$^5$ The original proposals are based on idealised 100% spin injection efficiencies which would provide large current modulation, however recently achieved injection efficiencies ~40-80% significantly reduce the output current on-to-off ratio and potential usefulness of such a device.
where $|U_{kk'}|^2$ is the probability of scattering from a state $k$ to $k'$ through an angle $\theta$ [34,80]. $\tau_i$ coincides with the momentum scattering lifetime $\tau_p$ which is related to the mobility $\mu$ of the 2DEG obtained from simple Hall measurements (see chapter 5). The lifetime $\tau_s$ is a more ambiguous quantity. The ratio $\tau_s/\tau_i$ is a measure of the effectiveness of momentum scattering in randomizing the precession vector $\Omega(k)$, and in general (i) for isotropic scattering where neither depend on $\theta$, all scattering times are equal to the elastic momentum scattering time and $\tau_s/\tau_i = 1$, whereas (ii) for small-angle scattering we have $1 - \cos n\theta \approx (n\theta)^2/2$ and $\tau_s/\tau_i = 1/n^2$ [34].

The approximation made by Kainz et al. [105] is simply that of (i) i.e. $\tau_s \sim \tau_i$. As demonstrated in [6] and in chapter 5, the low temperature carrier mobilities in modulation doped InSb/InAlSb QW heterostructures are controlled by long-range (small angle) remote ionized impurity scattering (RIIS). Thus in the structures considered here we are in the limit of case (ii). To investigate this ratio further, one requires knowledge of the scattering potential. Assuming that the results of Ref. [6] stand, this can be gained by manipulating the expression for the scattering rate associated with RIIS to match the form of $\tau_s^{-1}$ given above (for $n = 1$). The appropriate scattering probability $|U_{kk'}|^2$ can then be extracted and substituted into the expressions for $\tau_s^{-1}$ to yield an estimate for the ratio $\tau_s/\tau_i$. It can be shown that for the structures considered here the ratio $\tau_s/\tau_i$ typically varies between 0.12 to 0.28. To ease the following calculations, an average value of $\tau_s/\tau_i = 0.2$ is used.

From inspection of the expression for $\tau_{s[1\bar{1}0]}$, we see that for small carrier densities (e.g. $n_{2D} < 0.5 \times 10^{15} \text{ m}^2$) and/or small $\gamma$, the $k_F^4$ and $k_F^6$ terms become negligible and $\tau_{s[1\bar{1}0]}$ is dominated by the $k_F^2$ terms involving only $\alpha$ and $\beta$ parameters. This is the limit considered by Schleimann and Loss and Cartoxia.
where \( \tau_{d[1\bar{1}0]} \) approaches infinity when \( \alpha = -\beta \) as demonstrated by the black line in figure 4.9 [18].

Experimentally, the sensitivity of the spin lifetime to the carrier density has been demonstrated, both electrostatically (i.e., by a gate) [85,106], or via the doping conditions [20]. However, the modulation of \( \alpha \) whilst maintaining a constant carrier density can be achieved experimentally by the combined use of a top and ‘back’ gate as demonstrated by Nitta et al. [93]. This is the essentially the scenario considered for the original SL-FET operation. For this reason two approaches shall be considered separately: (i) constant carrier density; using \( \alpha \) as a free variable for a given \( k_F \) to calculate \( \tau_{d[1\bar{1}0]} \) as a function of \( \beta/\alpha \) and (ii) varying carrier density; using the results for \( \alpha, \beta \) and \( \gamma \) as a function of carrier density from the previous in section (this is most appropriate to the structures studied here).

It is emphasized that the first condition (i) is not appropriate for the structures which have been modelled, but it is instructive as a tool for independently exploring the effects of well width and carrier density on the behaviour of \( \tau_{d[1\bar{1}0]} \).

### 4.5.1 Modifications to the spin lifetime FET in InSb QWs

Case (i) in the above discussion can be explored by treating \( \beta \) and \( \gamma \) as fixed for a given carrier density and well width. The condition for maximum spin lifetime is found from \( \partial \tau_{d[1\bar{1}0]}^{-1} / \partial \alpha = 0 \), giving

\[
\alpha = \frac{1}{4} k_F^2 \gamma - \beta \quad \text{and} \quad \frac{\beta}{\alpha} = \frac{k_F^2}{k_F^2 - 4 \beta / \gamma} - 1
\]  (4.28)

It can seen that equation 4.28 reduces to the case of \( \alpha = -\beta \) in the limit of small \( k_F \) or \( \gamma \). Figure 4.9 shows the spin lifetimes \( \tau_{d[1\bar{1}0]} \) as a function of the ratio \( \beta/\alpha \) for a
15 nm (green line) and 30 nm (green line plus symbols) QW using SO parameters obtained from the \( k.p \) calculations at \( k_F = 1.26 \times 10^8 \text{ m}^{-1} \) with \( \tau_l = 1.2 \text{ ps} \) and \( m^* = 0.014 \ m_0 \). The corresponding SO parameters used in the calculations are \( \beta = 0.0768 \text{ eV}\AA \) and \( 0.0314 \text{ eV}\AA \), and \( \gamma = 385 \text{ eV}\AA^3 \) and \( 442 \text{ eV}\AA^3 \) for the 15 nm and 30 nm QWs respectively.

It is evident from these results, that the inclusion of terms involving \( \gamma \) suppresses and shifts the maximum spin lifetime. Substitution of equation 4.28
into the expression for the spin lifetime (equation 4.26) yields a maximum spin lifetime of

\[
\tau_{\text{max}}^{[1\bar{1}0]} = \frac{\hbar^2}{2k_F^2\gamma^2\tau_3},
\]

controlled by the parameters $\gamma$, $k_F^2$, and $\tau_3$. The appearance of a finite maximum is consistent with a qualitative picture of the spin configuration in the 2DEG plane. In the idealized case where $\gamma = 0$ and $\alpha = -\beta$ the component of an injected spin along $[1\bar{1}0]$ is always parallel to the direction of $\Omega(k_\|)$. However, with the inclusion of $\gamma k^3$ terms in the spin lifetime, the orientation of $\Omega(k_\|)$ is always changing with $k$ even when the SIA and BIA couplings are balanced according to equation 4.28. Thus the component of spin is never aligned with $\Omega(k_\|)$ and a finite spin relaxation will be experienced. Departure from the ideal case then increases with the magnitude of $\gamma$ which accounts for the different dependence on $\beta / \alpha$ observed for different QW widths.

Surprisingly, the width of the peak in $\tau_{\text{max}}^{[1\bar{1}0]}$ for the 30 nm QW is significantly broadened in comparison to the 15 nm QW data. Perhaps more importantly from a device perspective is that because of the broadening in $\tau_{\text{max}}^{[1\bar{1}0]}$, the potential current modulation from the ‘on’ to ‘off’ states in this structure from tuning $\alpha$ would be greatly reduced from that of a narrower well structure. A significant peak in $\tau_{\text{max}}^{[1\bar{1}0]}$ for the 30 nm well is recovered only for very small $n_{2D}$, i.e. the conditions of the original proposals of the SL-FET where $\gamma$ is neglected.

The effect of carrier density on the variation of $\tau_{\text{max}}^{[1\bar{1}0]}$ with $\beta / \alpha$ is demonstrated for the 15nm QW by comparison of the red, green and blue and lines in figure 4.9 for which $k_F = 0.8, 1.26$ and $1.5 \times 10^8$ m$^{-1}$ respectively (each data set is generated using different values of $\beta$ and $\gamma$ according to the $k.p$ calculations for the different $n_{2D}$). As $k_F$ is reduced the behaviour of the spin lifetime peak
4.5. D'yakonov Perel' spin relaxation

approaches that for the idealised case of $\gamma = 0$ (indicated by the black line in figure 4.9). These results demonstrate the sensitivity of the position and magnitude of the maximum spin lifetime to $k_F$ (and $n_c$), which is evident from the $k_F^2$ and $k_F^6$ dependences in the respective expressions.

From the point of view of engineering a structure for maximum spin lifetime ($\tau_{s[1\bar{1}0]}^{\text{max}}$), minimising the SIA and BIA coefficients and the ratio of lifetimes $\tau_3/\tau_1$ is required. Minimising $\alpha$ can be achieved by lowering the carrier density. In general though, these requirements are difficult to meet since $\gamma$ increases as the carrier density is reduced (although from equation 4.29 we see that $\tau_{s[1\bar{1}0]}^{\text{max}}$ is most sensitive to carrier density). The peak lifetime $\tau_{s[1\bar{1}0]}^{\text{max}}$ is independent of $\alpha$ and $\beta$ and requires a small $\gamma$ which in these structures is best met by narrow wells. Intriguingly, counter to the general understanding of the DP relaxation mechanism, equation 4.29 reveals there is no explicit momentum scattering (mobility) dependence on the maximum lifetime. How to directly engineer $\tau_3$ is unclear. Its explicit link to the scattering potential in the momentum lifetime implies that in general, reducing the momentum scattering lifetimes $\tau_i$ will result in increased spin lifetimes. In modulation doped structures this can be achieved by reducing the spacer thickness.

4.5.2 Results for varying carrier density

In the structures studied here, tuning $\alpha$ with an external field also changes the carrier density. The following results represent the calculations of $\tau_{s[1\bar{1}0]}$ using all three SO parameters and carrier densities associated with each SPM solution. Since for RIIS limited transport lifetimes, $\mu$ varies explicitly with spacer thickness and doping density the results are presented in terms of the product $\tau_{s[1\bar{1}0]}/\mu$. It should be emphasized that the results presented here are for solutions at zero bias so that the carrier density is varied through the doping conditions and not through an external field.
The results of $\tau_{s[\bar{1}0]}$ for the various well widths are presented in figure 4.10. Data for the 15 nm, 20 nm and 25 nm QW structures exhibit a strong non-monotonic behaviour at moderate $n_{2D}$ as observed in [105] and [107]. The turning points in the data indicate that the SIA and BIA induced couplings have been balanced over the range of carrier density considered; this is equivalent to the peaks observed in figure 4.9 although the condition for maximum lifetime is less trivial because $\alpha$, $\beta$ and $\gamma$ are now a function of $n_{2D}$. No turning point is seen in the results for the 30nm QW.

To understand these results, recall that the magnitudes of $\alpha$ and $\beta$ are comparable at moderate $n_{2D}$ in the 15 nm, 20 nm and 25 nm QW structures (see figure 4.2) which facilitates the observed peak in the spin lifetime (note that the
maximum spin lifetime is observed at lower $n_{2D}$ than the points at which $\alpha = -\beta$ due to the influence of $\gamma$). Accordingly, it can be inferred that a turnover in $\tau_{d^{[110]}\mu}$ for the 30nm well occurs at smaller $n_{2D}$ than is considered here, when $\alpha$ is smaller.

The results for $\tau_{d^{[110]}\mu}$ in the 20 nm QW can be quantitatively compared to those of Kainz et al. [105] for a 20 nm InAs/GaAlSb and GaAs/AlGaAs QWs. Using the same momentum scattering time of $\tau_\Gamma = 0.1$ ps and taking $m^* = 0.014m_0$ for InSb corresponds to a mobility of $\mu = 1.25$ m$^2$/V$^{-1}$s$^{-1}$. The carrier densities at which the peak spin lifetime is observed are consistent, however, a large disparity is found between the maximum values estimated from [105] as $\sim 33$ ns and $\sim 10$ ns for the InAs and GaAs QW systems respectively compared to a much smaller value of $\approx 0.44$ ns calculated here. This again is due to the large $k^3$ Dresselhaus parameter $\gamma$ present in these InSb/InAlSb heterstructures which significantly reduces the spin lifetime. Although it is unclear which values of $\gamma$ were used in the calculations of [105], typical values of $\gamma$ in the bulk InAs and GaAs systems are $103$ eVÅ$^3$ and $25$ eVÅ$^3$ respectively [49,84] (which would be further reduced in a heterostructure) which are substantially smaller than those calculated here.

The results presented here strongly indicate that narrow well structures exhibit longer spin lifetimes over the majority of realistic carrier densities ($n_{2D} > 2 \times 10^{15}$ m$^{-2}$) compared to those in wider well structures which are predicted to be greater only at smaller $n_{2D}$. This is in qualitative agreement with recent measurements of the spin lifetime in 30 nm InSb QWs which suggest short spin lifetimes of $\tau \approx 0.3$ ps [108], far shorter than those measured in 15 nm QWs of $\tau \approx 0.3$ ps [109]. Although the finer structure of the spin lifetime characteristics is dependent on the interplay between all three SO parameters, this trend in the variation with well width is primarily attributed to the smaller value of $\gamma$ in the narrow wells. It has been demonstrated here in both the scenarios of ($i$) constant
4.5. D'yakonov Perel spin relaxation

and (ii) varying carrier density that this parameter has a significant influence on the spin lifetime maximum in the [1 1 0] direction.

4.5.3 Results for [001] and [110] orientations

The corresponding expressions for the spin relaxation rate in a degenerate 2DEG for spin oriented parallel to the [110] and [001] directions are given by [80]

\[
\frac{1}{\tau_{s(110)}} = \frac{2\tau_1}{\hbar^2} \left[ (\alpha - \beta)^2 k_F^2 + \frac{1}{2} \gamma (\alpha - \beta) k_F^4 + \frac{1 + \tau_3/\tau_1}{16} \gamma^2 k_F^6 \right]
\] (4.30)

and

\[
\frac{1}{\tau_{s(001)}} = \frac{4\tau_1}{\hbar^2} \left[ (\alpha^2 + \beta^2) k_F^2 - \frac{1}{2} \gamma^4 k_F^4 + \frac{1 + \tau_3/\tau_1}{16} \gamma^2 k_F^6 \right].
\] (4.31)

Figure 4.11: Comparison of the spin lifetime multiplied by the mobility in the three orientations [1 1 0] (black line), [1 1 0] (green line) and [001] (red line) for the 20 nm QW.
Results from the calculation of $\tau_s \mu$ for the [110] and [001] directions as a function of carrier density are presented in figure 4.11 for the 20 nm QW with the results for the [1 1 0] direction for comparison.

Spins injected parallel to the [001] and [110] directions experience approximately equal spin relaxation rates which are, typically, over an order of magnitude greater than those in the [1 1 0] direction (also true in InAs and GaAs QWs [105]).

This may have significant implications for spintronic devices as many spin lifetime measurements are performed by optically creating spins in the [001] direction by pumping circularly polarized light perpendicular to the surface. The spin lifetime for carriers injected through a ferromagnet contact magnetized in the [1 1 0] direction in a spin transistor type two-terminal device may experience far less spin relaxation than is measured optically in the [001] direction. This also highlights the importance in the orientation of the ferromagnetic contacts in such a device to achieve maximum spin lifetime.

Since the [001] orientation is the most accessible orientation for optical measurements of spin lifetime, it is interesting to examine these results further. For spins parallel to the [001] direction, $\tau_{s[001]} \mu$ shows little variation with well widths over the range of carrier densities considered. The separate contributions to $\tau_{s[001]} \mu$ from the first two terms (red data) and the first term alone (green data) in equation 4.31 are shown in figure 4.12 for a 15 nm QW. The total contribution to the spin lifetime in this direction is controlled predominantly by the first two terms proportional to $n_{2D}$ and $n_{2D}^2$ in the expression for $\tau_{s[001]}$. In fact, in this direction, to a fairly good approximation, one can disregard terms involving $\gamma$ which also simplifies the analysis of experimental data somewhat. This is the case for all well widths considered (results for a 25 nm QW are shown in the inset).
Also shown in figure 4.12 is the contribution from terms proportional to $\alpha$ alone (blue data). This demonstrates that disregarding both $\beta$ and $\gamma$ terms does not approximate well the spin lifetime. However, this approach becomes increasingly valid as $\alpha$ is enhanced e.g. in wide QWs or increased carrier density, as demonstrated by the corresponding results for the 25 nm QW shown in the inset.

From an experimental point of view, provided that the spin relaxation is controlled by the DP mechanism, using experimentally determined values for the momentum scattering time (which in the absence of electron-electron scattering can be determined from the mobility) and the spin lifetime for optically oriented
4.5. D'yakonov Perel' spin relaxation

spins in the [001] direction, equation 4.31 can be used to extract an effective spin splitting parameter involving all three coefficients. In the case where $\alpha$ dominates, the Rashba parameter can be estimated [110].

4.6 Summary

Using the established $k.p$ formalism of Pfeffer and Zawadski [45], the inversion asymmetry spin-orbit coupling parameters have been calculated for the ground state subband in a wide range of asymmetric $n$-InSb/Al$_x$In$_{1-x}$Sb quantum well heterostructures using the electrostatic potentials and wavefunctions generated from a self consistent Schrödinger-Poisson model [68]. Crucially this work contributes to previous studies in this system by considering realistic structures and taking into account the penetration of the wavefunction into the barriers.

It is found that for the realistic InSb structures that are grown (at QinetiQ Malvern), for a given carrier density the Rashba parameter is largest in wide 30 nm QWs. However, narrower well structures can have higher carrier densities before the second subband becomes occupied. At these elevated densities, the Rashba parameter in narrow well structures is large and can exceed that in wide wells.

By evaluating the spin splitting at the Fermi energy it was demonstrated that contrary to common understanding, the bulk inversion asymmetry contribution (Dresselhaus) is significant and can exceed that from the Rashba interaction. Shortfalls in the commonly used expressions for the two dimensional Dresselhaus parameters $\beta$ were highlighted. In the extreme case of the infinite barrier approximation $\beta$ is overestimated by over a factor of two.

The angular dependence of the spin splitting in the plane of the 2DEG exhibits a characteristic anisotropy as found in previous studies, however, it is found that under certain conditions when $2\beta / \gamma k^2 < 1$ a $\pi/2$ phase shift in the anisotropy should occur which if detected experimentally could provide an alternative method for determining the ratio of BIA parameters $\beta/\gamma$. 
The D'yakonov-Perel' spin relaxation rates were computed using the parameters obtained in section 4.2 which showed a strong dependence on carrier density for spins in the [1\bar{1}0] direction. In general the spin lifetime is inversely proportional to the magnitude of the spin splitting, however, in agreement with previous reports, the spin lifetime reaches a maximum over a narrow range of carrier densities when the Dresselhaus and Rashba interactions interfere destructively. It is found that the large bulk Dresselhaus splitting parameter in InSb significantly reduces the maximum spin lifetime compared to wider gap materials GaAs or even InAs. For optical measurements of the spin lifetime, spins are oriented in the [001] direction. It is shown that spins in this direction experience over an order of magnitude greater spin relaxation than in the lateral [1\bar{1}0] direction. This is significant since most functional spin based device geometries injection spins in the plane of the 2DEG and hence will have lifetimes greater than that measured in the traditional fashion.

The inherently large SO coupling in the InSb/InAlSb system compared to other materials increases the significance of the higher order terms in the expressions for spin lifetime, which as a result has considerable effect on the operating conditions of the SL-FET and the maximum achievable spin lifetime. The results of the calculations presented provide valuable insight into the engineering of heterostructures for spintronic applications.
Magnetotransport in 30 nm InSb quantum wells – Experimental determination of the Rashba splitting

Whilst two dimensional electron gases formed in narrow gap InSb QWs have long been considered a promising candidate for spintronic applications such as the Datta Das spin transistor due to a large tunable Rashba interaction, few experimental reports on the extraction of the Rashba or zero field spin splitting exist.

The work presented in this chapter details the experimental approaches relevant for the investigation of electron transport and spin phenomena in narrow gap materials using the magnetoresistance technique. A comprehensive study of a range of high mobility gated $n$-type InSb/InAlSb quantum well heterostructures is presented in order to extract information on the SO coupling. Beating effects are observed in the low field Shubnikov de-Haas oscillations for the first time in this system and Rashba parameters are extracted from three samples as a function of gate bias. It is found that inhomogeneous Landau level broadening plays an important role in the observed beating phenomena and is analysed by means of numerical simulations of the magnetoresistance which reproduce well the
5.1 Introduction

The electron transport properties which characterise a semiconductor such as carrier density, \( n_{2D} \), and mobility, \( \mu \), can be probed by recording the response to electric and magnetic fields using a simple four-point measurement of the longitudinal resistance and the Hall effect (see section 5.2.2). Electron transport in a magnetic field, so-called magnetotransport can be broadly separated into two regimes, low field and high field measurements. In low magnetic fields, electron transport may be analysed in terms of the classical description of Drude [50]. Simple low field Hall measurements often requiring only one non-zero magnetic field data set enable a fast and simple method for extracting \( n_{2D} \) and \( \mu \) (discussed in section 5.2). In high magnetic fields, the density of states becomes quantised into Landau levels and a classical approach to transport is insufficient to describe the observed phenomena such as periodic oscillatory magnetoresistance (e.g. Shubnikov-de Haas effect [111]).

It was shown by Onsager [112], that the frequency of the magneto-oscillations for \( B > 0 \) is related to the extremal cross-sectional area of the Fermi
5.1. Introduction

surface in a plane normal to the magnetic field at B = 0. As a result, magnetotransport experiments have proved to be an important method for analysing the Fermi surface of various semiconductor materials. In addition, the removal of the ground state spin degeneracy in zero magnetic field due to inversion asymmetry can lead to anomalous magneto-oscillations in the form of beating patterns [38]. Consequently, the study of magneto-transport in 2D systems also provides valuable insight regarding the band structure parameters in zero field [37,72].

Values for the Rashba parameter calculated in chapter 4 for structures similar to those studied by Khodaparest et al. [44] predicted smaller values of α in the range 2-7x10^{-12} eVm. In addition, it was shown in Chapter 4 that the BIA contribution to spin splitting can be of significant and comparable value to the SIA contribution dependent on the details of the heterostructure (particularly the carrier density) [68]. Experimental evidence in support of this concept was recently given by Akabori et al. [113] by analysis of magnetotransport measurements in a narrow gap InGaSb/AlInSb QW indicating that the Dresselhaus SO interaction was dominant. Clear discrepancies exist between experiment and theory of spin splitting in narrow gap systems and further investigation of samples with a range of carrier densities is required to develop the understanding in this intriguing system.

5.2 Electron transport in low magnetic fields

This section describes the basic methods used for characterising semiconductor samples based on the semi-classical approach of Drude. The temperature dependence of the mobility in a typical InSb QW sample is analysed with a transport model which considers various scattering mechanisms. Some basic transport equations are derived which provide a basis for interpreting the results.
5.2. Basic transport equations

Consider a quasi-free electron system. When an electric field \( E \) is applied, electrons experience a force \(-eE\) which accelerates them in a direction opposite to \( E \). In the Drude model, it is assumed that between collisions, electrons move as free particles and their motion under external forces is governed by Newton's equations of motion [51]. Thus, in the time \( \tau_p \) between collisions, electrons acquire a drift velocity \( v_d = -eE\tau_p / m^* \) which is proportional to the electric field applied [114] (vector notation has been dropped for simplicity). The proportionality factor defines the electron mobility \( \mu \)

\[
\mu = \frac{e\tau_p}{m^*}.
\]  

(5.1)

Values of the mobility can differ by orders of magnitude for various material systems due to the scattering mechanisms present which determine \( \tau_p \) (e.g. see table 1.1).

From Ohm's law we have the classic expression for the current density \( j = -nev \) where \( n \) is the density of carriers and \( v \) is the velocity. By substituting in for the drift velocity we can relate the current density to the applied electric field by \( j = \sigma_0 E \), where \( \sigma_0 \) is the conductivity in zero magnetic field given by

\[
\sigma_0 = \frac{ne^2\tau_p}{m^*} \quad \text{and} \quad \sigma_0 = \frac{1}{\rho_0} = ne\mu
\]  

(5.2)

where \( \rho_0 \) is the resistivity of the material in zero magnetic field (units of \( \Omega m \)), related to resistance of a 3D conductor by \( R = \rho_0 L / A \), where \( L \) is the length of the conducting channel and \( A \) the cross-sectional area. In a 2DEG, motion is
quantised in the $z$-direction and $A$ is replaced by just the width of the sample $W$ such that $R = \rho_0 L/W$ ($\rho_0$ now has the units $\Omega/cm$). Equation 5.2 relates the macroscopic measureable quantity $\rho_0$ to microscopic quantities such as the carrier density and mobility.

An instructive parameter for a semiconductor is the mean free path between scattering events $\lambda_p = \sqrt{D \tau_p}$, where $D$ is the diffusion constant in two dimensions equal to $v_F^2 \tau_p / 2$ and $v_F$ is the Fermi velocity. It sets the scale of the device and is important in the study of ballistic transport in mesoscopic devices. For very small devices with transit lengths $L \ll \lambda_p$, electrons traverse the device without scattering and theories based on steady state diffusive transport (i.e. several scattering events) no longer apply. This is the ballistic transport regime and requires a purely quantum mechanical approach. It is therefore not surprising that a correct derivation of $\lambda_p$ goes beyond the classical description of Drude. At small electric fields, the mean free path, also known as the ballistic length can be estimated by\(^6\)

$$\lambda_p = \frac{1}{h} \left( \frac{dE(k)}{dk} \right)_{E=E_F} \tau_p \quad (5.3)$$

Evaluating equation 5.3 for the non-parabolic dispersion derived in chapter 2 yields

$$\lambda_p = \frac{h \sqrt{2 \pi}}{e(1 + 2\lambda E_F)} \mu \sqrt{n_{2D}} \quad (5.4)$$

\(^6\) For sufficiently large electric fields, the additional drift velocity can enable the electrons to reach the ballistic regime even when the transit length $L > \lambda_p$. 
5.2. Electron transport in low magnetic fields

Figure 5.1: Schematic illustration of the Hall Effect in a generic slab of material. $E_y$ is the Hall field

where $\lambda = 1/E_g$ and we have made use of the relationship $k_F = \sqrt{2m_{2D}}$. Thus, the mean free path is proportional to the mobility and the square root of the carrier density.

5.2.2 The Hall effect

The carrier density of the 2DEG may be determined by measurement of the Hall Effect. This phenomenon, observed by Hall in 1879, is the build up of a transverse voltage along a current carrying wire subject to a magnetic field.

A schematic of the Hall Effect in a slab of material with width $W$ and thickness $t$ is shown in figure 5.1. An electric field $E_x$ in the $x$-direction produces a net current flow in the same direction $J_x$. By applying a magnetic field perpendicular to the sample, $B_z$, electrons are subject to a Lorentz force which deflects the motion of electrons in a direction perpendicular to $E_x$ and $B_z$, i.e. in the (negative) $y$-direction $F_{Lor} = (-eE_x, -ev_B, 0)$. This results in an accumulation of negative charge at one side of the sample leaving a positively charged region at the other. This generates the Hall field in the $y$-direction which opposes the Lorentz force i.e. $F_H = (0, eE_H, 0)$. In equilibrium, the forces balance and current flows only in the $x$-direction [114].
When probed, a transverse ‘Hall’ voltage $V_H$ is measured. If the carriers had a positive charge, the carrier velocity would be reversed and the Lorentz force is unaltered. In this case the Hall field would be reversed. Thus the sign of the Hall voltage can be used to determine the polarity of the charge carriers - importantly this introduces the concept of positive charge carrier or ‘holes’.

The quantity of interest is the magnitude of the Hall field. Since the size of $E_y$ is determined by balancing the Lorentz force, intuitively one would expect it to be dependent on $B_z$ and also the current $j_x$. The Hall coefficient is defined by $R_H = E_y / j_x B$. It can be shown that the Hall coefficient depends only the carrier density and is given by [114]

$$R_H = \frac{1}{n_{2D} e} \quad (5.5)$$

The Hall voltage $V_y = E_y W$ is then given by $V_y = -B j_x / n_{2D} e$ where here $t$ is the thickness of the sample (in the $z$-direction). In the case of a 2DEG, the Hall voltage is given by [51]

$$V_y = \frac{-B j_x}{n_{2D} e} \quad (5.6)$$

Therefore, by measuring the magnetic field dependence of the Hall voltage, one can find the carrier density $n_{2D}$. With an additional measurement of the zero field resistivity $\rho_0$ (obtained from a four point measurement of the resistance along the channel) one can readily determine the carrier mobility using equation 5.2.

In theory, a sample of arbitrary shape with four electrical contacts can be used as a Hall device [115]. However, certain device geometries are more desirable than others. A geometry which allows simultaneous measurement of the Hall Effect and resistivity is the Hall bridge (see figure 3.3). Importantly, the Hall bridge approximates very well to an infinitely long Hall bar so that geometric
effects on the Hall voltage can be neglected [115]. For these reasons the Hall bridge is used in this thesis.

5.3 Characterisation of transport in 2DEGs

The samples described in chapter 3 were processed into gated Hall bridges and characterised by low field Hall Effect measurements at zero gate bias to determine the carrier density and mobility of the samples. The data for 2 K and at 290 K are listed in Table 3.1.

It is noteworthy that the wide well samples investigated here exhibit the highest low temperature mobilities reported in InSb QWs and also the highest room temperature mobilities reported in all III-V QW systems to date.

5.3.1 Temperature dependence of mobility

To characterise the transport in the 2DEGs, the temperature dependence of the mobility is analysed. The momentum scattering time, or transport time, $\tau_p$, depends on the energy and temperature of the carrier. In general, several scattering mechanisms may be present in a sample, each with an individual and well characterised dependence on carrier energy and temperature. In particular, certain scattering mechanisms may dominate at high or low temperatures and so analysis of the temperature dependence of the mobility can provide insight to the dominant scattering mechanism in a 2DEG in these regimes which can be used to engineer or maximise the mobility for various applications such as magnetic sensing and ballistic transport [6,116]. If each are characterised by the scattering rates $\tau_i^{-1}$, the resultant mean scattering rate is given within the relaxation-time approximation by Matthiessen's rule [6,114];

$$<\tau_p^{-1}> = \sum_i \tau_i^{-1}. \quad (5.7)$$
5.3. Characterisation of transport in 2DEGs

where the notation $\langle \tau_p^{-1} \rangle$ represents the average over the different mechanisms. This relationship assumes that each scattering mechanism $i$ is independent of the other. It also shows that the total scattering time $\langle \tau_p \rangle$ is less than any of the contributing scattering times $\langle \tau_i \rangle$.

A typical measurement of the carrier density and mobility in a modulation doped InAlSb/InSb QW (sample 2509A) over a range of temperatures from 2 K to 290 K is shown in figure 5.2(a) and (b) respectively. The mobility exhibits a relatively temperature independent behaviour at low temperatures $T < 30$ K and strong temperature dependence at high temperatures $T > 30$ K.

Figure 5.2: Measured temperature dependence of (a) carrier density and (b) mobility of a 30nm InSb QW sample 2509A.
which we will see can be accounted for by analysis of individual scattering mechanisms.

5.3.2 Transport lifetime model

The scattering mechanisms in III-V semiconductors are well established and can be broadly separated into two categories; lattice-phonon scattering and scattering from ionised impurities via the Coulomb interaction [51]. In QW heterostructures, the Coulomb scattering from ionised impurities which results from intentional doping can be reduced by separating the charge centres from the 2DEG, (see also chapter 3 [6]). The scattering from this mechanism is sensitive to the range of the interaction and so offers some degree of freedom for engineering the mobility. In contrast, scattering from phonons is unavoidable and dominates at high temperatures [117].

The two main phonon scattering processes important in III-V semiconductors are (i) deformation potential acoustic phonon scattering and (ii) polar-optical phonon scattering. The scattering from deformation potential acoustic phonons in a 2DEG with a QW of width $w$ has been considered by several authors and is given by [117]

\[
\frac{1}{\tau_{ac}} = \frac{3k_B T}{2} \frac{m^* \Xi^2}{\hbar^3 \rho_d u_s^2 w},
\]

where $\Xi$ is the deformation potential constant (related to the strain in the crystal [51]), $\rho_d$ the crystal density, and $u_s$ the longitudinal sound velocity. A large uncertainty exists in the value of the deformation potential in InSb. Several values have been quoted in the literature in order to achieve agreement with experiment (here we consider 7.2 eV and 30 eV [118]). Because the acoustic phonon scattering rate is proportional to $\Xi^2$ the use of either particular value can alter the magnitude of $\tau_{ac}$ significantly. This is discussed later in the section.
The scattering rate of electrons by absorption of polar-optical phonons is given by [117,119]

$$\frac{1}{\tau_{\text{ac}}} = \frac{e^2 m^* \omega_0 N(\omega_0) \omega}{4 \pi \varepsilon_0 \hbar^2}$$  \hspace{1cm} (5.9)

with $\varepsilon_p^{-1} = \varepsilon_{\infty}^{-1} - \varepsilon_s^{-1}$, where $\varepsilon_{\infty}$ and $\varepsilon_s$ are the high frequency and static dielectric constants. $h\omega_0$ is the optical phonon energy and $N(\omega_0) = [\exp(h\omega_0/k_bT) - 1]^{-1}$ is the number of phonons given by the Bose-Einstein distribution.

At low temperatures, the scattering rate from phonons is reduced and scattering from ionised impurities becomes significant. These originate from (i) a 3D background distribution of density $n_{\text{imp}}^{(3D)}$ or (ii) in modulation doped heterostructures, from a remote 2D sheet of ionised donor atoms separated from the 2DEG by a distance $S$ with a density $n_{\text{imp}}^{(2D)}$. Dependent on the quality of material, either of these mechanisms may dominate the transport at low temperatures, but in general, separating the charged impurities from the 2DEG significantly improves the carrier mobility [6]. The scattering rate associated with remote ionised impurities (RII) following the approach of Davies [120] is given by [6]

$$\frac{1}{\tau_{\text{RII}}} = n_{\text{imp}}^{(2D)} q_{\text{TF}} \left( \frac{e^2}{4 \varepsilon_0 \varepsilon_s k_F^2} \right)^2 \int_0^{2k_F} \frac{q^2}{(q + q_{\text{TF}})^2} \sqrt{1 - (q / 2k_F)^2} dq$$  \hspace{1cm} (5.10)

where, $q_{\text{TF}} = m^* e^2 / 2 \pi \hbar^2 \varepsilon_0 \varepsilon_s$ is the Thomas-Fermi screening wavevector and $q = 2k \sin(\theta / 2)$ is the scattering wave vector related to the scattering angle $\theta$. In a degenerate 2DEG at low temperature, scattering from an initial state to a final state can be considered to take place on the Fermi circle, in which case $q = 2k_F \sin(\theta / 2)$. The limits of the integral between 0 and $2k_F$ include all
scattering angles between $\theta = 0^\circ$ and $\theta = 180^\circ$ (i.e. back scattering). The scattering probability function is peaked towards small scattering angles due to the long-range nature of the Coulomb interaction.

The scattering rate associated with background impurities with a density $n_{\text{imp}}^{(3D)}$ is given by [6]

$$\frac{1}{\tau_{\text{imp}}} = n_{\text{imp}}^{(3D)} q_{\text{TF}} \left( \frac{e^2}{4\varepsilon_0 \varepsilon_s k_F^3} \right) \int_0^{2k_F} \frac{1}{(q + q_{\text{TF}})^2} \frac{q}{\sqrt{1 - (q / 2k_F)^2}} dq \quad (5.11)$$

We see that there is no explicit temperature dependence in equation 5.10 or 5.11; the only (weak) temperature dependence originates indirectly from the temperature dependences of the parameters $k_F$ and $m^*$ (and $\varepsilon_r$). Given that the carrier density changes significantly only for $T > 77$ K (shown in figure 5.2) at which point the scattering from phonons dominates, for the purpose of the analysis attempted here, values for $\tau_{\text{imp}}$ and $\tau_{\text{bi}}$ are calculated at $T = 2$ K and approximated to be fixed for all $T > 2$ K.

**TABLE 5.1:** Parameters for InSb used in the transport lifetime model taken from [4,6,116,118].

<table>
<thead>
<tr>
<th>Parameters for InSb</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Static dielectric constant $\varepsilon_r$ (F/m)</td>
<td>16.85</td>
</tr>
<tr>
<td>High-frequency dielectric constant $\varepsilon_{\infty}$ (F/m)</td>
<td>15.7</td>
</tr>
<tr>
<td>Lattice density (kg m$^{-3}$)</td>
<td>5790</td>
</tr>
<tr>
<td>Longitudinal sound velocity (ms$^{-1}$)</td>
<td>3700</td>
</tr>
<tr>
<td>Acoustic deformation potential (eV)</td>
<td>7.2</td>
</tr>
<tr>
<td>Optical-phonon energy (meV)</td>
<td>25</td>
</tr>
</tbody>
</table>
5.3. Characterisation of transport in 2DEGs

In figure 5.3 the transport model (indicated by the open diamonds) is compared to the experimental temperature dependent mobility from an InSb QW sample 2509A with a 20 nm spacer (indicated by the solid red line). Data from this sample is representative of all the 30 nm QW samples studied in this thesis (see also [6]). The parameters used in the calculations are listed in table 5.1.

The good agreement with the experimental data over the entire temperature range confirms the validity in this approach. Also shown are the
contributions to the mobility from individual scattering mechanisms. It is evident that the temperature dependence of the mobility in these modulation doped structures originates from phonon scattering, which dominates at high temperatures. At lower temperature, these are suppressed and the scattering by remote ionised impurity scattering is dominant.

The effects of band non-parabolicity have been taken into account using the Kane model in two ways. Using the same argument as before, for the ionised impurity scattering rates, the low temperature carrier density is used to calculate the effective mass $m^*(E_F)$ according to the method described in chapter 2 which is then used for the entire temperature range. For the phonon scattering calculations, the experimental temperature dependence of the carrier density, along with the temperature dependent band gap $E_g$ should be used to calculate $m^*(E_F,T)$. The main effect of non-parabolicity is of course to lower the Fermi energy and increase the effective mass. This shifts the mobility curves downwards, however, the functional dependence of the high temperature phonon scattering rates is also slightly altered.

Interestingly, it is found that when incorporating the effects of band non-parabolicity, good agreement with experiment can only be found using a deformation potential $\Xi = 7.2$ eV in accordance with Dutta, Chattopadhyay and Nag [116,118]. On the other hand, if in the parabolic band approximation the low temperature band edge effective mass is used $m^* = 0.014m_0$ and assumed temperature independent, then it is only possible to achieve a good fit with $\Xi = 30$ eV (obtained by Haga and Kimura [121]) as done by Orr et al. [6]. The theoretical fit using the parabolic approximation is indicated by the open circles in figure 5.3 for comparison.
5.3.3 Gate dependence of carrier density and mobility

The electric field across the QW was modified using the top gate electrode on the Hall bridge over a bias range $10 \text{V} \leq V_g \leq 10 \text{V}$. The carrier density, $n_{2D}$, and mobility, $\mu$, in samples 2509A, 2509B, 2504A and 2504B were modulated over a range of values which are presented in figure 5.4 (obtained at $T = 2 \text{K}$). Due to difficulties in reproducing reliable low leakage gate dielectrics, samples 2504A and 2504B were fabricated with a nominally thicker dielectric layer (for details see table 3.1). This is reflected in the smaller modulation of $n_{2D}$ with gate bias shown in figure 5.4(a).

![Figure 5.4](image)

**Figure 5.4:** (a) Sheet density $n_{2D}$ (closed symbols, left axis) and mobility $\mu$ (open symbols, right axis) for samples 2509A (squares), 2509B (circles), 2504A (upward triangle) and 2504B (downward triangle) as a function of gate bias $V_g$ at $2\text{K}$. (b) The $2\text{K}$ mobility as a function of carrier density for all samples and gate biases showing a linear relationship. The dashed line is a guide for the eye.

---

Data presented in figure 5.4 is determined from FFT analysis of the SdH oscillations, which agreed well with simple Hall effect measurements, indicating that no parallel conduction paths are present at low temperatures.
In fact, the gate electrode for one sample (2526) did not function at all due to excess leakage current. Subsequent discussions and analysis in the proceeding sections focus on the remaining four samples.

For each device as $n_{2D}$ is increased, $\mu$ increases monotonically. This behaviour is presented more clearly in figure 5.4(b) (the dashed line is a guide to the eye). This is typical for modulation doped heterostructures dominated by remote ionised impurity scattering, whereby the increasing Fermi velocity in the 2DEG reduces the effectiveness of the Coulomb scattering from remote ionised impurities and subsequently increases the momentum scattering lifetime [122].

### 5.4 Electron transport in high magnetic fields

The effects of perpendicular magnetic field on the band structure of the semiconductor can be included in the effective mass Hamiltonian (see equation B.1) using the substitution $\hbar k \rightarrow p + eA$ where $p = \hbar \mathbf{v}$ is the momentum operator and $A = (0, Bx, 0)$ is Landau Gauge vector potential giving magnetic field in the $z$-direction [51]. The equation to be solved is then

$$
-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left(\frac{1}{m^*_{cb}(z)}\frac{\partial}{\partial z}\psi_n(z)\right) + \frac{1}{2m^*_{cb,1}}(-i\hbar \mathbf{v} + eA)^2 + V(z)\psi_n(z) = E_n\psi_n(z).
$$

The motion of the particles is analogous to that in a harmonic oscillator potential and the solution takes the form [51],

$$
E(B,N) = \hbar \omega_c \left(N + \frac{1}{2}\right) \quad N = 0, 1, 2, ...
$$

where $\hbar \omega_c = \hbar eB/m^*$ is the cyclotron energy. With increasing magnetic field, the motion in the $x$-$y$ plane is forced into quantised orbits forming a series of discrete
5.4. Electron transport in high magnetic fields

Energy levels known as Landau Levels separated by the energy $\hbar \omega_c$. Each integer $N$ corresponds to a separate Landau level. For cyclotron motion in the $x$-$y$ plane, the allowed states in $k$-space are located on circles of radius $k_x^2 + k_y^2 = \frac{2m^*}{\hbar^2} \omega_c (N + 1/2)$. The radius of the orbits (in metres) is then defined as $l_N = \sqrt{\frac{\hbar(2N+1)}{eB}}$, where the radius of the ground state ($N = 0$) orbit is commonly referred to as the magnetic length, $l_m$ [123].

**Figure 5.5:** Landau fan chart of the first eight energy levels in a 2DEG in the presence of perpendicular magnetic field and Zeeman splitting ($g^* = -35$). Black and red dashed lines indicate the result for parabolic and non-parabolic bands respectively. The $N = 0$ spin split Landau level is labelled. The oscillating Fermi energy for the parabolic and non-parabolic system for $n_2D = 3.5 \times 10^{15} m^{-2}$ and $\Gamma = 0.5 meV$ are indicated by the solid bold black and red lines respectively.
Now let us consider the influence of the Zeeman effect on the electron energy states. When the Zeeman term (equation 4.1) is included in the derivation of the Landau level energies, an additional term appears on the right hand side of equation 5.13 [48];

\[ E_z(B, \sigma) = \pm \frac{g^* \mu_B B}{2}, \quad (5.14) \]

for spin up (+) and down down (-) respectively, where \( g^* \) is the effective Landé g-factor and \( \mu_B \) is the Bohr magnetron. The Zeeman splitting lifts the spin degeneracy of the energy level and introduces a spin splitting \( \Delta E = g^* \mu_B B \) proportional to the total magnetic field applied (see chapter 4).

The position of the spin-split Landau levels as a function of magnetic field is presented figure 5.5 by the black lines. Landau levels fan out from the subband edge \( E_l \). Here, the energy axis has been normalised to \( E_l \) and an arbitrary \( g \)-factor of \( g^* \sim -35 \) was used.

5.4.1 Landau levels in a non-parabolic system

As discussed in chapter 2, the effective mass approximation neglects various properties such as non-parabolicity and spin-orbit coupling. The energy spectrum of electrons in the ground state subband of narrow gap semiconductors with non-parabolic bands is given within the effective two-band model by [124]

\[ E(N, B)[1 + \lambda E(N, B)] = \hbar \omega_c \left( N + \frac{1}{2} \right) \pm \frac{g^* \mu_B B}{2}. \quad (5.15) \]

Solving for the energy (with \( \lambda = 1/\epsilon_g \)) results in
5.4. Electron transport in high magnetic fields

\[ E(N, B) = -\frac{E_g}{2} + \left\{ \frac{E_g^2}{4} + E_g \left[ \hbar \omega_c \left( N + \frac{1}{2} \right) \pm \frac{g^* \mu_B B}{2} \right] \right\}^{1/2} \]  

 Due to the energy dependence of the effective mass, the Landau levels as a function of \( B \) are no longer linear, but are bent downwards as the cyclotron energy gap becomes smaller with increasing energy. This is illustrated by the red dashed lines in the Landau fan chart of figure 5.5. For these calculations, the low temperature parameters for the band gap \( E_g = 0.24 \text{ eV} \) an effective mass \( 0.014 m_0 \) are used [4].

### 5.4.2 Two-dimensional density of states (\( B \neq 0 \))

In a clean system with no impurities, the energy quantisation resulting from perpendicular magnetic field transforms the DoS function into a series of \( \delta \)-functions located at the energies of each Landau level. In a real system, the presence of scattering potentials from impurities and material inhomogeneities broadens these delta functions into energy bands [123] which in most qualitative analysis are assumed to be of Gaussian form [125,126].

Since the energy separation between adjacent Landau levels \( \hbar \omega_c \) is proportional to the magnetic field applied \emph{perpendicular to the 2DEG}, when a finite level broadening exists, only at sufficiently large fields do the Landau levels become completely resolved. This is illustrated in figure 5.6 by the black and red lines which show the DoS at a magnetic field of 0.5 T and 2 T, respectively - initially with no Zeeman splitting (details of the calculation are given in appendix A). The effect of Zeeman splitting is illustrated by the green and blue lines in figure 5.6 showing the DoS at 2 T using \( g \)-factors of \( g^* = -25 \) and \( g^* = -50 \), respectively. Similarly, one can see that only at sufficiently large magnetic fields does the Zeeman splitting become resolved (this field depends on the broadening and the \( g \)-factor). Each Landau level has a degeneracy \( D = eB/h \) (allowed states per unit area).
5.4. Electron transport in high magnetic fields

Figure 5.6: Two-dimensional density of states (multiplied by the Fermi distribution function at $T=2$ K) in magnetic fields 0.5 T (black line) and 2 T (red line) calculated from equation A.2. Sharp highly degenerate peaks are formed. The increasing resolution of Zeeman splitting with $g$-factor (at $B=2$ T) is demonstrated as $|g^*|$ increases from 0 (red line) to 50 (blue curve). An arbitrary broadening of $\Gamma=1.5$ meV is chosen. $E_1$ is the subband edge and $E_F$ is the Fermi level.

Assuming a constant carrier density, in non-zero field a finite number of Landau levels will be occupied beneath the Fermi level dependent on the magnetic field. This dimensionless quantity is the filling factor of the system and is given by [50,123]

$$\nu = 2\pi n_{2D} J_m^2.$$  \hspace{1cm} (5.17)

The Fermi level is considered pinned to localised states in the highest occupied Landau level. As the magnetic field is increased, the degeneracy of each occupied
Landau level beneath the Fermi energy increases. The Fermi energy moves with the highest occupied Landau level until a critical field is reached (dependent on the carrier density in the system) when the highest Landau level becomes depopulated and the Fermi energy drops abruptly to the adjacent lower lying Landau level. The Fermi level is therefore oscillates as it switches from the \(N^{th}\) to the \((N-1)^{th}\) Landau level. This is illustrated by the solid black line in the Landau fan chart shown in figure 5.5 (corresponding to a carrier density of \(n_{2D} = 3.5 \times 10^{15}\) m\(^{-2}\)). The oscillation of the Fermi level can be interpreted as the adjustment required to maintain a constant carrier density, \(n_{2D}\).

The corresponding Fermi energy for the non-parabolic system is shown in figure 5.5 by solid red line for the same carrier density. By comparison to the parabolic result (solid black line) two features are observed; (i) due to the increased effective mass in the non-parabolic system, the Fermi energy is reduced and (ii) the separation/resolution of the Landau levels is also reduced in the non-parabolic system because the increased mass reduces the Landau level separation \(\hbar \omega_c\).

5.4.3 Shubnikov-de Haas oscillations and the quantum Hall effect

As the magnetic field is increased, Landau levels are swept through the Fermi energy resulting in a periodic oscillation of the DoS at the Fermi energy. This manifests itself in the macroscopic oscillations in the magnetoconductance \(\sigma_{xx}\) and magneto-resistance \(\rho_{xx}\) of a semiconductor known as Shubnikov-de Haas oscillations [111,127]. These are analysed in detail in section 5.6 and are introduced here for completeness.

Figure 5.7 shows a typical example of the Shubnikov-de Haas (SdH) oscillations observed in \(\rho_{xx}\) from an \(\text{In}_{0.85}\text{Al}_{0.15}\text{Sb/InSb/ In}_{0.9}\text{Al}_{0.1}\text{Sb}\) 30nm QW structure (sample 2504A) at \(T = 2\) K. The longitudinal resistivity \(\rho_{xx}\) and conductivity \(\sigma_{xx}\) both go through a maximum when the Fermi energy lies in the
5.4. Electron transport in high magnetic fields

Figure 5.7: Temperature dependence of the experimental longitudinal $\rho_{xx}$ (left axis) and Hall $\rho_{xy}$ (right axis) resistivity in units of $h/e^2$ as a function of perpendicular magnetic field $B$ for InSb QW sample 2504A. Data demonstrates the dampening effect of temperature and the integer quantum Hall effect.

centre of a Landau Level where the extended (mobile) states are available to scatter into. This counter-intuitive phenomenon is possible because $\sigma_{xx}$ and $\rho_{xx}$ become proportional to each one another at high magnetic fields (see appendix A).

As seen in figure 5.7, at sufficiently high magnetic fields the longitudinal resistivity $\rho_{xx}$ is vanishingly small and the transverse (Hall) resistivity $\rho_{xy} = -R_{\Omega}$ shows plateaus over finite ranges of $B$ where the Fermi energy lies between two Landau Levels [125]. This quantisation of the Hall effect was first observed by von Klitzing et al. [128] in a Si-MOSFET inversion layer in 1980. This effect,
and similarly the SdH effect, is observable only at high fields and low temperatures.

\[ N(E) \]

![Figure 5.8: Illustration of impurity broadening and mobility gaps in Landau levels](image)

The Hall resistivity \( \rho_{xy} \) at the plateaus is quantised into values \( \rho_{xy} = \frac{h}{e^2 i} \), with \( i = 1, 2, \ldots \) and is therefore referred to as the Integer Quantum Hall Effect (IQHE) (at extremely high fields, there exists a Fractional Quantum Hall Effect where plateaus occur for fractional values \( i \) [123]). For the \( i = 1 \) plateau this is about 25.8 KΩ. Interestingly, within a quantum Hall plateau, nearly all momentum relaxation processes are suppressed, resulting in a high quality ballistic conductor with extraordinarily long mean free paths. This is because electron states carrying current in opposing directions are localised at opposite sides of the 2DEG channel, significantly reducing the effects of back scattering regardless of the sample purity [50].

It was shown by Laughlin [129] that plateaus in \( \rho_{xy} \) should appear at these given values due to the presence of a mobility gap, regardless of the details of the material system, geometry or impurities. From his approach, and that of Aoki and Ando [130], it was shown that as long as the Fermi level lies within the energy band of localised states, \( \rho_{xy} \) is constant. For a more detailed discussion on the QHE the reader is pointed towards reference [123].
A feature of SdH oscillations in $\rho_{xx}$ is that they are periodic in $1/B$. In an ideal spin degenerate system i.e. no Zeeman splitting, a Fourier transform (FT) of the oscillations taken with respect to $1/B$ will result in a single peak corresponding to the fundamental frequency $f_{SdH}$ of the oscillations (and peaks of diminishing amplitude at the harmonic frequencies thereafter). In most systems Zeeman splitting is present and at some field the spin splitting is resolved in the SdH oscillations. A FT of data including these spin split oscillations results in an additional peak appearing at twice the fundamental frequency. For 2D systems, a simple relationship holds for determining the 2D carrier density $n_{2D}$ from the frequency $f_{SdH}$ (Tesla) of the SdH oscillations (after Onsager), given by [112],

$$n_{2D} = \frac{2e}{h} f_{SdH}.$$  

(5.18)

(Note that the factor of 2 must be removed when using the single spin frequency).

5.5 Anomalous magneto-oscillations

Zero field spin splitting results in unequal carrier populations $n_{\pm}$ for each spin subband. The total carrier density in the system $n_{2D}$ is the sum of both populations, such that $n_{2D} = n_{+} + n_{-}$. It can be assumed that for $B > 0$, the Landau levels can be partitioned into two independent sets, each giving rise to a separate series of SdH oscillations with frequencies given by $f_{SdH} = n_{\pm} h / e$. Since the spin splitting is small compared to the Fermi energy, the difference in frequencies $f_1$ and $f_2$ is small and a beating pattern in $\rho_{xx}$ will result (see for example figure 1.2). The FT of such a pattern will be a narrowly split peak corresponding to $f_1$ and $f_2$.

Beating patterns may also arise from alternative mechanisms which are entirely unrelated to zero field spin splitting. To establish a beating pattern requires the presence of two sets of oscillations with similar frequencies and amplitudes. This implies that the carrier densities and effective masses associated
with the two sets of carriers must be similar. This situation may be achieved in samples with a spatially inhomogeneous carrier density. For example, Brosig et al. [101] studied the density dependence of SdH oscillations in InAs/AlSb QWs using the persistent photoconductivity effect - beating patterns were only observed in large devices (1 mm) immediately after illumination (the effect was not observed in smaller devices of 200 μm), from which it was concluded that inhomogeneous carrier density was the origin of beat patterns.

In low density samples, the requirement that the two species of carriers having similar densities generally discounts the origin of beating patterns being the occupation of a second confined subband since this will be relatively unpopulated compared to the ground state. However, it has been demonstrated that the occupation of the second subband i.e. \( E_f > E_2 \) can induce a second set of oscillations in \( \rho_{xx} \) (also periodic in \( 1/B \)) due to elastic scattering between the two subbands, known as the magneto-intersubband scattering (MIS) effect [131]. The amplitude of the MIS oscillations are relatively temperature insensitive compared to that of SdH oscillations which allows the two components to be distinguished from one another. In an important paper by Rowe et al. [40] it was demonstrated that MIS was responsible for beat patterns observed in high density InAs/GaSb QWs where large zero field spin splitting is expected. It was also shown that the MIS component is persists even for \( E_f < E_2 \) (i.e. some thermally excited carriers exist) highlighting the wide range of carrier densities over which beating effects can be misinterpreted as a signature of zero field spin splitting.

### 5.5.1 Methods of analysis

Assuming that the two SdH series originated from a spin-splitting of the ground state subband rather than alternative mechanisms, Lou et al. [36] proposed a simple model for estimating the magnitude of the spin splitting from the experimentally determined difference in carrier densities \( \Delta n = |n_+ - n_-| \) given by \( \Delta E_{so} = 2\Delta n / N(E) \), where \( N(E) \) is the DoS (in zero field). This approach was
developed by Engels et al. [39] who derived a spin-dependent correction to the
doS \textit{in zero magnetic field} from the Rashba dispersion model (equation 4.12). Accordingly, the Rashba spin-orbit coupling parameter $\alpha$ is then given by the expression [39];

$$\alpha = \frac{\Delta n \hbar^2}{m^*} \sqrt{\frac{\pi}{2(n_{2D} - \Delta n)}}$$

(5.19)

involving only three variables, $\Delta n$, $n_{2D}$ and $m^*$ which are readily extracted from experiment. This model is particularly useful when the SdH data exhibit beating over a small range of fields and where only one or two beat 'nodes' are distinguishable. The model does however have a number of shortfalls, principally that it is derived from the Rashba model for the energy dispersion in \textit{zero field}, whilst data over which the FFT is performed and $\Delta n$ is extracted from is in non-zero fields (i.e. Zeeman term is neglected). Consequently, it neglects the field dependence of the Rashba splitting and the presence of Zeeman effect. Ignoring the Zeeman splitting is not a bad approximation for wider gap materials but is flawed for systems with large $g^*$ and leads to overestimations of $\alpha$. Nevertheless, the FFT method provides a straightforward method of analysing the strength of the Rashba parameter and has been applied to numerous results in narrow gap systems InAs and InGaAs [132-134]. Note that although equation 5.19 is derived from the parabolic dispersion, it can be shown that incorporating the effects of band non-parabolicity using the effective two band model yields the same result. This topic will be revisited in section 5.6.

Alternatively, when more than three beat nodes are observed, a more accurate analysis of the spin splitting can be made following the approach of Das et al. [35] who analysed the modulation of the SdH amplitude. By approximating the amplitude with $A \sim \cos \left( \frac{\delta \pi}{h \omega_c} \right)$ where $\delta$ is the spin splitting of the Landau levels including Zeeman splitting, node points will occur when $\delta / h \omega_c$ is equal to
5.5 Anomalous magneto-oscillations

Half integer values [38]. Plotting the node positions against 1/B therefore provides information on the size of the zero field spin splitting and $g^*$ from which $\alpha$ can be estimated. Importantly, from this analysis it can be shown that no beating effects should be expected in the absence of zero field spin splitting [35,38] (but the beating can be modulated by the size of the Zeeman term).

5.6 Investigation of spin-dependent phenomena in InSb quantum wells

Figure 5.9 shows a typical low temperature recording of the longitudinal resistivity $\rho_{xx}$ for samples 2509B (red line) and 2504B (blue line) for $V_g = 0$. Clear single-period oscillations are observed indicative of single subband occupation. SdH oscillations are resolved at filling factors up to $v = 46$ in the higher mobility sample (2504B) indicated by the solid arrows. The emergence of Zeeman splitting can be resolved at odd filling factors as high as $v = 15$ indicated by the dashed arrows, demonstrating the presence of a large $g$-factor. Data from these samples can be compared to that of Khodaparest et al. from a 20nm InSb QW with similar carrier density where Zeeman splitting was resolved at $v = 5$ [44].

A clear example of the integer quantum Hall effect observed in these samples along with the effect of temperature on $\rho_{xx}$ and $\rho_{xy}$ is given in figure 5.7. It can be seen that both the SdH oscillations and quantum Hall plateaus are strongly dampened with increasing temperature. Reducing the temperature below 5 K gave no significant improvement in the resolution of the low field SdH oscillations (not shown). This is consistent with measurements made on similar InSb samples down to lower temperatures ($T = 300$ mK) [135], and indicates that the SdH oscillations are limited by inhomogeneous level broadening rather than thermal broadening. This is discussed further in the following section.
Figure 5.9: Low field region of $\rho_{xx}(B)$ for samples 2509B (upper trace) and 2504B (lower trace) indicating the onset of SdH oscillations (solid arrows) and the emergence of Zeeman splitting (dotted arrows) at odd filling factors as high as $v = 15$. Clear single period oscillations are observed.

From examination of figure 5.7 and figure 5.9 it can be seen that there is a distinct non-oscillatory background magnetoresistance present in these samples which is temperature dependent. At low fields $\rho_{xx}$ contains at first negative and then a positive magneto-resistance, which becomes approximately linear at high fields. The magnetoresistance in the low field region in figure 5.9 is consistent with the effects of electron-electron interactions in the presence of Zeeman splitting as described by Lee and Ramakrishnan [136], although this mechanism will not be examined further in this thesis. The high field quasi-linear magnetoresistance has previously been observed in InSb epilayers and was attributed to the intrinsic magneto-resistance originating from sample inhomogenieties [66,137].
The magnitude of the effective $g$-factor $g^*$ which is expected to be large in InSb can not be commented on simply from the field at which the splitting is resolved since this field ($B_z$) is itself determined by both $g^*$ and $\Gamma$. This is highlighted by results in the literature from the extensively studied GaAs/AlGaAs QW systems where Zeeman splitting has been resolved at filling factors ranging from $\nu = 23$ (at $B_z \sim 0.16$ T) [138] to $\nu = 3$ (at $B_z \sim 10$ T) [125] with extracted values of $g^*$ corresponding to $g^* = 7.6$ and $g^* = 2.6$ respectively (these values are somewhat greater than the bare $g$-factor $g_0 = 0.52$ due to effects of exchange enhancement [139]). These measurements were performed using elegant tilted field techniques, first performed by Fang and Stiles [140] (see for example [139]). Tilted field measurements could not be performed using the current sample probe in the CFM system (chapter 3), and so no further analysis of the $g$-factor will be made.

5.6.1 Estimation of Landau level broadening

The extent of the low field SdH oscillations (of interest) is strongly influenced by the broadening of the Landau levels, $\Gamma$. This is indicted by the position of the solid arrows in figure 5.9 and is observed to vary between samples. Here a quantitative analysis of the broadening in these samples is given which reveals a large variation and dependence on carrier density. We shall see that the level broadening is large in these high mobility InSb QW samples compared to other material systems. This will be discussed further in the context of spin splitting in section 5.6.3.

Landau levels are resolved in the DoS when the energy separation of adjacent levels exceeds the level broadening. Therefore, under the assumption that the level broadening has negligible contribution from thermal excitation, a simple estimate for $\Gamma$ can made from the critical field at which SdH oscillations become resolved in $\rho_{xy}$, denoted here by $B_{\text{SdH}}$. Thus we have
This simple approach has the advantage that it makes no assumptions of the scattering potential. However in practice, it is limited by the ability to accurately determine $B_{SdH}$ from experimental data e.g. poor signal-to-noise ratio in the data limits the resolution of $B_{SdH}$ and leads to an overestimation of $\Gamma$. This technique therefore provides an upper limit for $\Gamma$ as indicated by the error bars in figure 5.10.

In order determine the broadening from $B_{SdH}$ the effective mass must be known. This is calculated according to the method outlined in chapter 2 which takes into account the effects of the band non-parabolicity in InSb. Careful examination of both the first and second derivatives of $\rho_{xx}(B)$ versus $1/B$ is required in order to determine $B_{SdH}$.

**Figure 5.10:** Landau Level broadening parameter $\Gamma$ for each sample at different gate biases as a function of carrier density as determined from the critical SdH field $B_{SdH}$. Closed symbols represent data obtained at zero gate bias. The dashed line is a guide for the eye.
The results of this analysis for each sample at each gate bias measured are plotted against carrier density in figure 5.10.

A relationship between $T$ and $n_{2D}$ is found such that data from different samples appear to fall close to a single line. The magnitude of $T$ in these samples which ranges from 1.5-3 meV. This is surprisingly large compared to typical values reported in the GaAs/AlGaAs and InAs/GaSb systems of $\Gamma \sim 0.05-0.7$ meV [138,139] and $\Gamma \sim 0.4-1.5$ meV [37,101], respectively. The effect of large broadening on the extraction of the spin splitting is discussed later in the section. It is somewhat counterintuitive that $T$ is large and yet the carrier mobility $\mu$ is high, suggesting that the scattering processes which influence the level broadening do not adversely affect the mobility. This observation is perhaps not surprising however, since the broadening of the Landau levels is related to the single-particle relaxation rate which does not affect the momentum scattering [141]. The broadening is related to the single particle relaxation rate by

$$\Gamma \propto \frac{\hbar}{\tau^{\eta}}$$  \hspace{1cm} (5.21)

where generally $\eta = 1$ or $\eta = \frac{1}{2}$ dependent on the nature of the scattering [141]. In remote doped structures, the single-particle relaxation time $\tau$ is typically an order of magnitude smaller than the momentum scattering time, whereas the two are approximately equal in uniformly doped structures [142].

The nature of the level broadening depends strongly on the range of the scattering potentials involved [141]. Given that at low temperatures, transport in these samples is dominated by remote ionised impurity scattering [6], it is reasonable to suggest that the large broadening in these sample could arise from the long-range nature of the scattering potential. In this regime, $\Gamma$ is susceptible to, and determined by inhomogeneities in the local potential felt by the carriers [141]. Such inhomogeneities may result from spatial variations in well width and/or interface roughness and perhaps reflects the difficulty in the growth of
high quality InSb heterostructures on highly mismatched GaAs substrates. However, it is interesting to note data taken from a similar InSb QW sample grown from a different MBE source [44] appears to show similar levels of broadening to those found here. It is also worth pointing out that this conjecture is clearly not universal for remote doped heterostructures; Akabori et al. [113] reported a narrow broadening of $\Gamma \sim 0.6$ meV in a structurally similar InGaSb/AlInSb sample with a large 50nm spacer layer. In the case of [113] the mobility was relatively small compared to those studied here ($\mu = 9.8$ m$^2$V$^{-1}$s$^{-1}$) and it is likely that (short range) alloy scattering in the InGaSb 2DEG influenced the transport.

5.6.2 Observation of beating patterns

Measurements from all samples at each gate bias show no obvious signs of beating in the low field $\rho_{cx}$ data, as has been the case in previous reports of magnetotransport in InSb QWs [44]. However, careful inspection of the first and second derivative of the $\rho_{cx}$ data with respect to B reveals a weak modulation in the SdH oscillation amplitude, away from the onset of resolved Zeeman splitting. This is demonstrated in figure 5.11(a) and (c) which shows raw data from sample 2504A (upper left panel) compared to the second derivative of the same data which exhibits a weak beating pattern (lower left panel). This weak beating is exhibited for all gate biases in samples 2504A and 2504B but only in the $V_s = 10$ V data from sample 2509A. Beating is not observed in samples 2509B or 2526, which can be attributed to the magnitude of the level broadening and is discussed in a later section.

The corresponding Fourier spectra of the data in figures 5.11(a) and (c) are shown in figures 5.11(b) and (d), respectively. A clear double peaked structure is observed consistent with the effects of zero field spin splitting (c.f section 5.5). The resolution of this structure is enhanced when performing the FFT on higher order derivatives.
Figure 5.11: (a) (Upper left panel) Low field region of $\rho_{xx}$ plotted against inverse field $1/B$ for sample 2504A at $V_g = 0$ V and $T = 2$ K. (b) (Upper right) FT of the data in (a). (c) (lower left panel) Second derivative of the same data from (a) showing a clear beating pattern – node indicated by the arrow. (d) (lower right) FT of the data in (c).

Note that in order to resolve the structure from $\rho_{xx}$ data, a $1/B$ field window must be chosen that excludes Zeeman split oscillations. Resolving the structure from the $d^2\rho_{xx}/dB^2$ data is less susceptible to the inclusion of Zeeman split oscillations as demonstrated in the data of figure 5.11(d) which exhibits the double peak structure even in the presence of a significant amplitude at the Zeeman split (double) frequency at $\sim 14$ T. The carrier densities associated with each peak,
labelled $n_1$ and $n_2$, are extracted according to $n_{1,2} = f_{1,2} e / h$ [see figure 5.11(b)]. Here $f_{1,2}$ is the FFT frequency (in Tesla) of the two peaks (at this point the assignment of spin cannot be made). An asymmetry in the peak amplitudes is observed in all cases and is discussed in a later section. The sum of the two densities $n_1$ and $n_2$ agrees well with the carrier density $n_{2D}$ obtained from the low field Hall effect, providing strong evidence that the two SdH series originate from a spin-split subband rather than the occupation of a second subband. The relatively poor resolution of the FFT spectra (due to the small number of oscillations in these low density samples) introduces uncertainties in the peak positions $f_{1,2}$ corresponding to an error in the densities of $\delta n_{1,2} \sim \pm 3 \times 10^{13} \text{ m}^{-2}$. These errors are taken into account in the determination of $\Delta n$.

Following the discussion in section 5.5, it is important to rule out erroneous identifications of zero-field spin splitting simply from the observation of beating, which can also arise from inhomogeneous carrier density and the MIS effect. All measurements presented here were performed in the dark, and since the length scale of the device is small < 200 μm, following [101] it can be assumed that the beat patterns do not originate from regions of spatially inhomogeneous carrier densities. Beating patterns may also arise from the mixing of the SdH series from the ground state subband and a MIS oscillation. MIS scattering only occurs when the second subband becomes occupied. In the samples studied, no evidence for second subband occupation is found in the FFT spectra or in the gate dependence of the carrier mobility; this is supported by self-consistent band profile calculations. In order to quantify this further the temperature dependence of the FFT amplitude is analysed. Figure 5.12(a) shows the FFTs of the low field $\rho_{xx}$ data of sample 2504B at $T = 2$, 5 and 10 K. The field window over which the FFT was taken remained fixed for each temperature.
The SdH series is distinguished from the MIS series by a rapidly decaying amplitude with temperature according to [143]

\[ A(T) \approx \frac{X}{\sinh(X)}, \]  

(5.22)

where \( X = 2\pi^2 k_b T / \hbar \omega_s \). The inset to figure 5.12(a) shows the temperature dependence of the Fourier amplitude for both the \( n_1 \) peak (open squares) and \( n_2 \) peak (red triangles) normalised by their value at 2 K. It can be seen that both peaks exhibit approximately the same temperature dependence that is well fit by the thermal damping term in equation 5.22 indicated by the dashed line (using \( m^* = 0.022 m_0 \)). The two peaks therefore correspond to two narrowly split SdH series and in the following analysis are attributed to the zero field spin splitting phenomenon.

Calculations of the spin splitting parameters presented in chapter 4 showed that the \( k \)-linear (\( \beta \)) and \( k \)-cubic (\( \gamma \)) Dresselhaus coupling parameters in these wide well structures are large (\( \beta \approx 3 \times 10^{12} \text{eVm} \) and \( \gamma \approx 430 \text{eVÅ}^3 \) at \( 3 \times 10^{15} \text{m}^{-2} \)) and contribute significantly to the spin splitting at low carrier densities. Their significance decreases rapidly with increasing carrier density due to the enhancement of the Rashba effect (see for example figure 4.7) [68]. At the higher carrier densities where beating is observed in these samples, the spin splitting associated with the Rashba effect is 200-300% larger than that from the BIA terms. From this it can be assumed that the Rashba term is the dominant mechanism contributing to the spin splitting.

With only one (or two) beat nodes distinguishable in the data the Rashba parameter can not be determined using the method of Das et al. [35]. Instead, the Rashba parameter is extracted from the difference in the spin populations \( \Delta n \) (inferred from the FFT spectra) using the method of Engels et al. [39] (equation 5.19).
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Figure 5.12: (a) (Upper panel) Fourier transforms of the low field $\rho_{xx}$ of sample 2504B for various temperatures. Inset shows the normalised FT amplitudes of the $n_1$ (left peak) and $n_2$ (right peak) versus temperature – dashed line indicates the decay according to equation 5.22. (b) (lower panel) Values for the Rashba parameter $\alpha$ (obtained using equation 5.19) versus carrier density $n_{2D}$ for samples 2509A, 2504A and 2504B. The dashed line shows the calculated values of $\alpha$ following chapter 4.
The results of this analysis for all data sets where splitting in the FFT spectra was distinguishable are presented in figure 5.12(b) as a function of carrier density.

Figure 5.12(b) shows that the Rashba parameter extracted from samples 2404A and 2504B increases monotonically with carrier density. This is in contrast to the results of Nitta et al. [93] Engels et al [39], Schapers et al. [133] and Hu et al. [134] obtained in the InGaAs system which report the value of $\alpha$ to decrease with carrier density. This is expected due to the reversed asymmetry in their samples - data in the above references was also obtained from top (front) gated structures with the doping layer positioned below the QW. Consequently the electric field across the QW is reversed relative to that in the samples studied here. (Both of these dependences are fully accounted for by theoretical treatments that take into account finite barriers such as that presented in chapter 4 [45,68]).

A second feature of figure 5.12(b) is that data from all three samples appear to lie on a common line. This result is consistent with the calculations made in chapter 4 showing that when varying the electrostatic potential in heterostructures via the doping density and spacer thickness (or indeed gate bias), data for the same QW width (and barrier compositions) fall onto a common curve (see figure 4.2).

**Comparison to theory and previous experiments**

Since the Rashba parameter depends strongly on the carrier density, a comparison with samples of similar density is most meaningful. Due to the reduced density of states in the InSb system and the requirement of single subband occupation in these wide QWs, the carrier density in these samples is significantly lower than most previous studies of spin splitting from beating effects in InAs and InGaAs QWs. A direct comparison is limited to just a few cases. The values of $\alpha$ in figure 5.12(b) agree well with the results of Khodaparest et al. [44] obtained from a similar 30 nm InSb QW ($\alpha \sim 1.3 \times 10^{-11}$ eVm). Furthermore, both these values are larger than those extracted from wider gap materials at comparable densities. For
example, Guzenko et al. studied beating effects in a low doped InGaAs/InP QW [144] and Holmes et al. in an InGaAs/InAlAs QW [145] finding $\alpha \sim 6.5 \times 10^{-12}$ eVm ($n_{2D} \sim 3 \times 10^{15}$ m$^{-2}$) and $\alpha \sim 9 \times 10^{-12}$ eVm ($n_{2D} \sim 2 \times 10^{15}$ m$^{-2}$), respectively. These results are consistent with the trend in the literature and the expectation that the Rashba parameter scales inversely with band gap after de Andrada e Silva [79].

The dashed line in figure 5.12(b) shows the calculated dependence of $\alpha$ on carrier density in the 30 nm InSb QWs using the method described in chapter 4. It can be seen that the experimental values of $\alpha$ exceed the theoretical calculation by a factor of $\approx 2$ [68]. The dependence of $\alpha$ on $n_{2D}$ is also stronger than calculations predict (which is attractive for spintronic applications [16]). It is likely that the discrepancy in magnitude is related the method of analysis. However, the neglect of the confinement energy (see chapter 2) in the calculation of $m^*$ will lead to a small over estimation of $\alpha$ of the order 10-20%. This would lower the range of $\alpha$ from $1.3-1.5 \times 10^{-11}$ eVm to approximately $1-1.2 \times 10^{-11}$ eVm.

As discussed in section 5.5, despite its extensive use in the literature the Engels expression used to determine $\alpha$ (equation 5.19) has the number of shortcomings, namely the neglect of Zeeman splitting and the field dependence of the Rashba splitting [38]. Consequently this method should be considered an overestimate (particularly in narrow gap systems where $g^*$ is large). Furthermore, $\Delta n$ which reflects the polarisation of the system oscillates with field. Ideally, one requires data of small amplitude oscillations that exhibit a number of beat nodes persisting to very low fields (minimising the Zeeman contribution) over which the analysis can be performed. This condition requires high density and extremely high purity samples. The large $g$-factor in InSb along with a large broadening makes the observation and analysis of beating patterns particularly challenging due to the small number of oscillations which may be analysed (discussed in detail in the following section). The Fourier analysis performed here was applied to data which did not show evidence of Zeeman splitting – this meant that the $1/B$
field window began just before the beat node at \( \approx 1.5 \, \text{T}^{-1} \) [c.f. figure 5.11(c)] and contained a small number of oscillations.

In addition, many body effects such as the exchange interaction enhance the spin splitting [146] and are not included in the models (both the zero field calculations and the Engels model). This may be significant following a recent report of large exchange enhancement of the g-factor in similar InSb QW structures [147].

5.6.3 Influence of Landau level broadening on beating patterns

It is speculated that the absence of beating in samples 2526, 2509B and 2509A for \( V_g < 10 \, \text{V} \) can be attributed to the combination of *large broadening* \( \Gamma \) *and a large Zeeman splitting* which limits the field range \( B_{\text{SDH}} < B < B_z \) over which the effects of SO splitting are observable. For \( B > B_z \) spin splitting in the 2DEG is dominated by the Zeeman effect [87]. The number of oscillations below \( B_z \) depends on both \( \Gamma \) and the carrier density \( n_{2D} \) and so it follows that only in samples with the greatest number of oscillations are the effects of beating detectable. It will be shown that this conjecture can be quantitatively supported by simulations of the SdH oscillations in the presence of Rashba SO splitting using the method described in appendix A.

Initially the broadening is taken to be spin independent by setting \( \Gamma_+ = \Gamma_- = \Gamma \) in equations A1 and A2. The magnetoresistance is simulated with narrow and large broadening parameters at a fixed carrier density \( n_{2D} = 3.3 \times 10^{15} \, \text{m}^{-2} \) and spin splitting \( (\alpha = 1.3 \times 10^{-11} \, \text{eVm} \) and \( g^* = -30 \)). The simulation using \( \Gamma = 1.6 \, \text{meV} \) is shown in the lower trace in figure 5.13 which exhibits a pronounced beating pattern. In contrast, we see that the simulation of data with \( \Gamma = 2.5 \, \text{meV} \) shown by the upper trace in figure 5.13 shows no discernible beating pattern. The disappearance of beating with larger broadening in these simulations is consistent with the observations made in our samples and
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**Figure 5.13:** Numerical simulations of the $\rho_{xx}$ for fixed carrier density and spin splitting with input parameters $\Gamma_+ = \Gamma_-= 1.6$ meV (lower trace) and $\Gamma_+ = \Gamma_-= 2.5$ meV (upper trace). The disappearance of beating patterns at larger broadening is demonstrated.

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provides at least a semi-quantitative basis for interpreting the absence of beating in the majority of our samples.\textsuperscript{8} In addition to the influence of broadening, due to competing spin splitting mechanisms which dominate in different regimes [68], the Dresselhaus splitting may not be negligible at lower carrier densities (where the broadening is large) and will also influence the observed beating patterns. It is worth commenting that Brosig et al. reported the absence of beating in high quality InAs/AlSb and InAs/AlGaSb QWs over a range of carrier densities [101]. In their samples however, SdH oscillations were resolved at fields as low as $B \sim 0.15$ T with a narrow broadening of $\Gamma \sim 0.4$ meV and so the absence of beating in their samples can not be attributed to the same broadening mechanism.

\textsuperscript{8} Although it is expected that the Rashba parameter will be reduced for lower carrier densities, which would in turn reduce the appearance of beating further.
Interestingly, the numerical simulation of a narrow broadened sample (lower trace figure 5.11) using the experimental value for the Rashba parameter does not reproduce the features in the experimental data. Good agreement has been found previously in data from InGaAs QWs [93]. The beating pattern in the simulation has a zero amplitude beat node and is far stronger than that observed experimentally indicating that the experimental value of $\alpha$ used is larger than that in our samples [better agreement is found for smaller $\alpha$ as shown in figure 5.14(a)]. The discrepancy between the simulated and experimental data and the origin of the non-zero amplitude beat node in the samples is discussed below.

5.6.4 Spin-dependent scattering rates

The observation of a non-zero beat node amplitude in these InSb QW samples indicates that the SdH series originating from the spin-split subband oscillate (at the Fermi energy) with different amplitudes. This conjecture is strongly supported by the unequal amplitudes of the spin split peaks in the FFT spectra (see figure 5.12).

The observation of non-zero beat node amplitude has previously been made by Lou et al. [37] in a 10nm InAs QW. This data was qualitatively interpreted by introducing the concept of a spin-dependent scattering process which suppresses the oscillation amplitude of one spin more than the other (although the nature of the mechanism was not discussed). This interpretation is based on the understanding that at low temperatures, the SdH amplitude in the low field region is predominantly determined by the single-particle relaxation time $\tau$ [143]. In this interpretation there is a different scattering time $\tau_s$ associated with each spin. By varying the component of the magnetic field perpendicular to the sample in a tilted field configuration (to vary the Zeeman splitting), Lou et al. [37] demonstrated that the disparity between the two scattering times was proportional to the total spin splitting in the system.
Figure 5.14: (a) Simulations of $\rho_{xx}$ with $\alpha = 9 \times 10^{12} \text{eV/m}$, $n_{2D} = 3.3 \times 10^{13} \text{m}^{-2}$ and $\Gamma_+ = \Gamma_- = 1.6 \text{meV}$ (upper trace) compared to the results when using a spin dependent broadening $\Gamma_+ = 1.6 \text{meV}$ and $\Gamma_- = 1.4 \text{meV}$. (b) Corresponding FFT spectra of the numerical simulations shown in (a) showing an asymmetry in the peak amplitudes with spin dependent broadening (solid line) compared to a symmetric structure with equal broadening for both spins (dashed line). (c) FFT spectrum from a simulation when the spin dependent broadening parameters are switched demonstrating the opposite asymmetry in peak amplitude.

(from the SO interaction or external field). Thus the appearance of such features in our samples is consistent with the presence of a large spin splitting. Experimentally, $\tau$ is commonly extracted from the field dependence of the oscillation amplitude $\Delta \rho_{xx} \propto \exp\left(-\pi \omega \tau / \rho s\right)$ [142,148], however, this is difficult when the two sets of oscillations are superimposed in the low field region.

To quantitatively explore the concept of spin-dependent scattering rates, it is recalled that the broadening of the Landau levels is related to the single-particle relaxation rate according to equation 5.21. Therefore, the effects of a
5.6. Investigation of spin-dependent phenomena in InSb...

spin-dependent scattering rate on the SdH oscillations can be incorporated into the numerical simulations by introducing a *spin-dependent level broadening* i.e. by setting $\Gamma_+ \neq \Gamma_-$. The effect of this on the SdH oscillations is demonstrated in figure 5.14(a) for the case where $\Gamma_+ > \Gamma_-$. with $\Gamma_+ = 1.6$ meV and $\Gamma_- = 1.4$ meV (lower trace) compared to the case of identical broadenings $\Gamma_+ = \Gamma_- = 1.6$ meV (upper trace). In these simulations a smaller Rashba parameter of $\alpha = 9 \times 10^{-12}$ eV m has been used which gives better agreement with the features of the experimental data. Note that this is approximately 2/3 smaller than that extracted experimentally indicating that the FFT method overestimates the magnitude of $\alpha$ (this value of $\alpha$ is within 30% of the theoretical value). These results clearly demonstrate that a spin-dependent broadening can indeed produce a non-zero beat node amplitude.

The corresponding FFT spectra of the simulations with $\Gamma_+ > \Gamma_-$ and $\Gamma_+ = \Gamma_-$. are shown in figure 5.14(b) by the solid and dotted lines respectively. It can be seen that a spin dependent broadening $\Gamma_+ > \Gamma_-$. introduces an asymmetry in the spin-split FFT peak consistent with that observed experimentally giving confidence on this interpretation.

This provides compelling insight to the nature of the spin-dependent scattering in these samples. Based on these simulations we can determine that the majority (low-energy) spin state is the spin up state which undergoes greater scattering events than the minority (high-energy) spin down state i.e. $\tau_+^{-1} > \tau_-^{-1}$. The uniqueness of this interpretation is demonstrated by reversing the asymmetry of the input broadening parameters i.e. $\Gamma_- > \Gamma_+$. The resulting FFT spectrum from this simulation (with $\Gamma_+ = 1.4$ meV and $\Gamma_- = 1.6$ meV) is shown in figure 5.14(c), which clearly exhibits the opposite peak asymmetry. The assignment of the relative spin energies is expected for a system with a negative $g$-factor. However, it is interesting to note that Lou et al. reported the opposite in the InAs QW using a more indirect method [37].

From this analysis it can not be determined whether the spin-dependent scattering rates originate from a spin-dependent scattering mechanism or simply
from the differing densities associated with each spin population which could be related to self-screening or even many body effects. No magnetic materials are intentionally incorporated during the growth of these heterostructure (magnetic impurities may preferentially scatter one spin orientation more than another). Although the conclusions drawn here and those of Lou et al. [37] differ, their samples are also structurally and electrically very different compared to those studied here; narrow QWs with high carrier densities and relatively low mobilities. A more appropriate comparison is made to the work of Holmes et al. who studied a wide (30 nm) InGaAs QW with low carrier density [145]; the authors present FFT data which exhibit the same asymmetry as presented here (although no analysis of this feature was made in that paper). This suggests that both the structure and carrier density play a significant role in the relative spin scattering rates. Further study would be required to isolate any particular mechanism for this phenomenon and would benefit from measurements in tilted field.

5.7 Summary

High field magnetotransport data from a range of high mobility InSb QW samples was presented as a function of temperature and gate bias. A detailed analysis of the level broadening in these samples was made indicating a clear relationship with the carrier density. With the use of a top gate electrode the carrier density in the 2DEG was able to be modulated and a weak beating pattern was detected in $d\rho_{xx}/dB$ and $d^2\rho_{xx}/dB^2$ data for a number of samples. This is the first observation of beating patterns in InSb QWs. By quantitatively ruling out alternative mechanisms for beating such as MIS, the observed beating patterns could be attributed to the Rashba spin splitting phenomenon. Values for the Rashba parameter were extracted from the difference in spin population according to the approach of Engels et al. [39] which yielded values in the range $1.3-1.5 \times 10^{-11}$
eV mA which are consistent with the only other previous extraction of the Rashba parameter in the InSb QW system [44].

Numerical simulations of the SdH oscillations were used to explore the influence of various parameters on the beating patterns. The following points were demonstrated: (i) The absence of beating in many of the samples and in those reported previously in this system can be attributed to the combination of large inhomogeneous broadening combined with the presence of a spin dependent scattering rate. This phenomenon is shown to manifest in systems with large spin splitting. (ii) Good agreement with the experimental data was only obtained when using values of $\alpha = 9 \times 10^{-12}$ eV mA that are $\approx 2/3$ smaller than those extracted experimentally highlighting the shortcomings in the FFT method. This value is within 30% of the theoretical value calculated in chapter 4. (ii) By comparing the FT of the experimental and simulated data, it could be determined that the low-energy (majority) spin state is the spin up state, consistent with the presence of a negative $g$-factor, and this has a greater relaxation rate than the high-energy (minority) spin down state.
Chapter 6

InAlSb tunnel contacts

The main prerequisite for a functional hybrid ferromagnetic/semiconductor spintronic device is the efficient injection and subsequent detection of spin polarised carriers through an integral tunnel barrier. This can be in the form of a fabricated ultra thin dielectric film or a Schottky barrier which forms naturally at the interface. As discussed in chapters 4 and 5, modulation doped InSb quantum well (QW) heterostructures are particularly attractive for these applications and it is therefore crucial for the development of spintronics in this material system to investigate the viability of using the InAlSb Schottky barrier as an efficient spin injection contact.

This chapter describes the experimental and theoretical approach to characterising the transport across Ti/InAlSb Schottky barriers at low temperature where tunnelling is dominant. Section 6.1 describes some of the main concepts of the Schottky barrier and the tunnelling process relevant for this investigation. Section 6.2 describes the criteria set out by Rowell for identifying single-step tunnelling – the satisfaction of which is crucial in the context of spin injection contacts. In section 6.3 experimental current-voltage characteristics for the Schottky barriers measured are presented and analysed using various tunnelling models. It is demonstrated that the tunnelling characteristics of the Ti/InAlSb Schottky barrier satisfy the Rowell criteria and are suitable for use as an efficient
spin injector. In section 6.4 possible techniques and recipes for engineering the Schottky barrier to meet the conditions for efficient spin detection in the Fert and Jaffres model [149] are discussed. With the use of a self-consistent Schrödinger-Poisson model, it is shown that with careful engineering of the doping in the barrier, the interface resistance can be optimised for electrical detection. These results are summarised in section 6.5.

6.1 Metal-semiconductor interfaces - Relevant concepts

Schottky barriers have long been used successfully for device applications due largely to the high degree of control over the carrier transport across the metal-semiconductor interface that can be achieved through either the choice of materials, operating bias or the doping. Room temperature measurements of electrical transport across Ti/InAlSb interfaces in InSb/InAlSb quantum well heterostructures have been reported [90], confirming the presence of a Schottky barrier. Characterisation of the low temperature transport of such barriers has not been reported and is important since this is where tunnelling is predominant. A detailed understanding of the barrier transport characteristics is essential for developing useful spin injection/detection devices in this material system [150].

The transport across metal-semiconductor interfaces has been extensively studied over the last 50 years [151]. Well established classical models have been developed which account for the current-voltage characteristics at high and low and intermediate temperatures [152-154]. An energy band diagram is illustrated in figure 6.1 for a moderately doped $n$-type semiconductor contact under reverse bias, $V$. The electron distribution in the metal at high and low temperatures is illustrated by the dot-dashed lines.
The three main mechanisms for traversing the barrier are (a) thermionic emission over the barrier, (b) quantum mechanical tunnelling through the barrier above the Fermi energy (thermionic field emission) and (c) quantum mechanical tunnelling through the barrier at the Fermi energy (field emission). For thermionic emission (TE) over the barrier the minimum energy required to surmount the barrier is $e\phi_b + E_F^m$. Due to its narrow band gap, and consequently low barrier height, TE dominates carrier transport across InAlSb Schottky barriers at substantially lower temperatures than in wider gap semiconductors. However, it will be shown experimentally that TE is negligible in the temperature range investigated and so this mechanism will not be discussed in detail.

Deviations from the standard transport formalisms in heavily doped semiconductors are frequently encountered and a number of alternative transport
phenomena have been proposed in order to account for the observed anomalous behaviour e.g. image force lowering of the barrier [155], variable range hopping [156], trap assisted tunnelling and band-tailing [157] have been proposed to account for the observed behaviour [151]. In general, and particularly in the case of spin injection, these transport mechanisms are detrimental to the application and efforts are generally made to minimise them for optimal device performance. Experimental data from some devices presented in this chapter exhibit a number of anomalous behaviour that can not be explained by the standard processes illustrated in figure 6.2.

Three main concepts of metal-semiconductor interfaces are relevant to the InAlSb Schottky barrier at low temperature; these are surface states, image force corrections and the process of tunnelling itself. An overview of these concepts will be given here to compliment the experimental results and discussions presented in section 6.3.

6.1.1 Surface states and Fermi level pinning

An ideal Schottky contact is rarely formed in most real semiconductor-metal interfaces due to the existence of a finite density of surface states (per unit area per unit energy) at the semiconductor surface, unrelated to the metal. Surface states are believed to result from the reduced symmetry of the 3D crystal lattice at the terminated surface i.e. dangling bonds left from the crystal growth, defects or interface states generated from a thin native oxide and constitute available states for electrons i.e. positive charge. These states are confined to the region of the surface due to the decay of their wavefunctions into the bulk crystal and the vacuum. Charge neutrality at the surface requires that these surface states are filled with electrons from the conduction band up to an energy level coincident with the Fermi level in the bulk. Therefore, in this (rather general) case a potential barrier is formed at the semiconductor surface even in the absence of a metal. If the density of the surface states is sufficient to accommodate any extra charge
from the formation of the Schottky barrier without substantially changing the Fermi energy, the potential barrier in the semiconductor will remain the same i.e. independent of the metal or work function [158]. In this case, the Fermi level is considered pinned by the surface states at a value above the valance band, determined only by the surface properties of the semiconductors. In most III-V semiconductors such as InSb (or InAlSb) the Fermi level is pinned near the middle of the band gap [158]. InAs is a well known exception to this; in this case the distribution of surface states pins the Fermi level inside the conduction band. The assumption of mid-gap pinning in InAlSb was consolidated by high temperature Schottky barrier transport measurements which determined the barrier height to be approximately half the band gap [90]. The low temperature measurements presented in this chapter compliment previous work on these structures.

6.1.2 Image force lowering of barrier height

Knowledge of the electrostatic potential in the vicinity of the barrier is crucial for any transport analysis. As evidenced in the analysis of high temperature transport in numerous material systems [90,159], it is important to consider the image force corrections to the Schottky barrier in the reverse bias regime. This is equally important in low temperature transport, which is discussed in the following section.

A free electron charge positioned at a distance $z$ from a metal surface ($z = 0$) induces an equal and opposite (positive) charge at the metal surface, but the Coulomb attraction between them acts as if the positive charge was positioned at $-z$. This is the image charge. The potential energy of the electron at a distance $z$ from the metal surface is simply
Figure 6.2: Schrödinger-Poisson band profile of an InAlSb Schottky barrier (black line) in the vicinity of the interface \((z = 0)\) under zero bias. Effect of image force lowering is shown by the red line. Inset shows the approximately linear relation between the image force lowering of the barrier and reverse bias.

\[ E_{im}(z) = \frac{e^2}{16\pi\varepsilon_0 z} \]  \hspace{1cm} (6.1)  

where \(\varepsilon_0\) is the permittivity of free space. In a uniform electric field, the total potential is the sum of the image force potential and the applied potential and results in an effective lowering of the metal work function by an amount \(\Delta\phi\) (which can be evaluated from \(dE(z)/dz = 0\)).
This concept is equally applicable to a metal-semiconductor interface where now a positive charge resides in the depletion region of the Schottky barrier and the electric field is the Schottky barrier potential, $e\psi(z)$ ($\varepsilon_0$ is now replaced by the permittivity of the semiconductor $\varepsilon_0 \varepsilon_s$, equal to 16.45$\varepsilon_0$ in In$_{0.8}$Al$_{0.2}$Sb). The potential energy in the barrier incorporating the effect of image force is thus given by $e\psi^*(z) = e\psi(z) - E_{im}(z)$ which has the effect of lowering and narrowing the Schottky barrier height and width as shown in figure 6.2. The coulomb attraction is largest at the interface where $z \to 0$. To a good approximation, the electric field in this region of the barrier is constant, denoted here by $\xi = d\psi(z = 0)/dz$. Thus the potential of the barrier in the vicinity of the interface, can be expressed by

$$\psi^*(z) = (\phi_b + z\xi) - \frac{e}{16\pi\varepsilon_0 \varepsilon_s z}$$

(6.2)

where $\phi_b$ is the un-lowered barrier height. By evaluating the derivative of Eq. 6.2 it can be shown that the potential maximum occurs at a finite distance inside the semiconductor and is lowered by an amount equal to

$$\Delta \phi(V) = \sqrt{\frac{e\xi(V)}{4\pi\varepsilon_0 \varepsilon_s}}.$$  

(6.3)

For a sufficiently forward biased junction, the image force lowering is small because the potential drop in the semiconductor reduces the electric field $\xi(V)$ at the interface. Conversely, the image force lowering is enhanced in the reverse bias regime where the electric field at the interface is maximal e.g. in the TE formalism, the current in reverse bias (normally constant) acquires a bias dependence which accounts for the experimentally observed deviation from simple TE [90]. As indicated in inset of figure 6.2 the barrier height can be lowered by as much 40 meV at a moderate bias of $V = -200$ mV.
6.1.3 Tunnelling current

At low temperatures electrons have insufficient energy to surmount barrier and field emission (process (c) of figure 6.1) through the potential barrier may contribute significantly to the transport, especially in heavily doped Schottky barriers where the electric field in the barrier is high and the depletion width is narrow.

The field emission from a metal to a semiconductor under reverse bias, \( J_F \), is implicitly dependent on the quantum transmission coefficient of the barrier \( T(E) \), the probability of occupied states in the metal \( F_m(E) \) and the probability of unoccupied states in the semiconductor \( 1 - F_{sc}(E) \), where \( F_m(E) \) and \( F_{sc}(E) \) are the Fermi-Dirac distribution functions for the metal and semiconductor respectively. This can be described quite generally by the integral [150]

\[
J_F^{m \rightarrow s} = q \int \phi \frac{N(E)\nu(E)T(E)F_m(E)(1 - F_{sc}(E))}{2} dE
\]

where \( N(E) \) is the 3D density of states in the metal and \( \nu(E) \) is the carrier velocity at the energy \( E \) in the direction of transport. The integral runs over all energies lower than the barrier height. Tunnelling occurs in the interval between the classical turning points of the barrier \( z_1 \) and \( z_2 \) when \( e\psi^\ast(z_1, V) = E \). The exact transmission coefficient of the barrier can be obtained by solving the Schrodinger equation for the potential profile of the Schottky barrier. However, when the potential profile of the barrier varies slowly on the length scale of the electron wavelength, the transmission of the barrier for carriers at an energy \( E \) can be calculated adequately using the Wentzel-Kramers-Brillouin (WKB) approximation [158]
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\[
\ln T_{\text{WK}}(E) = -\frac{2\sqrt{2m}}{h} \int_{a}^{b} dz \sqrt{e^{\psi(z,V)} - E} \tag{6.5}
\]

In simple cases such as rectangular or triangular barriers which are applicable for MTJs and metal-insulator-semiconductor junctions, the transmission coefficient can be solved analytically. For a Schottky barrier the situation is less trivial, especially in the case of heterostructures where the potential profile is often obtained from self-consistent calculations.

Various models have been developed for the analysis of MTJs and superconductor-insulator-superconductor (S-I-S) systems which provide information on the height, shape (asymmetry) and width of the potential barrier from fits to experimental data (see [160] and [161]). In general these are based on approximations centred around finding analytical forms of the tunnelling probability \( T_{\text{WK}}(E) \) (equation 6.5). Whilst the magnitude of the parameters extracted may hold significant ambiguity, they have the benefit of being easily implemented and are useful for comparing the tunnelling characteristics of similar devices and identifying trends.

6.2 The Rowell criteria

A set of criteria were set out by Rowell et al. in 1969 to indentify single-step elastic electron tunnelling through S-I-S structures [162]. Only three of these are relevant when neither electrode is superconducting [163]:

\( i \) An exponential dependence of the conductance on the barrier thickness,

\( ii \) A parabolic dependence of the conductance on bias \( G(V) \) that can be well fitted using either rectangular (Simmons [164]) or trapezoidal (Brinkman Dynes and Rowell [161]) barrier models.
A weak insulating-like temperature dependence of the zero bias resistance $R_d(T)$.

Historically in metal tunnel junction (MTJ) literature the first and second criteria are most frequently used, however, compelling evidence was recently provided by Akerman and co workers [163,165] that only the third Rowell criterion can be regarded as a definitive test of an integral tunnel barrier. It was shown that successful fits could be made to the current and conductance data over a range of biases using the Simmons’ and Brinkman Dynes and Rowell (BDR) models (yielding sensible barrier parameters) even when barriers were subsequently shown to include pin holes via the application of the third criterion. Accordingly, in the analysis of the reverse biased InAlSb Schottky barriers presented in this chapter, the third Rowell criterion is considered to be most important.

6.3 Electrical characterisation of InAlSb Schottky tunnel barriers

In this section three-terminal Schottky barrier transport measurements performed on a 15 nm InSb/InAlSb QW heterostructure are presented. Details of the measurement technique, sample structure and device fabrication are found in chapter 3.

6.3.1 Forward bias characteristics

A set of forward $J(V)$ characteristics of the Ti/InAlSb Schottky barrier for devices A, B, C and D is shown in figure 6.3 on a semi-log plot in the temperature range 4.5 K to 100 K. For clarity, only six curves are shown with temperature increments of 20 K, i.e. 4.5 K, 20 K, 40 K etc.
In general, the measured current densities across the InAlSb barriers are larger than those typically reported in wider gap systems, for example GaAs [166] and GaN [167] Schottky barriers, due to the lower barrier height (taking for example \( e\phi_b \approx E_g/2 \)).
6.3. Electrical characterisation of AlInSb Schottky tunnel barriers

Figure 6.4: (a) The TE ideality factor as a function of inverse temperature for each device. Note that \( n \gg 1 \) at 100 K. (b) Zero-bias barrier height determined by extrapolating the exponential region of the J-V plot to \( V = 0 \) according to the TE theory.

Data from all devices exhibit exponential behaviour at high biases with slopes close to \( 1/k_bT \) at \( T = 100 \) K. Rectifying behaviour is observed in all cases.

In these heavily doped Schottky barriers at low temperatures, TE over the barrier is expected to be negligible. In order to substantiate this, the TE ideality factor defined as \( n = q/k_bT[dV/d\ln J] \) was determined as a function of temperature for each device; for 'ideal' TE, \( n \) is equal to 1 and the slope of \( \ln J \) is proportional to \( 1/k_bT \). The results of this analysis are presented in figure 6.4 as a function of inverse temperature and show strong deviation from ideal TE \( (n = 1) \) over the entire temperature range. Proceeding with this analysis within the TE formalism, the zero-bias barrier height, \( \phi_{bo} \), can be extracted from the TE saturation current \( J_0 \) (determined from the straight line intercept of \( \ln J \) with \( V = 0 \)) [168]. This is shown in figure 6.4(b) as a function of \( n \). Values of \( \phi_{bo} \) from different devices appear to fall onto a single trend line, which increases with
decreasing $n$ and reaches a maximum value of $\phi_{b0} = 107$ meV at 100 K. This is well below the expected barrier height of $\sim 240$ meV \cite{90}, however from extrapolation towards $n = 1$ (shown by the solid line), i.e. increasing temperature, one can see that sensible values for $\phi_{b0}$ would be obtained. Therefore, with some certainty, the TE emission process can be ruled out as a transport mechanism for forward and reverse bias in the temperatures considered here.

Ideality factors $> 1$ can originate from several effects such as (i) image force lowering of the barrier and (ii) field emission (FE) and thermionic-field emission (TFE), as well as (iii) interface states at a thin native oxide at the metal-semiconductor interface and (iv) generation-recombination currents within the depletion region. Werner et al. \cite{168} showed that barrier height fluctuations can also account for ideality factors greater than one and also the frequently observed discrepancy between barrier heights determined from $J(V)$ measurements and capacitance-voltage $C(V)$ measurements. Generation-recombination can immediately be ruled out since it is only important in lightly doped semiconductors. Given the low temperature, the first three effects are likely candidates for the observed deviation from ideal TE.

Padovani and Stratton considered the field and thermionic-field emission across a Schottky barrier in detail \cite{153}. Their approach builds on the foundations of the Stratton model \cite{154,169} who considered the Taylor expansion of the WKB tunnelling probability about the Fermi energy, where most of the transport takes place. The resulting analytical solutions provide a useful quantitative approach to analysing experimental data.

Before proceeding with the analysis of Padovani and Stratton, it is important to note the main assumptions used. These are, (i) the parabolic potential approximation which assumes a uniform ionised donor density in the barrier region and $d\phi/dz = 0$ for $z > W$, where $W = [2\varepsilon_0\varepsilon_r(\phi_b - V + E_F)/eN_d]^{1/2}$ is the depletion layer width which describes the band bending. The assumption of a uniform charge distribution in the depletion region is generally not a good one for modulation doped structures. However, in the InAlSb barriers investigated here,
the Te doping is segregated throughout the barrier and bears closer resemblance to the idealised case than a true δ-doped barrier which is triangular. \(\text{(ii) The effects of image force lowering and narrowing of the barrier are ignored.}\) Despite these assumptions, quantitative comparison can still be made.

For sufficiently large forward biases, the current density can be expressed as [169],[153]

\[
J_{FE} = J_s \exp\left(\frac{eV}{E_{00}}\right) \tag{6.6}
\]

where \(J_s\) is a saturation current and \(E_{00}\) is an energy related to the transmission of the barrier. For the parabolic potential barrier \(E_{00}\) is a material constant related to the donor density by \(E_{00} = \frac{e\hbar}{2} \left( \frac{N_d}{m^* \varepsilon_0 \varepsilon_s} \right)^{1/2}\) such that for \(E \to 0\) the WKB transmission \(T_{WKB} \propto \exp(1/E_{00})\). At large forward bias, a semi-log plot of the \(J-V\) characteristic will yield a straight line with a slope \(\ln J/dV\) equal to \(e/E_{00}\). In addition, because \(E_{00}\) is a material dependent parameter, it is expected to be temperature independent. Figure 6.5(a) shows the experimental temperature dependence of the inverse slope for devices A, B, C and D. One can see that in the devices shown, the inverse slope is approximately constant at low temperatures (\(T < 20 \text{ K} \) for A and B, and \(T < 50 \text{ K} \) for C and D) and begins to increase as the temperature is raised further. At low temperatures, the data agrees with the predictions of FE theory and it is tempting to assign the low temperature value of the inverse slope to \(E_{00}\), yielding \(E_{00} \approx 24 - 30 \text{ meV}\). These values are comparable to those reported in the literature for InS \((E_{00} \approx 26 [170])\) and GaAs \((E_{00} \approx 14 [153])\) Schottky barriers, and would imply an impurity density of \(N_d \approx 1 \times 10^{18} \text{ cm}^{-3}\) (using \(m^* = 0.034m_0\) and \(\varepsilon_s = 16.45\)). Note that this is higher than typical densities used in the SP model.
The increase of the inverse slope at intermediate temperatures can be explained by the TFE mechanism. Here, carriers have sufficient thermal energy to tunnel through the barrier at energies greater than the Fermi energy. According to Padovani and Stratton, the forward bias $J-V$ characteristics for TFE across a Schottky barrier can be expressed similarly by [153]

$$J_{TFE} = J_{sTFE} \exp\left(\frac{eV}{E_0}\right)$$  \hspace{2cm} (6.7)

where now $J_{sTFE}$ is the (modified) saturation current density and $E_0$ is a temperature dependent energy related to $E_{00}$ by

$$E_0 = E_{00} \coth\left(\frac{E_{00}}{k_bT}\right).$$  \hspace{2cm} (6.8)
i.e., a plot of $\ln J$ versus $V$ will yield a straight line of slope $e/E_0$. The temperature dependence of the inverse slope is shown in figure 6.5(b) normalised by its low temperature value. The temperature dependence of equation 6.8 is too weak to describe the data when using the low temperature inverse slope as $E_{00}$. In order to reproduce the experimental temperature dependence smaller values of $E_{00}$ are required. These fits are indicated by the dashed lines in figure 6.5 were made using the parameters $E_{00} = 11.8$ meV, 11 meV, 19.5 meV, 18.5 meV for devices A, B, C and D, respectively. Justification for using values of $E_{00}$ less than the experimental low temperature inverse slope in equation 6.8 is based on the neglect of image force lowering and narrowing of the barrier in the approach of Padovani and Stratton and the non-uniform impurity density in the barrier (this is equivalent to the empirical ideality factor $n$ introduced to the TE process).

Rideout and Crowell [155] showed that the inclusion of image forces causes deviation of the $\ln J-V$ from a straight line and that TFE and TE is enhanced compared to the un-lowered case (it was also shown that when image force lowering is included, ideality factors always exceed unity). Hasegawa et al. [167] similarly found that the extracted values of $E_{00}$ from measured data were too large to describe their data and a modified version of the TFE expression was derived to take into account a non-ideal barrier profile. This is consistent with the conjecture proposed here and reflects the inadequacies of the idealised parabolic barrier model.

Intriguingly, the disparity in the temperature dependences of the inverse slopes from devices A and B, and C and D indicate very different barrier transmissions, which may not be realistic; The above analysis suggests that devices A and B have lower barrier transmissions (i.e. lower conductance) than devices C and D. Following this, one would intuitively expect lower tunnelling currents in these devices. However, this is contrary to the magnitude of the current densities seen in figure 6.3. This strongly indicates that the above TFE analysis is inappropriate for these high conductance devices and that the enhanced temperature dependence in devices A and B originates from an
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alternative temperature dependent transport mechanism. It is speculated that this mechanism is trap assisted tunnelling and is revisited later in this section.

The FE to TFE crossover is smooth and TFE is expected to become dominant when $E_{00} \approx k_b T$. Assuming that the TFE analysis is valid for devices C and D, this occurs at $T \approx 190$ K. From the good agreement between the temperature dependence of the inverse slope and TFE theory, one can conclude that at low temperatures FE dominates the forward bias $J-V$ characteristic while at intermediate temperatures $T > 50$ K TFE begins to influence the transport. It will be shown that the TFE mechanism also satisfies the Rowell criteria. Data from samples E, F, G, H and I will be analysed with respect to the temperature dependence of the zero bias conductance, discussed in a later section.

6.3.2 Reverse bias characteristics

Figure 6.6 shows the reverse bias $J-V$ characteristics of devices A, B, C and D between 4.5 K and 100 K. The vertical axes span four orders of magnitude for comparison to the forward bias data in figure 6.3. It can be seen that devices A and B exhibit greater temperature dependence compared to devices C and D, consistent with the trend observed in the forward bias regime. However, unlike the forward bias characteristics, the reverse data do not show an obvious exponential component at high bias.

In general, the analysis of the reverse bias region is considerably more complicated than the forward bias regime. The reverse bias expressions for FE derived by Padovani and Stratton are less transparent and less easily checked than for the forward bias case (i.e. no simple exponent). The $\ln|J|-V$ characteristics for FE and TFE that can be identified from the results of Padovani and Stratton (when image force lowering is neglected) are respectively (i) a sub-linear behaviour close to $V^{1/2}$ for FE and (ii) an exponential form at high bias according to $J_{TFE} = J_{stFE} \exp \left( \frac{eV}{\varepsilon'} \right)$ for TFE.
Thus, a linear region in the $\ln J-V$ plot is expected to develop with a slope $e/\varepsilon'$ as the temperature is increased ($\varepsilon'$ is the equivalent reverse bias energy to $E_0$). In the data presented in figures 6.6(a)-(d), non-linear $\ln J-V$ characteristics are observed for all devices in the reverse bias regime indicative of FE. The exponential region

**Figure 6.6:** Reverse bias $|J|-V$ characteristics of devices (a) A, (b) B, (c) C and (d) D as a function of temperature.
predicted for TFE is not manifested in the data recorded and one can conclude that an extension of the experimental bias range is necessary to further investigate the TFE regime in these devices.

In figure 6.7 the entire $|J| - V$ characteristic is shown for each device at 10 K for comparison. A large variation in the magnitude of the current density is observed. It should be re-emphasised that the devices originate from the same processed sample having undergone identical surface treatments. The disparity in the magnitude of the low temperature $|J| - V$ curves of the devices is therefore most likely due to variations in the Schottky barrier height and/or the presence of a spatially non-uniform interfacial layer such as an a native oxide at the InAlSb surface which is not removed by the surface pre-treatment techniques used (see chapter 3).
Devices H and I show anomalous changes of slope in the reverse bias regime. This is especially pronounced in device I which exhibits plateau-like structures as marked by the X arrow (weaker features are detectable in the forward bias data). Weak features in the \( \ln |I| - V \) characteristic (e.g. devices A and B) might be expected considering the potential profile of the ‘real’ Schottky barrier which has a non-uniform doping distribution. For example, consider the potential profile of the QW structure generated from the Schrödinger-Poisson model (SPM) shown in figure 6.2. The modulation doping causes a positive slope beyond the classic depletion width i.e. with reference to the parabolic approximation for bulk material, \( \partial V/\partial z \neq 0 \) for \( z > W \). The transmission of the barrier as a function of reverse bias therefore exhibits inflections due to the presence of the second (smaller) barrier which will be reflected in the tunnelling current. This effect will be more pronounced in the \( J-V \) characteristic at low temperatures when the injection energy distribution is narrow.

Clearly, this description of a single inflection does not account for the appearance of multiple current plateaus in device I. Similar features have been observed previously that were attributed to a distribution of barrier heights (see Tung [171]). Plateau features may equally be accounted for by the presence of energetically discrete trap states in the barrier which may originate from threading dislocations. These effects should become smeared at elevated temperature due the extension of the Fermi distributions which is indeed observed in the data. The fact that current plateaus are not observed in each device indicates spatially inhomogeneous barrier profiles and/or defects. If the latter mechanism is assumed, the discrete nature of the plateaus implies a discrete distribution of traps rather than a continuum e.g. Carrano et al. [172]. Atomic force microscopy studies of this material reveal typical threading dislocation densities of approximately \( 10^8 \text{ cm}^{-2} \). Assuming a spatially uniform distribution, for the small area junctions investigated here, this corresponds to the presence of single numbers of defects under the Schottky contact region (statistically one to three, dependent on contact area) which is in quantitative agreement with the
6.3. Electrical characterisation of AllnSb Schottky tunnel barriers

proposed interpretation of enhance tunnelling via a discrete distribution of defects/impurities within the barrier. This is discussed further in the following section.

Numerical calculation of tunnel current

The reverse bias tunnelling current for the devices can be calculated numerically using equation 6.4. In this calculation, the potential profile of the barrier is solved at each bias using a self consistent Schrödinger-Poisson model (SPM) e.g. figure 6.2 and the integral is evaluated using the finite difference method. Details of the SPM, the parameters and the assumptions used are found in appendix B. The result of the numerical simulation is indicated by the triangles in figure 6.7 and agrees well with the experimental $J-V$ characteristics in both magnitude and bias dependence indicating the validity of this model and the SPM. The error bars in this calculation take into account a 10% variation in top barrier width i.e. $\pm 5\text{nm}$; this spans an order of magnitude due to the exponential dependence of the tunnel current on the barrier width and thus encompass the majority of device characteristics. In addition, it is worth noting that there is a degree of uncertainty associated with the area of the Schottky contact as estimated from scanning electron micrographs of the devices; this may shift slightly the magnitude of the experimental current densities.

6.3.3 Conductance properties

A characteristic feature common to nearly all tunnel junctions is a parabolic dependence of the differential conductance $G = dI/dV$ on bias around $V = 0$ [162]. The observation of such behaviour is the 2nd Rowell criterion and is investigated here.

The differential conductance $G(V_b)$ of the Schottky barriers at 4.5 K are calculated numerically using six point linear averaging and are shown in figure
6.3. Electrical characterisation of AlInSb Schottky tunnel barriers

Figure 6.8: The differential conductance $\frac{\partial I}{\partial V_b}$ for devices A to G as a function of $V_b$ at 4.5 K. The dot-dashed lines represent fits to the BDR model (Equation 6.8).

6.8(a). The conductance properties vary substantially from device to device but clearly the result is that each device exhibits a parabolic dependence on reverse bias. A stronger dependence is observed in the forward bias regime due to the rectifying current-voltage characteristic of the Schottky barrier. The parabolic dependence on reverse bias indicates that the Schottky barrier height is approximately bias independent; conversely, the stronger dependence on forward bias reflects the bias dependence of the barrier height and width in this regime.

The parabolic dependence of the conductance is compared to the results of the BDR model obtained for trapezoidal barriers and (to second order in $V$) given by [161]
where $A_0 = t\sqrt{2m/3\hbar}$, $\Delta \varphi = \varphi_2 - \varphi_1$ represents the barrier asymmetry and the zero bias conductance $G_0 = 3.16 \times 10^{10} \frac{\varphi_{1/2}^2}{t} \exp(-1.025t\varphi_{1/2})$.

Note that in this form, the conductance $G(V) = dI/dV$ (Ohm cm$^{-2}$), the barrier thickness is in angstroms (Å) and the potentials are in volts. Although formulated for trapezoidal barriers which bear little resemblance to the Schottky barrier, the BDR model can be used to compare the conductance data of different devices. As the authors point out, emphasis should not be on the values of the extracted fitting parameters but rather the observation of parabolic conductance. Of particular relevance to Schottky barriers, the BDR model predicts that the position of the conductance minima, $V_{mn}$, depends on the barrier asymmetry i.e. $V_{mn} < 0$ for $\Delta \varphi < 0$. This is indeed observed in the experimental conductance data in figure 6.8.

The BDR model has been extensively used to extracted barrier parameters in MTJ literature, but as emphasised by Miller et al. [173] the expansion in equation 6.9 is only valid over a small bias range typically less than one half of the barrier height. With this in mind and due to the asymmetry of the conductance data from the Schottky barriers, the BDR model is fit to the experimental data in the range $-100$ mV $< V_b < 0$ mV.

The resulting least squares fit of the BDR model to the reverse bias data using equation 6.9 are shown in figure 6.8 by the dashed lines. To reduce the fitting parameters in this analysis, a triangular barrier is assumed by taking $\phi_2 = 0$ and thus $\Delta \varphi = -\phi_1$. Fitting of the BDR model to devices H and I did not yield sensible parameters and so results are not shown here. The extracted fitting parameters from the BDR model for devices A to G are summarised in table 6.1. Sensible parameters are extracted for each device apart from A and B whose barrier heights are particularly low (this could be interpreted as a result of the
reduced barrier transmission felt by electrons traversing the barrier via defect states). The extracted parameters appear consistent with the trends observed in the $J-V$ data in figure 6.7 i.e. devices with the lowest reverse bias current (E, F and G) yield higher and wider barriers than devices with greater reverse bias current (A, B, C and D). It should be noted that emphasis here is not on the extracted barrier parameters but rather the appearance and fitting of the parabolic conductance.

Notably, each device can be fit with the BDR model and so satisfy the 2$^{\text{nd}}$ Rowell criterion. This will be revisited in the following section.

**TABLE 6.1: Extracted barrier parameters from a least squares fit of the BDR model to experimental data for devices A to G. Parameters from the Stratton model are also included where possible.**

<table>
<thead>
<tr>
<th>Device</th>
<th>BDR</th>
<th>Stratton</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\phi$ (meV)</td>
<td>$d$ (nm)</td>
</tr>
<tr>
<td>A</td>
<td>128</td>
<td>20.2</td>
</tr>
<tr>
<td>B</td>
<td>102</td>
<td>19.2</td>
</tr>
<tr>
<td>C</td>
<td>367</td>
<td>22.2</td>
</tr>
<tr>
<td>D</td>
<td>334</td>
<td>19.9</td>
</tr>
<tr>
<td>E</td>
<td>357</td>
<td>40</td>
</tr>
<tr>
<td>F</td>
<td>402</td>
<td>26.5</td>
</tr>
<tr>
<td>G</td>
<td>250</td>
<td>30.0</td>
</tr>
</tbody>
</table>

6.3.4 Zero-bias resistance and conductance anomalies

Although good agreement between the numerical simulation of the tunnel current and the BDR model indicates that tunnelling is the predominant transport mechanism, it alone is insufficient to conclude that it is the dominant or sole mechanism. Analysis of the 3$^{\text{rd}}$ Rowell criterion i.e. a weak temperature dependence of the zero bias resistance is necessary to further determine the nature
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Figure 6.9: Specific zero-bias resistance as a function of temperature for each Ti/InAlSb barrier.

of the transport. Accordingly, in figure 6.9 the temperature dependence of the specific zero bias resistance \( R_0 A = \left( \frac{\partial J}{\partial V} \right)_{V \rightarrow 0} \) (\( \Omega \text{m}^2 \)) is presented for devices A to I. \( A \) is the junction area (listed for each device in table 3.2).

The specific resistance of the nine Ti/InAlSb Schottky barriers spans three orders of magnitude demonstrating clearly the variability of the barrier characteristics. The majority of data at low temperatures are grouped closely to \( 5 \times 10^{-5} \Omega \text{m}^2 \) e.g. devices A, B, C, D and G. Data which deviate significantly from this trend may therefore represent non-ideal Schottky barriers via the presence of either a thin interfacial oxide layer which increases the resistance (devices E and F) or defects/impurity states within the barrier which enhance tunnelling and reduces the junction resistance (devices H and I). Importantly, each device exhibits a decrease in zero bias resistance with increasing temperature, which is associated with a tunnelling mechanism rather than the metallic temperature.
dependence (an increasing resistance with increasing temperature) associated with a shorted barrier e.g. see Akerman et al. [165]. Nevertheless, three different temperature dependences can be distinguished from the data of figure 6.9: (i) a weak temperature dependence (devices C and D), (ii) an exponential dependence on temperature (device H), and (iii) a transition from a weak temperature dependence at low temperatures to exponential dependence at elevated temperatures (devices A and B). The origins of this dependence are discussed below.

The weak temperature dependence observed in devices C and D is described well by the Stratton model for the zero bias conductance \( G(T) \) given by [169]

\[
G_0(T) = \frac{A^*}{c_1 k_B} \exp(-b_1) \frac{\pi c_1 k_B T}{\sin(\pi c_1 k_B T)}
\]

where \( A^* \) is the effective Richardson constant and \( b_1 \) and \( c_1 \) are the coefficients defined by Padovani and Stratton for a parabolic Schottky barrier and can be expressed as [153]

\[
b_1 = \frac{\phi}{E_{\text{on}}} \quad c_1 = \ln\left(\frac{4\phi}{E_{\text{on}}}\right) - \frac{1}{2E_{\text{on}}}
\]

The experimental data for device C and D show an apparent drop in \( R_0A \) as the temperature is lowered below 10 K (see figure 6.10). This can be explained by considering a spatially inhomogeneous barrier height; according to Werner and Güttler [168], if \( \phi_b \) and \( \sigma_b \) are the mean value and standard deviation of the (Gaussian) distribution respectively, the barrier height acquires a temperature dependence \( \phi_b(T) = \bar{\phi}_b - e\sigma_b^2 / 2kT \). This expression for the temperature dependent barrier height is substituted into equation 6.10 for the fitting procedure. The resulting least squares fits to the data are indicated by the dashed lines in
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Figure 6.10: Zero bias resistance as a function of temperature for (a) devices C and D fit with the Stratton model and (b) device I which exhibits anomalous oscillatory temperature dependence.

Figure 6.10(a) yielding $\overline{\phi}_o = 256$ meV and 245 meV with a standard deviation of $\sigma_s = 7$ meV for devices C and D, respectively. Values of $E_{00}$ established from the forward bias characteristics were used.

It is therefore concluded that devices C and D satisfy the 3rd Rowel criterion and can be identified to support single step tunnelling.

Table 6.1 compares the extracted barrier parameters from the Stratton model and the BDR model (insufficient data from device E, F and G prevented a fit to the Stratton model). Lower barrier heights are extracted from the Stratton model. However, we see from figure 6.2 that the expected zero bias barrier height assuming mid gap pinning and taking into account image forces is $\phi_o \approx 280$ meV. Thus in this case it seems the Stratton model generates the more realistic parameters.

The stronger temperature dependences in the data of devices A, B, H and I can not be fit by the Stratton model. Closer inspection of the data from device I
6.3. Electrical characterisation of AlInSb Schottky tunnel barriers

reveal that the zero bias resistance oscillates with temperature below 25 K [see figure 6.10(b)]. This anomalous behaviour can not be explained by standard transport formalisms nor has it been reported previously.

To further investigate the nature of these low resistance Schottky tunnel junctions, the differential resistance spectra, $(dV/dI)^{-1}$, was examined for each device. Data for devices C, H and I are presented in figure 6.11 as a function of temperature.

Device C is representative of devices exhibiting a weak temperature dependence of the zero bias resistance and hence single step tunnelling. Data in figure 6.11(a) shows an asymmetric single peaked structure in the $(dV/dI)^{-1}$ spectra, characteristic of Schottky barriers [174]. Data for low resistance devices H and I are relatively featureless at high temperatures $T = 50$ K. In contrast to the data of device C, striking features are resolved in the data at low temperatures. A peak is present at zero bias with satellite features, one of which (at $V_b \approx -24$ mV) corresponds closely to the InSb LO Phonon energy $(E_{\text{LO}} = 24.4$ meV), as indicated by the arrows. The zero bias peak is strongly temperature dependent.
and is responsible for the enhanced temperature dependence of the $R_0A$ product compared to devices C and D. Zero bias anomalies along with the appearance of structure at the LO phonon energy have previously been observed in InSb Schottky barriers [175,176]. A peak at the phonon energy indicates a tunnelling process in which an LO phonon is emitted during passage across the barrier. The zero bias anomaly is frequently encountered in studies of MTJs and also GaAs Schottky barriers [28,174]. Carruthers [174] studied the resistance spectra of $p$-type GaAs Schottky barriers and observed that the zero bias anomalies coincided with the appearance of additional structure at the phonon energies. The author reviews the various theories for the origin of the zero bias anomaly from which it is argued that the feature is associated with impurity wavefunction overlap within the barrier. This model describes resonant-inelastic tunnelling via overlap in the barrier. Moreover, the resonant tunnelling picture predicts enhancements in the phonon-induced structure at energies $eV = \pm \hbar \omega_0$. Thus, the structure observed in devices H and I appear to support the impurity/trap assisted tunnelling mechanism. It is proposed that the enhanced temperature dependence in the zero bias resistance in devices A, B H and I is due to assisted tunnelling via a finite number of defects/traps in the barrier. This may be mediated by phonons in devices H and I.

Trap assisted tunnelling models have been proposed by various authors. Electrons may tunnel into deep level interface states associated with the presence of defects or impurities created by threading dislocations or the Ti adhesion layer incorporated into the contact metallisation process, then tunnel across the remaining barrier. Depending on the distribution of states within the barrier, electrons occupying the intermediate states may also be thermally excited to higher energy levels and traverse the barrier at higher energy with greater transmission. Importantly, in the context of spin injection, trap/impurity assisted tunnelling is an incoherent, spin-flip scattering process due to the mixing tunnelling electron wavefunctions with the unpolarised intermediate trap states. Such a process is detrimental to spin injection as evidenced by Jansen and
Moodera [177] who observed a significant increase in conduction and decrease in TMR of junctions containing nonmagnetic impurities.

The origin of the intermediate resistance peaks at \( V_b < -24 \) mV is less clear, as is the oscillatory temperature dependence of the zero bias peak in device I. It is noted that the position of the intermediate peaks in the spectra of devices H and I correspond closely to the LA \((E_{OILA} = 14.6 \) meV) and TA \((E_{OILA} = 5 \) meV) InSb phonon energies, respectively [176]. Unfortunately these observations are limited to only two devices, and the measurement of a larger number of Schottky barriers would be required to further investigate the origins of these phenomena which is beyond the scope of this thesis.

### 6.4 Engineering InAlSb Schottky tunnel barriers for spin injection and detection

The critical parameter for electrical injection and detection of spin is the specific resistance \((\Omega \text{m}^2)\) i.e. the resistance area product. Fert and Jaffres [31] showed that the spin polarization of current injected from a ferromagnetic contact into a bulk semiconductor through a spin dependent interface resistance \(r_{b^*}\) (tunnel barrier), is given by

\[
SP_i = \frac{\beta r_F + \gamma r_p^*}{r_p + r_N + r_b^*} \tag{6.11}
\]

where in this notation \(\beta\) is the spin polarization in the ferromagnet, \(\gamma\) is the spin asymmetry coefficient of the interface layer (characterising the spin dependence of the interface resistance), \(r_F\) and \(r_N\) are the product of the spin diffusion length \(\lambda_g\) and resistivity \(\rho\) in the ferromagnet and semiconductor, respectively. With no interface layer \((r_{b^*}=0)\), the spin polarization is proportional to \(r_F/r_N\) which is typically less than \(10^{-5}\) in magnitude i.e. negligible whereas a large spin polarisation can be obtained for large interface resistance such that \(r_{b^*} \gg r_N\).
This is suitable for a spin LED experiment requiring no electrical detection such as those described in section 6.1. For a spin-valve experiment where spins are injected and detected through electrical contacts, the situation is less trivial; \( r_b^* \) must lie within a narrow range determined by the material parameters and device geometry. For a two terminal structure such as that shown in figure 6.12 where the ferromagnetic electrodes (FM) are fabricated onto a semi infinite lateral 2DEG channel (see also Appendix C), \( r_b^* \) must satisfy [149]

\[
\frac{\rho_{sc} W t^2}{\lambda_{sc}} < r_b^* < \rho_{sc} \lambda_{sc} W
\]

where \( \rho_{sc} \) and \( \lambda_{sc} \) are the (2D) sheet resistivity and spin diffusion length of the 2DEG, and \( t \) and \( W \) are dimensions defined in figure 6.12. (Note that in the case of a 2DEG \( r_N \) is replaced by \( \rho_{sc} \lambda_{sc} W \)).

Typical values for \( r_b^* \) for the devices studied in the previous section that satisfy the Rowell criteria are of the order \( 10^{-5} \, \text{\Omega m}^2 \) at \( V_b = -50 \, \text{mV} \). For the purpose of spin injection, this is six orders of magnitude greater than the
threshold value $\rho_{sc}\lambda_{sc}W$ estimated to be $\approx 3 \times 10^{11}$ $\Omega \text{m}^2$ using values of $\rho_{sc}=108$ $\Omega \Box$ (cf. table 3.2), $\tau \approx 0.5$ ps [109] and $W = 500$ nm ($\lambda_{tr} \approx 540$ nm in this case). Thus the current material is suitable for a spin LED device to determine the spin injection as evidenced by Hanbicki et al. for the GaAs Schottky barrier [28]. The interface resistance is, however, too large for the purpose of spin injection and detection using the device configuration shown in figure 6.12. This is not surprising since the QW material studied here has a thick top cap of 50 nm with a Schottky barrier which was not designed specifically for such a purpose. The results in the previous section do however show that careful analysis is required to ascertain the transport characteristics. Of equal significance, the identification of thermionic field emission in forward bias means that the Schottky barriers are fundamentally suitable for spin detection [178].

The band bending of the electrostatic potential profile is entirely determined by the space charge distribution and thus via appropriate consideration of the extrinsic doping and upper barrier thickness one can engineer the shape and width of the Schottky barrier. Since the transmission of the barrier is exponential dependent on the extent of the barrier above which the electron is tunnelling (see equation 6.5) one can gain some control over the interface resistance $r_s^\ast$. In the following the considerations for an efficient injection and detection strategy in modulation doped InSb QWs are discussed briefly.

A band profile of a typical Schottky barrier is shown in figure 6.2. A distinctive feature of the modulation doped barrier is the conduction band minima (located at $z \approx 35$ nm on the scale in figure 6.2) that occurs within the depletion region. This feature is rarely observed in the widely reported bulk doped structures. In fact, spin injection into modulation doped heterostructures which are suitable for spin FET type lateral spin transport devices has not been reported to date. In a review article by Van Roy et al. [179], it was pointed out that an undepleted region in the Schottky barrier is undesirable for spin injection/detection since the injected carriers may accumulate in this region where a net unpolarised population reside, lowering the overall efficiency of spin transfer to the 2DEG.
Ideally this region of the barrier between the bottom of the barrier and the QW should be flat, although in practice this is hard to achieve just from simple electrostatic arguments. In any case, reverse biasing the junction depletes and flattens the region between the doping and the QW and efficient injection is restored. In the extreme case an unwanted bias dependence of the spin injection will result as evidenced in [179].

6.4.1 Fundamental constraints

The three parameters which impact the barrier transparency are (i) the In$_{1-x}$Al$_x$Sb cap thickness and (ii) the Al content of the In$_{1-x}$Al$_x$Sb cap which alters the Schottky barrier (assuming near mid-gap pinning) and (iii) the doping. With regard to (i), narrowing the top cap thickness reduces the confinement of the electronic states within the QW. Moreover, the wavefunction samples more of the ternary material which is shown to be detrimental to carrier mobility. Regarding (ii), the barrier height must be sufficiently high to ensure that tunneling is the dominant transport mechanism. Finally, the dopant layer should be sufficiently close to the 2DEG for efficient charge transfer and not too close to the free surface so that free carriers are lost to the surface states. Whilst some freedom is granted for the doping, in reality, the first two growth parameters tend to be restricted.

The lattice constant of In$_{1-x}$Al$_x$Sb varies considerably with alloy content $x$ compared to, say, Al$_x$Ga$_{1-x}$As (see figure 3.1). Note that the same is found in the In$_x$Al$_{1-x}$As and In$_x$Ga$_{1-x}$As systems. Assuming that the InSb QW grows pseudomorphically onto the lower In$_{1-y}$Al$_y$Sb barrier, there exists a critical thickness that the QW can be grown before the lattice relaxes and misfit dislocations form; therefore wide QWs require a low alloy content In$_{1-y}$Al$_y$Sb lower barrier ($y=0.1$ in the 30 nm QWs studied in chapter 5). In addition, to minimise strain in the upper In$_{1-x}$Al$_x$Sb barrier (so that its thickness is not a critical parameter), it is generally grown with an alloy content that differs by only
5% from that below the QW. For maximum confinement and carrier mobility the barrier alloy contents should be as high as possible for a given QW width and thus different QW widths are grown with varying upper and lower barrier compositions as discussed in chapter 4. With this in mind one should first decide which QW width is desirable before attempting to engineer the Schottky barrier. This is not straightforward to answer. It is desirable for a functioning all-electrical device to have a large Rashba effect in order to manipulate the spin orientation in the plane of the 2DEG in addition to fast transit times. The injected spin polarisation must survive longer than the transit time or the relevant transit length in order to be detected at the second contact (i.e. requiring long spin lifetimes/spin diffusion lengths). However we see from chapter 4 that these factors are tensioned against since in general, long spin lifetimes/diffusion lengths occur in systems with a small Rashba effect e.g. GaAs. Figure 6.13 shows the spin diffusion length as a function of carrier density for four different QW widths using the parameters obtained in chapter 4 according to

**Figure 6.13**: Calculated spin lifetime for InSb QWs as a function of carrier density using the parameters obtained in chapter 4.
\[ \lambda_s = \sqrt{D \tau_s} = \hbar \sqrt{\frac{m_{2D} \tau_p \tau_s}{m^*}}. \tag{6.13} \]

This indicates that under the growth requirements listed above and at moderate carrier densities, the longest spin diffusion lengths are found in the narrower QWs.

### 6.4.2 Designs for epitaxial spin injection-detection barriers

Engineering of the interface resistance in the 15 nm QW structure can be achieved by reducing the top barrier thickness to 30 nm and using two δ-doping layers; one to thin the barrier and one to supply carriers to the QW without occupying the barrier region. In addition, the alloy content in the upper barrier can be reduced from 20% to 15%, matching that in the lower barrier. This result is shown by the solid line in figure 6.14. Two doping layers, labelled A and B, are located 5 nm and 20 nm above the QW. δ-layer B is doped to a higher level than layer A in order to reduce the depth and broaden the conduction band minima in the barrier.

In this figure an additional band profile is shown for a structure with identical doping but with a 40 nm top cap (dot-dashed line). The acute influence of this parameter on the WKB transmission probability of the barrier \( T(E) \) is shown in the inset, evidenced by a four orders of magnitude increase in \( T(E) \) at low energies e.g. 70 meV by reducing the top cap by 10 nm. At a bias of -50 mV the interface resistance of the engineered 30 nm barrier is reduced to \( r^*_{\delta} = 1 \times 10^9 \ \Omega m^2 \). This is four orders of magnitude lower than the standard un-engineered barriers investigated in section 6.3 (10^5 \ \Omega m^2) and brings the interface resistance close to the desired range inferred from the Fert and Jaffres model, c.f. equation 6.12.
6.4. Engineering AlInSb Schottky tunnel barriers for spin injection...

For maximum change in resistance between parallel and anti parallel configurations, the FM electrode separation $t$ should be much less than the spin diffusion length $\lambda_{sf}$. If we consider reasonable parameters for a low density sample, $\rho_{sc} = 1000 \ \Omega \cdot \square$ and $\lambda_{sf} = 1 \ \mu m$ (reasonable for a low density) with a contact width of $W = 1 \ \mu m$ and separation of $t = 100 \ nm$ we find that the desired range is $1 \times 10^{-11} < r^*_b < 1.4 \times 10^{-9} \ \Omega m^2$. In fact, for small separations $t$ the lower limit is almost always satisfied. (Using the parameters for the device studied in section 6.3 shifts the upper limit to $5 \times 10^{-11} \ \Omega m^2$). The interface resistance of the engineered barrier can be further reduced by lowering the alloy content in the top barrier to 10% or reducing the layer thickness – the solution presented here is within the parameter space that is

**Figure 6.14:** Schrödinger-Poisson conduction band profile solution for a 15 nm QW with a 30 nm (solid line) and 40 nm (dashed line) top cap with the associated ground state wavefunctions (red lines). Inset shows the resulting WKB transmission probability of each barrier.
6.4. Engineering AlInSb Schottky tunnel barriers for spin injection... currently used in typical MBE wafer growths. Thus it is concluded that the interface resistance of a 15 nm QW can engineered to be suitable for a spin-value device. However, from inspection of figure 6.14, one can see that the conduction band minima within the Schottky barrier depletion region is unavoidable using the present modulation doping scheme.

An alternative design for a spin injection structure is that shown in figure 6.15. In growth order the structure consists of 1 µm In₀.₉Al₀.₁Sb (undoped)/5 nm $n^+$-In₀.₉Al₀.₁Sb (3x10¹⁷ cm⁻³)/10 nm In₀.₉Al₀.₁Sb (undoped)/40 nm InSb/10 nm $n^+$-In₀.₉Al₀.₁Sb (2x10¹⁸ cm⁻³). Here, to avoid the conduction band minima in the upper barrier, the δ-doped layer (A) is positioned below the QW (this would thus require the Te dopant to not segregate through the QW). A wide 40 nm QW is chosen so that the structure resembles that of a single heterointerface structure; the wavefunction (and electron distribution) is confined to the lower interface...
away from the free surface \((z = 0)\). This gives additional freedom for the width of the top barrier which can be thinned sufficiently to achieve the desired interface resistance. In this design, the top cap is 10 nm thick and uniformly doped (B) to reduce the width of the Schottky and to populate the QW.

The resulting interface resistance calculated according to equation 6.4 at a bias of -50 mV is \(r^* = 1 \times 10^{-11} \ \Omega m^2\) i.e. well within the desired range for efficient spin injection and detection. This approach also leaves scope for the growth of an additional ultra thin MgO tunnel barrier or higher alloy content InAlSb barrier on the surface. Most importantly, one can see that in this design the electrons tunnel directly into the QW region with no accumulation in the Schottky barrier.

6.5 Conclusions

In section 6.3 experimental current-voltage characteristics from nine different Ti/InAlSb Schottky barriers in an InSb quantum well heterostructure were analysed within the framework of various tunnelling models and the thermionic field emission (TFE) theory of Padovanni and Stratton and the Rowell criteria for single step tunnelling. Considerable variation in the \(J-V\) characteristics and the temperature dependence of the specific zero bias resistance was observed.

Barriers could be broadly separated into two categories, (i) low resistance barriers with strong temperature dependent characteristics and (ii) high resistance barriers with weakly temperature dependent characteristics. With the exception of the barriers H and I which exhibit anomalous conductance, the barrier conductance \(G(V)\) of the seven remaining barriers could be well fit with the Brinkman Dynes and Rowell (BDR) model yielding reasonable parameters, thus satisfying the 2\(^{nd}\) Rowell criterion. Devices C and D which exhibited a weak temperature dependence of the zero bias resistance \(R_0\) could be successfully fit with the Stratton model taking into account a narrow distribution of barrier heights. This observation satisfies the 3\(^{rd}\) Rowell criterion from which it is concluded that these high resistance barriers support single step tunnelling.
It was noted that each devices exhibited a tunnelling-like temperature dependence of $R_o$, however, it is argued that the stronger temperature dependence observed in devices A, B, H and I originates from the presence of defects in the barrier which promote trap assisted tunnelling. In the lowest resistance junctions H and I, what appears to be phonon structure in the differential resistance spectra is observed.

The observation of single step tunnelling along with the large interface resistance $r_b^*$ under reverse bias demonstrates that the InAlSb Schottky barriers are suitable for use as a spin injection medium [150]. Furthermore, good agreement between the forward bias characteristics of these devices and TFE theory demonstrates that these Schottky barriers are also suitable for electrical spin detection. In the forward bias regime, the interface resistance $r_b^*$ is $\approx 10^{-6}$ $\Omega m^2$ at 50 mV which is over an order of magnitude smaller than that under the equivalent reverse bias. Although this is too large for efficient spin detection, this bias asymmetry opens a new degree of control over the injection and detection properties for a lateral device.

Using a self consistent Schrödinger Poisson model to generate band profiles of the Schottky barrier and a tunnelling model which showed good agreement with experimental, it is shown that the resistance of the Schottky barrier can be engineered to be within the desired range for efficient spin injection and detection in a lateral spin value type device. Two designs are given for a 15 nm and 30 nm QW heterostructure, the latter is designed to remove the conduction band minima in the barrier region and maximise the efficiency of spin transfer into the QW. The fabrication of such structures is discussed in appendix C.
Chapter 7

Conclusions and further work

In this thesis a number of issues related to the use of InSb quantum wells (QWs) as a medium for spintronic applications were investigated. Three core activities were addressed:

(i) The measurement of gated Hall bars in high mobility 30 nm InSb quantum wells with the direct observation of the Rashba spin splitting.
(ii) Investigating of the use of InAlSb Schottky barriers as a tunnel barrier for spin injection and detection in two terminal spin valve type devices.
(iii) Calculations of the Rashba and Dresselhaus zero field spin splitting parameters and associated spin lifetime in realistic InSb heterostructures;
(iv) The fabrication of two terminal spin valve devices in InSb epilayers

The first three activities were detailed in chapters 4, 5 and 6. The fourth activity remains ongoing and although did not result in a working device, details of the fabrication, issues and steps made to overcome these problems are detailed in appendix C.
In this chapter the main implications of these activities are summarised and the future work that would be beneficial to the development of spintronics in narrow gap InSb QWs are highlighted briefly.

7.1 Conclusions

Calculations of the conduction band profile using a self consistent Schrödinger-Poisson model has proven to be a very useful tool during the course of this project, not only for investigating the influence of the doping parameters on the confined states and occupation in the QW but also the conduction band profile and the quantum state wavefunctions. These were used to evaluate the matrix elements of the eight-band $k.p$ model for the inversion asymmetry spin splitting parameters; $\alpha$, $\beta$ and $\gamma$. This work was presented in chapter 4. These calculations extend the work of Stanley et al. [67] by taking into account finite barriers. The main result was that contrary to common belief, the structural inversion asymmetry (SIA) or Rashba spin splitting is not always dominant in narrow gap QWs. The well known large bulk inversion asymmetry (BIA) or Dresselhaus splitting in bulk InSb plays an important role in the spin dynamics in InSb QWs. It was shown that the contributions to the spin splitting from terms linear ($\beta$) and cubic ($\gamma$) in the in-plane momentum associated with BIA can be significant and even exceed that from SIA, depending on the details of the heterostructure. The results highlight the importance of the heterostructure design on the spin splitting parameters and their impact on the spin lifetime. Evaluating the anisotropic Dyakonov Perel' spin lifetimes [80] using the calculated parameters $\alpha$, $\beta$ and $\gamma$, showed that the maximum spin lifetime is limited by the magnitude of the bulk BIA ($\gamma$) term – this is inherently large in InSb. Shortcomings in the commonly used expressions for $\beta$ are elucidated and the link with SIA is revealed.

In optical measurements of the spin lifetime, spins are oriented out of the plane of the QW into the [001] direction. Spins oriented in this direction as well as the [110] direction experience over an order of magnitude greater spin
relaxation than those in the [1-10] direction. Thus electrically injected spins in the [1-10] direction will have significantly greater spin diffusion lengths than would be inferred from optically determined spin lifetimes, which alleviates the device fabrication demands for a lateral spin transport device. In addition, this indicates a strong anisotropy in the plane of the 2DEG which is the driving force for the spin galvanic effect [96].

The 30 nm wide QWs studied in this thesis exhibit impressively high electron mobilities both at room and low temperature. A highest room temperature mobility of 6.93 m²V⁻¹s⁻¹ was recorded in sample 2504A which is the highest reported in III-V QWs to date. The temperature dependence of the electron mobility shows excellent agreement with a model taking into account scattering from phonons and ionised impurities. This analysis indicated that low temperature mobility is limited by remote ionised impurity scattering. Furthermore, it is shown [6] that this model is robust and describes a range samples with varying doping and growth parameters.

The spin dependent properties of a series of gated Hall bridges prepared from 30nm wide QWs were investigated in chapter 5 using high field magnetotransport measurements. Emphasis was on low temperatures where Shubnikov de-Haas oscillations and the quantum Hall effect are well resolved. Gated measurements were performed at 2 K with the aim of extracting information on the Rashba spin splitting. Using the gate electrodes, the carrier density in the QWs was varied over a limited range which itself varied from device to device due to difficulties encountered with the thin SiO₂ gate oxide used (primarily to stop unacceptable leakage currents from the gate to the drain contact). The gated measurements revealed three important features of these samples: (i) the mobility is proportional to the carrier density; consistent with the theoretical description of the scattering in the 2DEG being dominated by remote ionised impurities, (ii) the Landau level broadening in these samples is unexpectedly large (considering the high mobility) and shows a distinct dependence on the carrier density (or indeed the mobility) and (iii) in samples with narrower broadening, a weak beating pattern is distinguishable in the
derivatives of the longitudinal resistivity $\rho_{xx}$. A Fourier transform of the data exhibits an asymmetric split-peak structure from which a difference in spin populations $\Delta n = n_1 - n_2$ is extracted and subsequently used to estimate the Rashba spin splitting parameter $\alpha$ according to Engels et al. [39]. Data obtained for $\alpha$ as a function of carrier density demonstrate $\alpha$ varying between $1.3-1.5 \times 10^5$ eVm which agrees well with the only other experimental report of $\alpha$ in InSb QWs [44]. These values are greater than the calculations performed in chapter 4; which is attributed to the limitations of the Engels formula (section 5.5).

Numerical simulations of the resistivity (details of which are given in appendix A) were used to investigate the influence of broadening on the beating patterns. It is demonstrated that the absence of beating effects in the majority of samples can be attributed to large inhomogeneous broadening. The origin of the asymmetric Fourier transform peak was also investigated by simulating $\rho_{xx}$ with a spin dependent broadening $\Gamma_+ \neq \Gamma_-$ explicitly associated with spin-dependent scattering. Simulations show a non-zero beat node and reproduce the observed asymmetry in the Fourier transform peaks in the experimental data. The uniqueness of this approach was tested and confirmed, thus the findings provide insight to the spin dependent scattering in the 2DEG. Both the observation of beating effects and spin dependent scattering are significant steps in this material system and builds on the growing literature of spin dependent phenomena in InSb QWs.

The efficient electrical injection of spin into a semiconductor requires an interfacial layer with a large spin dependent resistance such as a tunnel barrier to be incorporated into the ferromagnetic-semiconductor contact. For a tunnel barrier to be suitable for use as a spin injection contact it must be (i) high resistance and (ii) support single-step tunnelling. In chapter 6 the viability of using InAlSb Schottky barriers as a tunnel barrier for spin injection into InSb QWs was investigated. Three point $I$-$V$ measurements of Ti/InAlSb Schottky barriers were performed on a series of nine devices fabricated from the same wafer. Although the conductance properties varied substantially from device to device, by applying
the Rowell criteria (section 6.2) it was shown that a number of devices show characteristics of single step tunnelling. The reverse bias $J-V$ characteristics of the majority of devices show good agreement with a numerical calculation of the tunnel current through a Schottky barrier potential obtained self-consistently with the SPM using the nominal growth details and experimental carrier density. Devices could be broadly categorised by the temperature dependence of the zero bias resistance $R_0(T)$; devices with weak temperature dependences satisfied the Rowell criteria, whereas devices with stronger temperature dependences did not. Of the devices which didn't satisfy the criteria, two devices stood out as anomalous, exhibiting pronounced features in the differential resistance spectra which are not consistent with standard transport mechanisms. Devices which show a strong temperature dependence of $R_0(T)$ are linked to defect assisted tunnelling across the barrier involving multiple steps and/or phonon emission.

The interface resistance of the barriers under a bias of -50 mV was typically $r_b^* \approx 10^{-5} \Omega m^2$. This is approximately six orders of magnitude greater than the threshold value according to the model of Fert and Jaffres [31] and are thus suitable for use as spin injection contacts. However, for electrical spin injection and detection, the interface resistance must lie within a narrow range of values [149] which in this case is not satisfied.

To satisfy the conditions for efficient spin injection and detection requires an engineered tunnel barrier. To-date electrical spin injection experiments have generally focussed on bulk epitaxial semiconductors or undoped QWs used for spin light emitting diodes structures. Issues related to the design of epitaxial barriers in QW heterostructures suitable for spin injection, transport and manipulation were discussed. In the modulation doped structures of the type considered in this thesis, an unavoidable conduction band minimum in the barrier is present which is detrimental to spin injection. Using the same SPM and tunnelling model that showed good agreement with the experimental data, the engineering of an epitaxial InAlSb tunnel barrier with the desired interface resistance was addressed. Taking into account realistic growth constraints and
with knowledge of the theoretical results obtained in chapter 4, two designs for epitaxial barriers in a 15 nm and 30 nm QW heterostructures were presented with the interface resistance in the required range \[149\] (some flexibility can be gained from the geometry of the electrodes).

### 7.2 Further work

There are clear areas of investigation that can progress from the work presented in this thesis. In addition to these, a number of the interesting observations that have been made may lead to additional research. These are outlined below.

(a) The difficulties encountered in fabricating hybrid ferromagnetic-semiconductor devices with thin film tunnel barriers are outlined in detail in appendix C. The problem ultimately stems from the thickness of the InAlSb lower barrier (3 μm) required to grow high quality InSb QWs (a technology issue). Deep etches are required to electrically isolate devices and form mesas. Deep wet etches that are routinely used to isolate devices are problematic when an interfacial layer is present and has so far impeded the development of electrical spin injection into InSb. Appendix C.3 describes a possible strategy to overcome this obstacle by fabricating spin valve devices from a Co/MgO/InSb structure without the need for any etching or mesa definition. The fabrication of these structures is the subject of future work.

(b) Gate electrodes on the Hall bridges used to investigate the Rashba effect in chapter 5 did not function efficiently and limited the modulation of the 2DEG density \(n_{2D}\) and the Rashba parameter \(\alpha\). The development of better gate electrodes using higher quality dielectrics is attractive; this would permit the use of thinner layers, extending the accessible range of both \(n_{2D}\) and \(\alpha\). In addition, the arguments regarding spin-dependent scattering would benefit from measurements in tilted fields i.e. by varying the relative magnitude of the total spin splitting one
can confirm the influence on the observed beating phenomena inferred from simulations.

(c) The high room temperature mobility in the 30 nm wide InSb QWs studied in chapter 5 makes them very attractive for the study of room temperature ballistic transport phenomena (this would be a milestone for the spin transistor [16]). However, the issue of electrical isolation commented on above is not restricted to hybrid spintronic devices, but also becomes evident as even simple devices are scaled down to sub-micron size; for example, a relatively standard structure used for investigating ballistic transport is the quantum point contact or a nano-Hall cross. Whilst nanoscale features can be defined using electron-beam lithography onto InSb, etching a mesa down to the substrate is difficult and can rule out the use of wet chemical processing (e.g. a 50 nm nano-wire would have an aspect ratio of \( \approx 60 \)). Substantial work on ballistic transport in the GaAs/AlGaAs system has been performed [180], and ballistic transport effects at room temperature were reported [181]. It is of note that these achievements are largely due to the technological ability to grow high quality lattice matched GaAs heterostructures as thin as 300 nm - enabling the definition of fully isolated nano-wires using relatively straightforward etching techniques. Reports of ballistic transport in InSb QWs have been made at low temperatures in shallow etched structures [182] but room temperature results remain elusive (the remaining material beneath the QW becomes increasingly conductive at high temperatures and can mask effects from the QW). The measurement of room temperature ballistic transport in the 30 nm InSb QWs is thus a clear avenue of future work that would be a significant technological and physical milestone. This will entail overcoming the current fabrication obstacles.

(d) Experimentally determined values of \( \alpha \) in chapter 5 are larger than estimates from the theoretical calculations performed in chapter 4. It was highlighted in chapter 4 that optical measurements of the spin lifetimes (e.g. using
the technique described in [109]) access spins oriented in the [001] direction. This lifetime is significantly different to orientations in plane of the QW applicable to lateral devices, but can yield information on the spin splitting parameters using the expressions for the D'yakonov Perel' spin relaxation according to [80] (equation 4.31) and the measured mobility. This approach was recently demonstrated in [183] for GaAs QWs. Provided one can justifiably assign the spin relaxation to be mediated by the Rashba term (i.e. structure, density or with gate modulation), this is an alternative method of experimentally determining the Rashba parameter and has the advantage that it is performed in zero external magnetic field - eliminating the influence of the Zeeman splitting (discussed in chapter 5) - and would provide a better test for the theoretical calculations in chapter 4.

(e) Finally, in order to gain information on the anisotropy of the zero field spin splitting with in-plane momentum $k_{||}$, the spin galvanic effect (SGE) can be used. A uniform non-equilibrium spin polarization, obtained electrically or optically produces a spin current in an unbiased sample. The SGE is driven by the asymmetry of the spin relaxation in the plane of the 2DEG. Thus from the theoretical results in chapter 4, a sample whose edges are aligned along the [110] and [110] direction will be suitable and exhibit a large SGE. The SGE effect has been studied in GaAs [96] and InAs QWs [94] and is expected to be larger in InSb. Currents models are based on only the spin splitting terms linear in $k$ ($\alpha$ and $\beta$), however, it is likely that the inherently large bulk Dresselhaus parameter $\lambda$ will play a significant role. It was noted in chapter 4 that a change in anisotropy of the spin splitting in the plane of the 2DEG occurs when the condition $2\beta/\gamma k_{F}^{2} = 1$ is passed. This observation could in principle be observed in a gated sample - given that both $\beta$ and $\gamma$ show a weak dependence on $n_{2D}$ and hence $k_{F}^{2}$, the asymmetry is controlled by the gate modulation of $n_{2D}$. The investigation of the SGE in InSb QWs is therefore attractive.
References


References


References


Appendix A

Modelling magneto-oscillations in a two-dimensional electron gas

Simulations of the magnetoresistivity $\rho_{xx}(B)$ provide valuable insight to the influence of the various parameters which effect the density of states (DoS). In the case of Rashba spin splitting, comparison of beating patterns in experimental $\rho_{xx}(B)$ data to simulations can yield quantitative information on the size of the zero field spin splitting in the system as shown by Lou et al. [1] and Nitta et al. [2]. These simulations were performed in Chapter 5 to help analyse the results obtained from the InSb quantum wells and are discussed here.

An established method of simulating magneto-oscillations which can be performed with relative numerical ease is the method of Englert et al. [3]. The authors proposed a phenomenological model for the magnetoconductance (based on theoretical results of Gerhardts [4]) in order to investigate the $g$-factor in a GaAs/AlGaAs 2DEG. This approach was then later developed by Lou et al. [1] by including the Rashba effect in the Landau level energies. The magnetoconductivity at $T = 0$ K is given by [1,3,4];

$$\sigma_{xx}(B) = \frac{e^2}{2\hbar} \sum_{N_{\pm}} \left( N + \frac{1}{2} \right) \exp \left( - \frac{(E_{F}(B) - E_{\pm}(N_{\pm}B))^2}{\Gamma_{\pm}^2} \right), \quad (A.1)$$
where $E_{\pm}(N,B)$ is the energy of the $N$th Landau level and here we denote $\Gamma_{\pm}$ as the broadening of spin up (+) and spin down (-) Landau levels, respectively. The broadening is taken to be independent of field. Equation A.1 demonstrates that $\sigma_{xx}$ reaches a maximum (minimum), when the Fermi Level lies in the centre of (between) the Landau levels. The general method is the following:

(i) For a given Landau level energy spectrum i.e. with or without Rashba splitting, the Fermi energy $E_F(B)$ is determined as a function of magnetic field by an iterative solution to the integral equation relating Fermi energy to the carrier density (c.f. equation 2.14). The carrier density is assumed to be constant with magnetic field [4]. The DoS is a series of Gaussian broadened Landau levels given by [4];

\[
N(E, B) = \frac{eB}{\hbar} \sum_{N=0}^{N=N_{\infty}} \frac{1}{\sqrt{2\pi \Gamma_{\pm}}} \exp\left( -\frac{(E - E_{\pm N})^2}{2\Gamma_{\pm}^2} \right).
\]  

(ii) Once the Fermi energy is obtained as a function of magnetic field, the magnetoconductivity of the two-dimensional electron gas (2DEG) is calculated from equation A.1.

(iii) The magnetoresistivity $\rho_{xx}$ is obtained from inverting the conductivity tensor expression yielding [1],

\[
\hat{\rho} = \frac{1}{\sigma_{xx}^2 + \sigma_{xy}^2} \begin{pmatrix} \sigma_{xx} & -\sigma_{xy} \\ \sigma_{xy} & \sigma_{xx} \end{pmatrix}.
\]

such that

\[
\rho_{xx} = \frac{\sigma_{xx}}{(\sigma_{xx}^2 + \sigma_{xy}^2)}.
\]

(Note that in equation A.3 use has been made of the Onsager reciprocal relations $\sigma_{xx} = \sigma_{yy}$ and $\sigma_{xy} = -\sigma_{yx}$ [5]). For simplicity the classic expression for the
transverse (Hall) conductivity $\sigma_{xy} = -en_{2D}/B$ is used, although it should be emphasised that this approximation is valid only in low fields.

Using this method, $\rho_{xx}$ can be simulated as a function magnetic field with various input parameters to the Landau level spectrum $E_n(N,B)$ such as; the $g$-factor, broadening, and the Rashba spin-orbit coupling parameter.

### A.1 Landau level spectrum in the presence of Rashba splitting

The Landau level energies in the presence of the Rashba interaction is given by Winkler as [6]:

$$E_z^R(N,B,\alpha) = \hbar \omega_c (N + \frac{1}{2} \pm \frac{1}{2})$$

$$\pm \frac{1}{2} \left( \hbar \omega_c - g^* \mu_B B \right) \sqrt{1 + \frac{8\alpha^2}{(\hbar \omega_c - g^* \mu_B B)^2} \frac{eB}{\hbar} \left(N + \frac{1}{2} \pm \frac{1}{2}\right)}$$  \hspace{1cm} (A.5)

The Landau level energy spectrum associated with the Rashba model is shown in the lower panel of figure A.1 in the vicinity of zero field using parameters $g = -35$ and $\alpha = 1.5 \times 10^{-11}$ eVm. The Landau levels for spin up and spin down electrons are indicated by red and black lines respectively for clarity.
The Rashba interaction causes the Landau levels to become highly non-linear. It can be seen that as the magnetic field is decreased the Landau levels converge to the subband edge ($E = 0$) and the two spin states are degenerate at $B = 0$. This is a feature of the Rashba model and occurs because the spin states are degenerate at $k = 0$ (see Chapter 4).

Exploring the limits of equation A.5 we see immediately that for $\alpha = 0$ the standard energy spectrum is recovered. It can also be shown that in the limit...
Figure A2: Spin splitting as function of magnetic field for fixed Fermi energy showing the pure Zeeman splitting (dashed line) and the cooperation of Zeeman plus Rashba splitting (solid line) ($n_{2D} = 3.5 \times 10^{13} m^2$, $\alpha = 1.5 \times 10^{11} eV m$).

$B \to 0$ for a fixed Fermi energy, i.e. varying both $B$ and $N$ to maintain a constant carrier density, the spin splitting at the Fermi energy, $\Delta E = E_{N+} - E_{N-}$ reduces to the pure Rashba spin splitting $\Delta E = -2|\alpha|k_F$. In the opposite limit of high magnetic field, it can be shown that the pure Zeeman spin splitting $\Delta E = g^* \mu_B B$ is recovered [6]. The model predicts a smooth transition between the two regimes which is illustrated in figure A.2 which shows the spin splitting at fixed Fermi energy as a function of field. The model reproduces the correct field dependence of the Rashba parameter in agreement with that of Das et al. [7].

Since the magneto-oscillations are determined by the field dependence of the Landau levels and the redistribution of carriers between them [7], it follows that the intersection of energy levels of different spin will lead to additional features in the oscillation patterns. In fact, the DoS now exhibits a beating pattern which is reflected in the field dependence of the Fermi Energy, shown in the top panel of figure A.1 by the bold black line. Since the magneto-oscillations are
related to the DoS at the Fermi energy, it can be seen that the Rashba model fully accounts for the beating effects observed in $\rho_{xx}$ by various authors.

References

Appendix B

Self consistent Schrödinger-Poisson model

The self consistent Schrödinger-Poisson model (SPM) is an invaluable tool for semiconductor device modelling allowing one to explore the influences of various growth parameters on the conduction band profile and electronic states in the quantum well (QW). The SPM used in this thesis was written by Dr. Mike Fearn at QinetiQ Malvern. Finer details of the program code and the various modifications made during its development are proprietary to QinetiQ, however details of the self-consistent method can be found elsewhere in the literature e.g. the reader is directed to references [1,2] and [3]. Due its fairly extensive use in this thesis in chapter 4, a brief outline of the model is given here for completeness.

The device heterostructures considered in this thesis could be separated into three regions, the Al$_x$In$_{1-x}$Sb lower barrier, the InSb QW and the Al$_x$In$_{1-x}$Sb upper barrier. Each region has a different band gap $E_g$ and effective mass $m^*$. The conduction and valance band offsets of the materials with differing band gaps introduce discontinuities in the potential energy at the heterointerfaces which form a QW. The total potential energy in the device consists of the conduction band offset step functions $dE_c(z)$ and the continuous electrostatic potential $e\phi(z)$ from the ionised donors and free carriers according to $V(z) = -e\phi(z) + dE_c(z)$. 

The entire structure is of finite length and is divided into a 'mesh' of discrete elements which are solved individually for the calculation.

## B.1 The Schrödinger equation

With the $z$-axis in the growth direction, the envelope wave functions of the $n$th subband $\Psi_n(z)$ satisfy the effective mass equation

$$-rac{\hbar^2}{2} \nabla \left( \frac{1}{m^*_cb(z)} \nabla \Psi_n(z) \right) + V(z)\Psi_n(z) = E_n \Psi_n(z) \quad (B.1)$$

where, $m^*_cb(z)$ is the position-dependent effective mass that varies in each region of the device, $V(z)$ is the total potential energy and $E_n$ is the energy eigenvalue. This is the equation that is solved in the one-band SPM. Note that band non-parabolicity is ignored in the effective mass approximation. Boundary conditions require that both $\Psi_n(z)$ and $1/m^*_cb(z)(\partial \Psi_n(z)/\partial z)$ are continuous across the heterointerfaces (the second boundary condition takes into account the variation of the Bloch function in each region and ensures continuity of the probability current). In addition, for bound states the wave function and its derivative must be zero at the left and right hand boundaries of the heterostructure and satisfy the normalization condition $\int_{-\infty}^{\infty} |\Psi(z)|^2 \, dz = 1$.

In the first instance the Schrodinger equation is solved for the case without space charge to yield the set of wavefunctions $\Psi_n(z)$. The electron density distribution and the wavefunction are related by [2]

$$n(z) = \sum_{n=1}^{n=m} |\Psi_n(z)|^2 n_n \quad (B.2)$$
where $m$ is the number of bound states and $n_n$ is the density of each state is found by integrating the density of states $N(E_n)$ and the Fermi function $F(E_n)$ according to

$$n_n = \int_{-\infty}^{\infty} N(E_n) F(E_n) dE.$$  \hfill (B.3) 

### B.2 The Poisson equation

The potential distribution and the electric field in the device are related to the charge through the one-dimensional Poisson equation

$$-\frac{d}{dz} \left( \varepsilon(z) \frac{d\phi(z)}{dz} \right) = e\rho(z)$$  \hfill (B.4) 

where $\varepsilon(z)$ is the permittivity of the semiconductor that varies with position and material composition, $\rho(z) = [N_d(z) - n(z)]$ is the net charge density and $N_d(z)$ is the doping density [2]. It is assumed that the Fermi energy is pinned at mid-gap on the semiconductor surface [4,5] which is enforced by the surface potential at the left hand boundary of the device ($z = 0$). The Poisson equation is solved for the charge distribution $n(z)$ obtained from the first solution to equation B.1 with the ionised charge from the doping to yield the electrostatic potential energy $e\phi(z)$. This is then fed back into the Schrödinger equation to generate the next solutions for $\Psi_n(z)$. This self-consistent iterative procedure is continued until the relative change in the energy eigenvalue from one iteration to the next is less than a specified value or a number of iterations are completed. Essentially the SPM can solve the conduction band profile for an arbitrary doping profile and heterostructure.
B.3 Material parameters

For the structures studied in chapter 4, a single δ-doping layer is located in the top barrier which is simulated by a dopant profile that decays exponentially in the growth direction following the results of secondary-ion-mass-spectroscopy (SIMS) data in these structures [6]. The exact functional form of the decay is not expected to affect the trend of the results presented in this thesis, but its presence is important since the potential profile of the barrier is altered. In the SPM it is assumed that all donors are ionised and that no inter-diffusion of atoms takes place at the interfaces.

The alloy compositions $x$ and $y$ are varied according to their dependence on the band gap and effective mass (these parameters are listed in table B.1). Material parameters used in the SPM calculations were derived from transmission spectroscopy performed by Dai et al. [7] to determine the band gap energies of $\text{In}_x\text{Al}_y\text{Sb}$. The $\text{InSb}$ QW is assumed to be lattice matched to the lower barrier and strained accordingly. Table B.1 lists the parameters used in the SPM calculations for each QW width considered. The conduction : valance band offset ratio is taken to be $62\% : 38\%$ following [4].

\textit{TABLE B.1:} Parameters used in the SPM model at 10 K [7]. Data for upper and lower barrier materials is indicated by the notation [Upp:Low].

<table>
<thead>
<tr>
<th>QW width $W$ (nm)</th>
<th>[Upp:Low] Barrier Al fraction $x:y$</th>
<th>[Upp:Low] Barrier band gaps $E_g$ (meV)</th>
<th>[Upp:Low] Barrier effective mass $m^*$</th>
<th>Strained QW band gap $E_g$ (eV)</th>
<th>[Upp:Low] Barrier $E_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>0.20:0.15</td>
<td>651.9:548.9</td>
<td>0.034:0.029</td>
<td>263.2</td>
<td>16.45:16.75</td>
</tr>
<tr>
<td>20</td>
<td>0.20:0.15</td>
<td>651.9:548.9</td>
<td>0.034:0.029</td>
<td>263.2</td>
<td>16.45:16.75</td>
</tr>
<tr>
<td>25</td>
<td>0.18:0.13</td>
<td>610.7:507.7</td>
<td>0.032:0.027</td>
<td>260.0</td>
<td>16.57:16.87</td>
</tr>
<tr>
<td>30</td>
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<td>548.9:445.9</td>
<td>0.029:0.024</td>
<td>255.4</td>
<td>16.75:17.05</td>
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</tbody>
</table>
References

Appendix C

Fabrication of spin injection devices in narrow gap semiconductors

C.1 Co/MgO tunnel barriers grown on InAs (001)

Work on the fabrication of amorphous metal-oxide spin injection barriers on 1 µm thick InAs (001) epilayers grown by MBE at QinetiQ Malvern was performed in parallel to the work described in previous chapters. The inversion layer at the surface of InAs forms a two dimensional electron gas (2DEG) resulting in very low interface resistances of $r_b^{*} \approx 10^{-12}$ Ωm² [1]. This is two to three orders of magnitude lower than the desired range for efficient spin injection-detection according to the model of Fert and Jaffres [2] and allows for purposeful engineering of an interfacial oxide barrier to take place.

Ultra thin MgO films (~1-2 nm) and Co ferromagnetic layers (20 nm) were grown deposited in situ onto the InAs epilayers by Dr. Laura Singh (Cambridge materials group). Various chemical pre-treatments were investigated to help minimise the surface roughness and optimise the barrier integrity. Atomic force microscopy and transmission electron microscopy studies of the structural and surface properties of the Co/MgO/InAs junction
Figure C.1: (left) Optical image of a fabricated TLM devices used to characterise the MgO barrier. (Right) Schematic view of the top contacting arrangement where the insulating SiO2 layer is not shown for clarity.

were performed by the Cambridge materials group (Singh et al. [3]) and the Imperial College materials group (Eustace et al. [4]), respectively.

Transmission line model (TLM) devices suitable for electrical characterisation of the barrier properties were fabricated at QinetiQ Malvern with the guidance of Dr. Steven Clowes and Dr. Phil Buckle. An optical micrograph of a fabricated TLM device is shown in figure C.1(a). The device geometry and structure ensured that all of the current passed through the Co/MgO/InAs interface rather than via a parallel path directly into the InAs as illustrated by the schematic diagram in figure C.1(b).

The entire TLM device was fabricated using only two photo lithography steps. Firstly, 5 µm wide strips of resist were defined by photo lithography and used as an etch mask for the removal of Co/MgO using an Ar⁺ ion beam mill process (IBM) and subsequent reactive ion etch (RIE) to form a 1 µm high InAs mesa. A SiO₂ layer >1 µm was then sputtered over the device to planarise the structure, the top of the mesa was exposed with a lift-off process. A second photo lithography step was required for metallisation of the Ti/Au electrodes and a final Ar⁺-IBM removed all of the Co along the mesa apart from that protected by the
Ti/Au electrodes which defined 5x5 \(\text{um}^2\) contacts. The IBM with *in situ* SIMS facility at QinetiQ Malvern allowed accurate determination of the etch time by monitoring both the Co and In counts simultaneously. A typical recording of the etch process is shown in figure C.3.

Three point *I-V* measurements of the Co/MgO/InAs junctions were performed using the transport system at QinetiQ Malvern (see chapter 3). Subsequent additional analysis was done at Imperial College by Dr. Fred Magnus and Dr. Steven Clowes; details of the electrical characterisation are given by Magnus *et al.* [5]. By application of the Rowell criteria (c.f. section 6.2.3) it was shown that with certain chemical surface pre-treatments, a continuous pinhole free MgO barrier (=1.2 nm) could be fabricated with an interface resistance \(r_0 \approx 10^{-9} \text{\Omega m}^2\) appropriate for spin injection/detection according to the Fert and Jaffres model [2] and thus demonstrating the feasibility of using Co/MgO tunnel contacts on narrow gap InAs for spintronics.

### C.2 InSb two-terminal spin-valve devices

In addition to the work carried out on InAs, a large effort was directed towards fabricating spin injection devices from InSb. Whilst InSb QWs are desirable for use as a spin FET type device because of the tunable Rashba interaction in the 2DEG, InSb epilayers are suitable for two-terminal spin valve devices such as that illustrated in figure 6.13 and in addition offer some advantages over QW heterostructures in terms of fabrication.

For example, the electrostatic and structural details of the Schottky barrier in modulation doped QW heterostructures are crucial for facilitating the efficient transfer of spins into the 2DEG and require careful engineering of the doping and hence multiple wafer growths to optimise which can be expensive. The interface resistance of a direct Ti/\(n\)-InSb epilayer contact is reported to be \(10^{-11} - 10^{-10} \text{\Omega m}^2\) [6]. This is larger than that on InAs due to the presence of a low Schottky barrier but still leaves some scope for the growth of an ultra thin MgO tunnel barrier. In
addition, the Ar$^+$-IBM method used for Co etching in the InAs TLM devices significantly degrades the mobility in the 2DEG (located 50 nm beneath the surface) and can not be used. This was demonstrated by Hall measurements on QW material exposed to Ar$^+$-IBM which showed that after 1 min the mobility was reduced by over an order of magnitude compared to the un-processed wafer. Thus alternative etching methods or a bottom up strategies (metal lift-off) are required to fabricate the Co electrodes in InSb QWs. In contrast, the thickness of the conducting layer in both InSb (3 μm) and InAs (1 μm) epilayers mitigates the detrimental affect of the Ar-IBM on the surface as shown by Hall measurements.

Lateral two-terminal spin injection devices have been used by various authors to gain information on the spin dependent transport in the semiconductor. Electron micrographs of a two-terminal device fabricated from InSb QW material are shown in figure C.2. The device is operated as a spin valve whereby a spin polarized current is passed between the two ferromagnetic (FM) electrodes (labelled 1 and 2 in figure C2) and a voltage is measured between the same electrodes. The two FM electrodes are designed such that they exhibit different magnetisation-reversal (coercive) fields. This ensures that upon application of in plane magnetic fields along the easy axis the magnetisation of the two electrodes are aligned either parallel or anti parallel. This is achieved by control of the aspect ratio of the electrodes c.f figure C.2. Thus injected spins that traverse the device arrive at contact 2 either parallel (low resistance) or anti-parallel (high resistance) producing a distinctive hysteresis loop in magnetoresistance [7]. This is referred to as the local measurement configuration. Equally, because the splitting between the electrochemical potential of the spin channels decays exponentially with the spin diffusion length $\lambda_S$ either side of the injection contact, provided the two
Figure C.2: Electron micrographs of a two-terminal test device fabricated from InSb QW material. Device has been electrically isolated with a wet chemical deep etch. The dashed lines in the upper image indicate the regions which are air-bridged.

FM electrodes are separated by less than $\lambda_f$, the same measurement can be performed in the non-local configuration i.e. current is passed between contacts 1 and 3 and voltage is measured between contacts 2 and 4 (see figure C.2). Koo et al. [7] demonstrated the spin transport in Fe/InAs spin valve using both these techniques.

Initial test structures were successfully fabricated from Co(20 nm)/InSb QW samples as evidenced in figure C.2. Electrodes in this device were 4 x 0.55 $\mu$m and 4 x 1 $\mu$m in dimension separated by $\approx 0.5$ $\mu$m. The parallel-bar electrodes were patterned onto the Co/InSb QW sample by e-beam lithography.
Figure C.3: Typical recording of the In (red line) and Co (blue line) counts from the SIMS during Ar-IBM of the Co layer in spin injection devices. X-axis scale is in ms.

using positive tone PMMA resist followed by evaporation of a Ti(10nm)/Au(80nm)/Ti(5nm) tri-layer. In the test structure Co was removed around the electrodes using Ar\(^+\)-IBM. The additional top Ti(10nm) layer serves as an etch mask to the IBM (Ti has a relatively high etch resistance compared to Au).\(^2\) The mesa was formed by wet chemical deep etch (lactic and nitric acid) which removed the 3 \(\mu\)m AlInSb buffer layer and electrically isolated the devices down to the GaAs substrate. This demonstrated the ability to define nanoscale parallel FM electrodes with submicron separations using standard lithography techniques. Various subtle design alterations were made to improve the lift-off of Ti/Au/Ti between the FM electrodes. The electrode widths and separations could be scaled down to 400 nm and 200 nm respectively. Note that both the damage caused to the 2DEG in this structure from the Ar-ion milling and the large
Schottky interface resistance (discussed in chapter 6) leave it un-functional as a device but it serves as a proof of principle.

Figure C.4: (Upper panel) Electron micrograph of a two-terminal devices fabricated from a Co/MgO/InSb layer using a wet chemical isolation etch. (Lower panel) Same structure processed with a modified two stage isolation etch method.

The fabrication of two-terminal devices from bulk $n$-InSb epilayers was also attempted. An ultra thin ($\approx 1.1$ nm) MgO film was grown by the Cambridge materials group under the same pre-treatment and growth conditions that produced integral barriers on InAs. The process used to fabricate the Co/InSb QW test structure was repeated. During the final processing step (isolation etch,)
it was observed that the wet etch preferentially etches along the length of the electrodes where the thin MgO film was present. This is indicated in the SEM of figure C.4 by arrows. Notably, no indication of preferential etching is found for electrodes where no MgO is present (circled by dotted lines in figure C.4). This clearly demonstrates the acute influence the presence of the MgO film has on the processing. Consequently, the devices fail at the wet etch stage.

The devices require a wet etch to form suspended metal air-bridges from the feed metal to the central mesa (electrical isolation is also required). This ensures that current is injected through the tunnel barrier into the mesa in the parallel bar region. To mitigate the preferential undercutting effect an alternative two stage etch process was developed consisting of a shortened wet etch, sufficient to form air-bridges, followed by a deep dry chemical reactive ion etch in methane and hydrogen (CH$_4$/H$_2$). To minimise the required wet etch time, the width of the air-bridges was reduced. Results of this process are shown in the lower panel of figure C.4. The device integrity is improved compared to the standard single etch method and allowed subsequent electrical measurements to be performed (not shown here). The disadvantage of using the CH$_4$/H$_2$ RIE is the polymer layer of reaction bi-products that is re-deposited onto the surface and sidewalls of the mesa. This is evidenced most clearly by the presence of 'fences' around the perimeter of the etched mesas; this is not conducting and is not expected to affect electrical measurements. This polymer film ultimately slows the etch rate and limits the achievable etch depth. In the process used to produce the device in figure C.4 this layer was minimised by performing a series of shorter (10 min) etches each followed by an oxygen plasma clean. Using this technique, an etch depth of 2.5 μm was achieved (total etch time of 1 hour).

C.3 Future work

The main problem with fabricating nanoscale devices from narrow gap InAs and especially InSb originates from the thickness of the
Figure C.5: Proposed un-isolated two-terminal spin valve device. Au leads contact a small area of the of the Co electrodes and are isolated from the semiconductor by oxide layer <100 nm thick.

heterostructure grown on top of the insulating substrate. Methods to electrically isolate devices and define conducting mesas which are routine in most standard electrical devices become problematic when an interface oxide barrier is present. It is clear that if one could remove the isolation etch step described in the previous section, significant progress could be made. Below a possible strategy for fabricating two terminal spin value structures without the need for wet or dry isolation etch is outlined.

Traditionally, in two-terminal ferromagnetic/semiconductor hybrid devices, the ferromagnetic electrodes are long, narrow and thin. This is to create a single domain, force the magnetisation into the direction of the long axis of the wire and further restrict the magnetisation into the x – y plane. Under these circumstances, the hysteresis loops in either R or M versus B are sharp and distinct. A semiconductor mesa is formed to confine the current carrying semiconductor away from the ends of the ferromagnetic bars where the stray
fields are present. This region is shown in figure C.5, generated using the OOMMF software.

![Figure C.5: 2D image plot of the total field in the parallel bars indicating the extent of the stray fields. Blue and red represent x and y components. Figure generated using OOMMF software.](image)

Consider two finite parallel ferromagnetic electrodes (with the long axis in the x-direction) patterned onto a semiconductor sample that extends indefinitely in the x−y plane. It is proposed that if the parallel electrodes are sufficiently long, the majority of the current flowing between electrodes is in the vicinity where the magnetisation is distinct and only a small proportion of the current spreads out beyond the boundaries of the electrodes where the stray fields are present. Then this portion of the total current will be a small contribution to the observed $R-B$ magnetoresistance response and could be neglected. In this scenario the device may still operate effectively as a spin valve.

To briefly investigate the viability of this proposal, the current distribution between the two electrodes is solved using ComSol Multiphysics to show the extent of the current at the ends of the parallel bars. Here the
Figure C.6: 2D image plot of the current density in the vicinity of the electrodes in the case when the whole top surface is biased at 50 mV. The scale is from $1.25 \times 10^8 \text{A/m}^2$.

dimensions of electrodes (1) and (2) are 500 nm x 4 μm and 300 nm x 4 μm, respectively (identical to that in figure C.5). The thickness of both electrodes is 20 nm. The Co electrodes ($\rho_{\text{Co}} = 7.5 \times 10^{-8} \ \Omega \text{m}$ [2], $\varepsilon_r = 1$) are positioned on top of a 1 μm thick layer of bulk InSb ($\rho_{\text{InSb}} = 2 \times 10^{-5} \ \Omega \text{m}$, $\varepsilon_r = 16.45$). In this problem, electrode (1) is common and electrode (2) is held at 50 mV. In the following simulations, emphasis should be put on the distribution of current density rather than the magnitude.

Figure C.6 shows the 2D image plot of the current density in the region of the electrodes. In this case the entire top surfaces of the electrodes are held at the potentials. The image represents a 2D slice of the current density just below the semiconductor surface. One can see that the majority of the current density is located along the central region of the electrodes where the magnetisation is parallel. Realistically, only a small area of the electrodes will be contacted which would lead out to a larger area contact pad. This situation is shown in the 2D image plot of figure C.7 a contact area of 100 nm x 200 nm.
Figure C.7: 2D image plot of the current density of the electrodes when they are contacted and held at potential of 50 mV. Scale is to $3 \times 10^{10}$ A/m$^2$.

In this case the current density extends over a smaller region near the electrical contacts where the magnetisation is parallel and definite. The contribution from the stray field would be minimal. Note, that in the simulations shown above, no knowledge of a high resistance tunnel barrier is given.

To simulate a structure closer to that which would be fabricated, a high resistance interfacial layer is included. Intuitively, one would expect the current to be more evenly distributed compared to the case of an ideal contact. For the purpose of this exercise, a high resistance barrier is simulated using an additional 10 nm layer ($\rho=10^5 \, \Omega m$) between the semiconductor and the Co electrodes. The result is shown in figure C.8. The current (smaller in magnitude) is indeed distributed along the length of the wire as expected. However, the main result is that the current density falls off rapidly beyond the boundaries of the Co electrodes where the stray field are present and constitutes only a small percentage of the total current density.
Figure C.8: 2D image plot of the current density between the electrodes contacted by a small area (100 nm x 200 nm) but with a high resistance layer between the Co and semiconductor. Scale is to $80\text{A/m}^2$.

References


Appendix D

The two-dimensional density of states in zero magnetic field

Consider an electron wave function travelling through a two dimensional periodic potential system such as a quantum well. For motion confined to the \(x-y\) plane, the electron wave function must be of the form [14]

\[
\phi(r, k) = u_k(r) \exp(ik \cdot r),
\]

where \(r = (x, y)\) and \(k = (k_x, k_y)\) and the function \(u_k(r)\) contains the lattice periodic part of the Bloch function and \(\exp(ik \cdot r)\) is the plane wave. The entire space can be considered to be made up of identical squares with length of sides, \(L\). The periodic boundary conditions \(\phi(x, y) = \phi(x+L, y)\), and \(\phi(x, y) = \phi(x, y+L)\) restrict the allowed values of \(k_x\) and \(k_y\) to discrete intervals [8];

\[
k_x = \frac{2\pi n_x}{L}, k_y = \frac{2\pi n_y}{L}.
\]
Figure D.1: Schematic representation of k-space and the geometry used for the DoS calculation.

Where \( n_x \) and \( n_y \) are integers. The area occupied by each electronic state in k-space is then \( \left( \frac{2\pi}{L} \right)^2 \). This is illustrated in figure D.1 where the discretisation of allowed states in k-space are indicated by solid dots. The density of states in a semiconductor is the number of states per unit area per unit energy.

For a circle in k-space, the area increment from \( k \) to \( k+dk \) is \( 2\pi k\,dk \) (see figure 2.7). The number of allowed states in the area between \( k \) and \( k+dk \) is then

\[
2\pi k\,dk \frac{A}{(2\pi)^2} = \frac{kA}{2\pi} \,dk \quad \text{(where } A = L^2 \text{ is the area).}
\]

Therefore, the number per unit area is just \( \frac{k}{2\pi} \,dk \). The number of states per unit area per unit energy between \( E \) and \( E+dE \) (i.e. the DoS), \( N(E) \), is then given by
\[ N(E) = \frac{k}{2\pi} \frac{dk}{dE}. \]  

From the **parabolic energy dispersion** (equation 2.1), the wave vector is related to the energy by

\[ k = \frac{\sqrt{2m^*E}}{\hbar}, \]

and

\[ kd\kappa = \frac{m^*}{\hbar^2} dE. \]  

where \( m^* \) is the effective mass at the conduction band edge. Substituting these expressions into equation D.3 gives the **2D DoS for parabolic bands** as

\[ N_p(E) = \frac{m^*}{\pi\hbar^2} \Theta(E - E_n), \]  

where a factor of two has been included for spin degeneracy. Here the subscript \( p \) refers to its derivation from a parabolic dispersion and \( \Theta(E - E_n) \) is the step function centred on the subband edge \( E_n \).

From the **non-parabolic energy dispersion** (equation 2.8), the wave vector is related to the energy by,

\[ k = \frac{\sqrt{2m^*E(1 + \lambda E)}}{\hbar}, \]

where \( \lambda = 1/E_g \) is the non-parabolicity factor. Performing the differentiation on both sides of equation 2.8 yields,
\[(1 + 2\lambda E) dE = \frac{\hbar^2 k}{m_{eb}} dk. \quad \text{(D.7)}\]

Substitution of equations D.6 and D.7 into equation D.3 gives the modified DoS for non-parabolic bands,

\[N_{np}(E) = \frac{m_{eb}^*}{\pi \hbar^4} (1 + 2\lambda E) \Theta(E - E_n), \quad \text{(D.8)}\]

where the subscript \(np\) refers to its derivation from non-parabolic dispersion.

References